

A CRITERION FOR THE BREAKDOWN OF QUASI-PERIODIC SOLUTIONS AND ITS RIGOROUS JUSTIFICATION

RENATO CALLEJA AND RAFAEL DE LA LLAVE

ABSTRACT. We formulate and justify rigorously a numerically accessible criterion for the computation of the analyticity breakdown of quasi-periodic solutions in Symplectic maps and 1-D Statistical Mechanics models. Depending on the physical interpretation of the model, the analyticity breakdown may correspond to the onset of mobility of dislocations, or of spin waves (in the 1-D models) and to the onset of global transport in symplectic twist maps.

The criterion we propose here works whenever there is an *a posteriori* KAM theorem that asserts the existence of a KAM torus provided that we can find a function that satisfies very approximately the invariance equation and satisfies some mild non-degeneracy conditions.

We formulate two precise theorems that implement these ideas: one which applies to statistical mechanics models (possibly with long range interactions) and another one which applies to symplectic mappings.

The proof of both theorems uses an abstract implicit function theorem that unifies several such theorems in the literature.

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1. INTRODUCTION

For a very long time, there has been interest in assessing whether a twist mapping has an invariant circle or not. It was observed long ago [Poi93, Bir17, Mos63, Sie42] that the existence of smooth invariant circles (or invariant tori) in twist mappings implies that the motion is localized. The converse, namely, that if there are no invariant circles the behavior is unbounded, was conjectured in [Chi79] and established in [Mat88]. The existence of smooth invariant circles (or invariant tori) in quasi-integrable systems was established by the well known Kolmogorov-Arnol'd-Moser (KAM) theory, [Mos66b, Mos66a, Lla01].

Twist mappings appear also in the study of models from Solid State Physics. For example, in the study of equilibrium solutions of models with nearest neighbor interactions. Again, the existence of smooth invariant circles play a very important rôle. In [ALD83], it is shown that transition from smooth quasi-periodic solutions, to discontinuous solutions has deep physical interpretations (depending on the meaning of the models) it could be that dislocations can move or that a deposited material does not stick to the substratum or that spin waves can travel.

The analyticity breakdown transition for twist maps has been the subject of intensive numerical study starting with the pioneering [Gre79].

The goal of this paper is to formulate a numerically accessible criterion for the computation of the analyticity breakdown of analytic tori in systems described by a variational principle, in particular in twist mappings. Roughly, the criterion asserts that an analyticity breakdown happens if and only if some appropriate norms of a hull function go to infinity. We recall that hull functions are the parameterizing by the internal phase of the equilibria.

In a practical implementation, we compute the hull functions on a family starting from the integrable case by continuation while we monitor the Sobolev norms of such hull functions. We approach the breakdown when this Sobolev norms blow up or other non-degeneracy conditions break down. See Section 3 for a precise formulation of the criterion. We have implemented this in [CdIL08], where we include algorithmic details. In the present paper, we concentrate on rigorous results.

The criterion presented here works whenever there is an *a posteriori* KAM theorem that asserts the existence of a KAM torus provided that we can find a function that satisfies very approximately the invariance equation and which also satisfies some mild non-degeneracy conditions.

In practical application, the approximate solutions are provided by numerical calculation. A careful numerical application has little trouble in producing solutions of a truncated version of the invariance equation up to a multiple of the round-off error of the machine. One can assess whether the approximate solutions of the truncated equations are indeed approximate solutions of the true invariance equation using rigorous computer bounds [dlLR91] and this leads to rigorous proofs. Even if one does not want to get full rigor, one can get good indications of their reliability using the standard methods of numerical analysis (results with different precision, level of truncations, etc.).

Of course, to measure the size of the error of a functional equation, we need to define appropriate norms. We will argue that the Sobolev norms are very appropriate for the numerical approximations. Hence, we will formulate *a posteriori* theorems in Sobolev norms.

The rigorous results of this paper are very well adapted to numerical methods in two ways:

- The theorems are based in repeating an step which produces a more accurate solution. We will specify these iterative steps as an algorithm. If these algorithms are implemented, they lead to extremely efficient algorithms [CdIL08, HdLS08]. The proofs of the theorems are just based on providing estimates of the Newton step. To prove convergence, we provide a rather

easy abstract Nash-Moser theorem, Theorem A.1, which shows that, given the estimates for the Newton step, we obtain the convergence of the scheme and the fact that the solution is close to the initial approximation.

- The rigorous theorems provide justification of the numerics. Given some numerical calculations, the rigorous theorem we prove provide precise condition numbers that ensure that the computation is reliable.

In this paper, we will present two such *a posteriori* theorems in Sobolev norms that apply two different types of models.

- a) Symplectic mappings.
- b) Equilibrium states in statistical mechanics models (a generalization of twist mappings).

Of course, there is a very important overlap between the models *a)* and *b)* (twist mappings for example). On the other hand, in [dIL08] one can find statistical mechanics models that cannot be written as a dynamical system. On the other hand, non-twist mappings [dCNGM96] can be treated as symplectic mappings but do not admit a variational formulation.

The very successful criteria of [Gre79, OS87] which are used for twist mappings, do not have an easy counterpart for equilibrium models, since it is not proved that all the invariant tori are approximated by periodic orbits nor what is the analog of dynamical stability of periodic orbits.

We note that there are also other *a posteriori* theorems such as the ones presented in [dILFS08, CC08, Zeh75]. In the appendix A, we formulate an abstract theorem that can be used to prove the results. From our point of view, the abstract theorem provides with a valuable guide to the strategy of the proof, emphasizing what needs to be estimates an in what order.

The estimates can be performed in Sobolev spaces or in analytic spaces with very few changes.

2. A POSTERIORI KAM THEOREMS

KAM theorems can be formulated as assertions that certain functional equations have solutions. The theorem with its proof can be interpreted as an implicit function theorem, [Zeh75, Zeh76, Bos86]. The functionals considered usually have derivatives (understood in some appropriately weak sense), and the existence of a formal perturbation theory (up to first order) can usually be formulated as existence of the inverse of this derivative. The difficulty of small divisors implies

that the inverse of the derivative is not bounded. In such cases it is impossible to apply the usual implicit function theorem for differentiable functions in Banach spaces, and indeed, in this generality, the result of an implicit function theorem is false. Even though some usual algorithms for the proof of the standard implicit function theorem do not converge in this generalized scheme, it was a deep observation that a variation of the Newton method can be used for our problems. By performing the proof of the implicit function theorem carefully, it is possible to find a finite set of explicit conditions [Kol54, Nas56] (non-degeneracy conditions) that guarantee that a *Newton method* started on a sufficiently approximate solution will converge to a true solution. In numerical analysis theorems of this type are often called *a posteriori estimates*. The prototype of such a theorem [dlLR91] is

Theorem 2.1. *Let $\mathcal{X}_0 \subset \mathcal{X}_1$ be Banach spaces and $\mathcal{U} \subset \mathcal{X}_0$ and open set. Consider the map*

$$\mathcal{F} : \mathcal{U} \subset \mathcal{X}_0 \rightarrow \mathcal{X}_1$$

and such that there exist computable functionals $f_1, \dots, f_n : \mathcal{X}_0 \rightarrow \mathbb{R}^+$ satisfying the following properties. Suppose that $x_0 \in \mathcal{X}_0$ satisfies

- (1) $\|\mathcal{F}(x_0)\|_{\mathcal{X}_1} < \varepsilon$
- (2) $f_1(x_0) \leq M_1, \dots, f_n(x_0) \leq M_n$
- (3) $\varepsilon \leq \varepsilon^*(M_1, \dots, M_n)$

Then there exists an $x^ \in \mathcal{X}_0$ such that $\mathcal{F}(x^*) = 0$ and*

$$\|x_0 - x^*\|_{\mathcal{X}_0} \leq C_{M_1, \dots, M_n} \varepsilon$$

This theorem assures the existence of a true solution close to an initial guess x_0 as long as a finite number of conditions are satisfied. For our applications it is quite important that the Newton method starts on an arbitrary approximate solution. Some versions of Nash–Moser implicit function theorems, notably those of [Zeh75, Sch60], have this feature, but they require extra conditions such as special structure in the equations or invertibility of the derivative of the functional in a neighborhood about the initial guess.

3. CRITERION FOR THE BREAKDOWN

The criterion for the breakdown of quasi-periodic solutions we propose is summarized in the following recipe.

- (1) Compute by continuation a parameterization of the invariant torus (hull functions) in such a way that it satisfies the functional equations up to round-off error.

- (2) Monitor the Sobolev norms of this computed solutions (and other non-degeneracy conditions).
- (3) We will approach the breakdown when these Sobolev norms blow up (or other non-degeneracy condition breaks down).

In practice, one can find that the on several cases norms blow up according to a power law. In that case, by fitting one can compute the breakdown point more accurately. Indeed, the Renormalization group predicts that there is a power law blow up, [dLL92].

We emphasize that the criterion is just a consequence of the *a posteriori* formulation of the KAM theorem in Sobolev spaces. For example [dLFS08] considers whiskered tori, [CC08] considering dissipative systems in analytic regularity. Adaptations and numerical implementation of them are in progress.

In the subsequent sections we present two complete implementations of the above ideas. We present two different contexts both of which lead to criteria for breakdown which are numerically affective.

In section 5, we present a KAM theorem for symplectic mappings based in *automatic reducibility*. A version for the analytic spaces was presented in [dLGJV05], but now we present a result for Sobolev spaces, which, is well suited for numerical implementations.

In section 6, we present another KAM theorem based on automatic reducibility for models in Statistical Mechanics. We present a version based on Sobolev spaces which is well suited for our criterion. The analytic version was presented in [dLL08].

Both theorems will be proved by applying an abstract Nash-Moser implicit function theorems which we present in Appendix A so that is can be read independently. Theorem A.1 combines features of the abstract theorems in [Zeh75, Sch69]. Of course, there is a large literature of implicit function theorems, which are useful in many contexts. For example, [Ser73, Ham82] but for us the feature of starting the iteration on just approximate solutions was very important.

For simplicity, in thir paper we will present results for mpas only, but there are analogous results for flows. [Dou82, dLGJV05] show how to deduce results for flows from results from maps.

4. SOME STANDARD DEFINITIONS AND RESULTS

In this section, we include some of the definitions that we will require for stating our breakdown criterion.

In the abstract discussion of an *a posteriori* theorem in section 2 and in the rigorous version in Appendix A, we have not specified which norm to use. This allows extra flexibility. There are several norms

which one can use in applications. In mathematical applications, one often encounters norms in analytic spaces or C^r norms. For numerical applications we have found convenient to use Sobolev norms.

4.1. Sobolev Spaces. We denote the Fourier expansion of a periodic mapping $u : \mathbb{T}^n \rightarrow \mathbb{R}^d$ by

$$u(\theta) = \sum_{k \in \mathbb{Z}^n} \hat{u}_k \exp(2\pi i k \cdot \theta),$$

where \cdot is the Euclidean scalar product in \mathbb{R}^n , and the Fourier coefficients \hat{u}_k can be computed

$$\hat{u}_k := \int_{\mathbb{T}^n} u(\theta) \exp(-2\pi i k \cdot \theta) d\theta.$$

The average of u is the 0-Fourier coefficient, we denote the average of u on \mathbb{T}^n by

$$\text{avg} \{u\}_\theta := \int_{\mathbb{T}^n} u(\theta) d\theta = \hat{u}_0.$$

Definition 4.1. We will denote by

$$H^m = \{u \mid \|u\|_m^2 = \sum_{k \in \mathbb{Z}^n} (1 + |k|^2)^m |\hat{u}_k|^2 < \infty\}$$

the Banach space of functions from $\mathbb{T}^n = \mathbb{R}^n / \mathbb{Z}^n$ taking values in \mathbb{R}^d . Here $|\cdot|$ represents the maximum norm on the spaces \mathbb{R}^d and \mathbb{C}^d , i.e. if $x = (x_1, \dots, x_d) \in \mathbb{C}^d$, then

$$|x| := \max_{j=1, \dots, m} |x_j|.$$

Similar notation for the norm will be also used for real or complex matrices of arbitrary dimension, and it will refer to the matrix norm induced by the vectorial one.

There are several advantages of using Sobolev norms for our applications

- In our computations, which involve handling of Fourier series, the computation of Sobolev norms is extremely fast and reliable. (the computation of C^r norms seems more involved and is more unreliable because it is affected by errors at one point. Sobolev norms are more immune to local errors since they are weighted sums of averages) [dILP02].
- Analytic norms involve the choice of a domain. It is known that near the breakdown the analyticity domain shrinks so that one gets different values of the breakdown depending on the domain

chosen to study (indeed the analyticity breakdown is defined as the value for which there is not any domain of analyticity)

- Sobolev norms transform well under rescaling transformations. It is easy to show that

$$\|D^r u \circ \lambda\| = \|D^r u\|_{L^2} \lambda^{r-1/2}$$

These scaling properties of Sobolev norms are very useful to study breakdown [CdIL08] since it is known that for the *universality class* the analyticity breakdown satisfies some scaling relations [Mac83]. The scaling relations of Sobolev norms allow us to identify more accurately the breakdown point for families in the same universality class. Checking the scaling relations can be used as a criterion to identify the boundary of the universality class [CdIL08].

- It has been shown in [dILGJV05, dIL08] that solutions of the invariance equations which are Sobolev of a sufficiently high order are analytic.

4.1.1. *Some properties of Sobolev spaces.* The Sobolev spaces we have introduced are a Banach Algebra for large enough m . The following result is proven in [Ada75] as a straight forward application of the Sobolev Imbedding Theorem.

Theorem 4.2. *Let $m > \frac{n}{2}$. There is a constant K_1 depending on m and n , such that for $u, v \in H^m$ the product $u \cdot v$, belongs to H^m and satisfies*

$$(1) \quad \|u \cdot v\|_m \leq K_1 \|u\|_m \|v\|_m$$

In particular, H^m is a commutative Banach algebra with respect to the pointwise multiplication and the equivalent norm

$$\|u\|_m^* = K_1 \|u\|_m$$

An elementary consequence of H^m being a Banach algebra under multiplication when $m > n/2$ is that if M is a matrix valued function $M, M^{-1} \in H^m$ and $\|M - \tilde{M}\|_m$ is sufficiently small, then $\tilde{M}^{-1} \in H^m$. The proof is just using the Neumann series

$$(2) \quad \tilde{M}^{-1} = \left[\sum_{n=0}^{\infty} M^{-1} (M - \tilde{M})^n \right] M^{-1}$$

and the Banach algebra properties.

It is also useful to have the following estimates on compositions (see for example [Tay97]).

Theorem 4.3. *Let $\mathcal{F} \in \mathcal{C}^m$ and assume $\mathcal{F}(0) = 0$. Then, for $u \in H^m \cap L^\infty$*

$$(3) \quad \|\mathcal{F}(u)\|_m \leq K_2(\|u\|_{L^\infty})(1 + \|u\|_m)$$

where

$$K_2(\lambda) = \sup_{|x| \leq \lambda, \mu \leq m} |D^\mu \mathcal{F}(x)|$$

In the case that $m > n/2$, if $f \in C^{m+2}$, we have that

$$(4) \quad \begin{aligned} & \|f \circ (u+v) - f \circ (u) - Df \circ (u)v\|_m \\ & \leq C_{n,m}(\|u\|_{L^\infty})(1 + \|u\|_m) \|f\|_{C^{m+2}} \|v\|_m^2 \end{aligned}$$

Notice that by the Sobolev Imbedding Theorem we also have that

$$(5) \quad H^m \subset \mathcal{C} \cap L^\infty, \quad \text{for } m > \frac{n}{2}$$

so if $\mathcal{F} \in \mathcal{C}^m$ and $u \in H^m$ with $m > \frac{n}{2}$ then the hypotheses of Theorem 4.3 are immediately satisfied.

4.2. Number Theory. A standard definition in KAM theory is the Diophantine condition.

Definition 4.4. *We say that $\omega \in \mathbb{R}^n$ is Diophantine if for some $\nu > 0$ and $\tau > n$ we have that*

$$(6) \quad |q \cdot \omega - p| \geq \nu |q|_1^{-\tau} \quad q \in \mathbb{Z}^n - \{0\}, \quad \forall p \in \mathbb{Z}$$

where $|l|_1 = |l_1| + |l_2| + \dots + |l_n|$. We define $D(\nu, \tau)$ as the set of all frequency vectors satisfying (6).

4.3. Cohomology equations. It is also standard in KAM theory to solve for φ in the equation

$$(7) \quad \varphi(\theta \pm \omega) - \varphi(\theta) = \xi(\theta)$$

where $\omega \in D(\nu, \tau)$ and ξ a function of zero average.

Estimates for (7) in Sobolev spaces are given by the following lemma, which is straight forward compared to the version in other spaces.

Lemma 4.5. *Let $\omega \in D(\nu, \tau)$. Given any function $\xi \in H^{m+\tau}$ satisfying $\text{avg} \{\xi\}_\theta = 0$ there is one and only one function $\varphi \in H^m$ satisfying*

$$(8) \quad \varphi(\theta \pm \omega) - \varphi(\theta) = \xi, \quad \text{avg} \{\varphi\}_\theta = 0$$

Moreover,

$$(9) \quad \|\varphi\|_m \leq C\nu^{-1} \|\xi\|_{m+\tau}$$

Proof. From (8) the Fourier coefficients of φ and ξ satisfy

$$\hat{\varphi}_k = \frac{\hat{\xi}_k}{e^{\pm 2\pi i k \cdot \omega} - 1}, \quad k \neq 0$$

So

(10)

$$\begin{aligned} \|\varphi\|_m^2 &= \sum_{k \in \mathbb{Z}} (1 + |k|^2)^m |\hat{\varphi}_k|^2 = \sum_{k \in \mathbb{Z}} (1 + |k|^2)^m \frac{|\hat{\xi}_k|^2}{|e^{\pm 2\pi i k \cdot \omega} - 1|^2} \\ &\leq C \sum_{k \in \mathbb{Z}} (1 + |k|^2)^m \frac{|\hat{\xi}_k|^2}{(2\pi k \cdot \omega)^2} \leq C\nu^{-2} \sum_{k \in \mathbb{Z}} (1 + |k|^2)^{m+\tau} |\hat{\xi}_k|^2 \\ &= C\nu^{-2} \|\xi\|_{m+\tau}^2 \end{aligned}$$

5. THE CRITERION FOR SYMPLECTIC MAPS

In this section we introduce a rigorous justification of the criterion of breakdown of analyticity for Symplectic maps with a Diophantine rotation vector. Similar result hold for vector fields. In [dLGJV05] it is shown how to obtain results for flows from results for maps. Hence, we have the straight forward adaptation of results and proofs to the reader.

The destruction of tori for symplectic maps has been studied extensively after [Gre79]. Another method was introduced by [OS87]. Both methods are based on locating periodic orbits, [Gre79] studies the stability properties and [OS87] studies the properties of stable manifolds. The obstruction method – if implemented taking care of round-off and truncation error – can establish rigorously the non-existence of invariant tori with a finite computation. The criterion of [Gre79] involves taking limits, which cannot be justified with a finite computation. Nevertheless, there are rigorous partial justifications of the Greene’s criterion, [FdLL92b, Mac92]. Furthermore, in [dlLO06] one can find the result that some conjectures on the properties of renormalization group imply that both the criteria of [Gre79, OS87] are sharp in a neighborhood of the non-trivial fixed point of renormalization.

Since both criteria depend on locating periodic orbits of high period they seem to have trouble when the potentials have different harmonics which lead to a plethora of orbits that collide with each other, [Wil87, Ket90, FdLL92a, KM94, LC06]. The present criterion seems to be immune to these complications since the quasi-periodic solutions are unique and there is little chance of confusion.

The criterion presented here (and, in particular Theorem 5.2) applies for symplectic maps in any dimension. The results in [Gre79, OS87]

were formulated in one dimension. Extensions of [Gre79] to higher dimensions were formulated and implemented in [Tom96a, Tom96b].

The present criterion works also in the context of Variational Problems in Statistical Mechanics discussed in Section 6 for which no analogue of periodic orbits and stable manifolds seems to be available.

The proof is based in the constructive proof for the analytic case presented in [dILGJV05]. The guiding principle of the proof is the observation that the geometry of the problem implies that KAM tori are *reducible* and approximate invariant tori are *approximately reducible*. This leads to a solution of the linearized equations without transformation theory. Here we will summarize the main ideas of the proof in order to construct and find the estimates for the quasi-Newton method.

5.1. Non-degeneracy conditions. The results for an exact symplectic map f of a $2n$ -dimensional manifold \mathbf{U} are based on the study of the equation

$$(11) \quad (f \circ K)(\theta) = K(\theta + \omega)$$

where $K : \mathbb{T}^n = (\mathbb{R}/\mathbb{Z})^n \rightarrow \mathbf{U}$ is the function to be determined and $\omega \in \mathbb{R}^n$ satisfies a Diophantine condition.

We will assume that \mathbf{U} is either $\mathbb{T}^n \times U$ with $U \subset \mathbb{R}^n$ or $B \subset \mathbb{R}^{2n}$, so that we can use a system of coordinates. In the case that $\mathbf{U} = \mathbb{T}^n \times U$, we note that the embedding K could be non-trivial.

Let $\Omega = d\alpha$ be an exact symplectic structure on U and let $a : U \rightarrow \mathbb{R}^{2n}$ be defined by

$$(12) \quad \alpha_z = a(z)dz \quad \forall z \in U$$

For each $z \in U$ let $J(z) : T_z U \rightarrow T_z U$ be a linear isomorphism satisfying

$$(13) \quad \Omega_z(\xi, \eta) = \langle \xi, J(z)\eta \rangle$$

where $\langle \cdot, \cdot \rangle$ is the Euclidean scalar product on \mathbb{R}^{2n} . Since Ω is antisymmetric, J satisfies $J(z)^T = -J(z)$.

Notice that (11) implies that the range of K is invariant under f . The map K gives a parameterization of the invariant torus which makes the dynamics of f restricted to the torus into a rigid rotation.

We will consider the set of functions $K : \mathbb{T}^n = (\mathbb{R}/\mathbb{Z})^n \rightarrow \mathbf{U}$ satisfying

$$(14) \quad K(\theta + k) = K(\theta) + (k, 0) \quad k \in \mathbb{Z}^n.$$

Notice that it is equivalent to say that K satisfies (14) than to say that $K(\theta) - (\theta, 0)$ is periodic. Hence, we can consider \tilde{H}^r as an affine space modelled on H^r .

Definition 5.1. Given a symplectic map f and $\omega \in D(\nu, \tau)$. A mapping $K \in H^m$ is said to be non-degenerate if it satisfies the following conditions

N1: There exists an $n \times n$ matrix-valued function $N(\theta)$, such that

$$(15) \quad N(\theta) (DK(\theta)^\top DK(\theta)) = I_n,$$

where I_n is the n -dimensional identity matrix.

N2: The average of the matrix-valued function

$$(16) \quad S(\theta) := P(\theta + \omega)^\top [Df(K(\theta))J(K(\theta))^{-1}P(\theta) - J(K(\theta + \omega))^{-1}P(\theta + \omega)]$$

with

$$P(\theta) := DK(\theta)N(\theta),$$

is non-singular.

N3: The $2n \times 2n$ matrix $M(\theta)$ obtained by juxtaposing the two $2n \times n$ matrices $Dk(\theta)$ and $J^{-1} \circ K(\theta)DK(\theta)N(\theta)$ as follows

$$(17) \quad M(\theta) := \begin{pmatrix} DK(\theta) & J(K(\theta))^{-1}DK(\theta)N(\theta) \end{pmatrix},$$

is invertible in H^{m-1} and that

$$\|M^{-1}\|_{m-1} < \infty$$

for some $m > n/2 + 1$.

We will denote the set of functions in \mathcal{P}_m satisfying conditions **N1-N3** by $\mathcal{ND}(m)$.

Remark 5.1. By the Rank Theorem, Condition **N1** guarantees that $\dim K(\mathbb{T}^n) = n$. For the KAM theorem, the main non-degeneracy condition is **N2**, which is a twist condition. Its role will become clear in 5.3. Note that **N1** depends only on K whereas **N2** depends on K and f .

Note also that by the observation of the Neumann series (2), the Condition **N3** is an open condition in H^{m-1} . As we will see condition **N3** will be implied for functions K which satisfy the invariance equation.

5.2. Statement of an *a posteriori* theorem for symplectic maps.

Theorem 5.2. Let $m > \frac{n}{2} + 2\tau + 1$ and $f \in C^{m+34\tau-17}$, $f : \mathbf{U} \rightarrow \mathbf{U}$ be an exact symplectic map, and $\omega \in D(\nu, \tau)$, for some $\nu > 0$ and $\tau > n$. Assume that the following hypotheses hold

H1. $K_0 \in H^{m+34\tau-17}$ (i.e. K_0 satisfies 5.1).

H2. The map $f \in C^{m+3}$ in \mathcal{B}_r , a neighborhood of radius r of the image under K_0 of \mathbb{T}^n for some $r > 0$.

H3. If a and J are as in (12) and (13), respectively,

$$\|a\|_{C^{r+3}(\mathcal{B}_r)} < \infty, \quad \|J\|_{C^{r+3}(\mathcal{B}_r)} < \infty, \quad \|J^{-1}\|_{C^{r+3}(\mathcal{B}_r)} < \infty.$$

Define the error function e_0 by

$$e_0 := f \circ K_0 - K_0 \circ T_\omega.$$

There exists a constant $c > 0$ depending on $\sigma, n, r, \rho_0, |f|_{C^2, \mathcal{B}_r}, \|a\|_{C^{r+3}}, \|J\|_{C^{r+3}}, \|J^{-1}\|_{C^{r+3}}, \|DK_0\|_{m-2\tau+1}, \|N_0\|_{m-2\tau+1}, |(avg \{S_0\}_\theta)^{-1}|$ (where N_0 and S_0 are as in 5.1, replacing K by K_0) such that, if $\|e_0\|_{m-2\tau}$ verifies the following inequalities

$$(18) \quad c\nu^{-4}\|e_0\|_{m-2\tau+1} < 1,$$

and

$$c\nu^{-2}\|e_0\|_{m-2\tau+1} < r,$$

then there exists $K^* \in H^m$ such that

$$f \circ K^* - K^* \circ T_\omega = 0.$$

Moreover,

$$\|K^* - K_0\|_m \leq c\nu^{-2}\|e_0\|_{m-2\tau+1}.$$

Remark 5.3. In [GEdlL08], it is shown that if f is analytic, $K \in H^m$, for $m \geq m_0$ and satisfies the invariance equation and Definition 5.1 then K is analytic. Here, m_0 depends on τ and n .

5.3. Quasi-Newton method for symplectic maps. Here we describe the procedure to improve approximate solutions in the case of symplectic maps. We use the methods developed in [dlLGJV05]

Since equation (11) can be formulated as finding zeros of

$$(19) \quad F(K) := f \circ K - K \circ T_\omega,$$

then the improvement $K + \Delta$ of an approximate solution K is given by solving from the linearized equation for Δ

$$(20) \quad DF(K)\Delta(\theta) = Df(K(\theta))\Delta(\theta) - \Delta(\theta + \omega) = -e(\theta)$$

with error function

$$(21) \quad e(\theta) = F(K)(\theta) \quad \forall \theta \in \mathbb{R}^n$$

In [dlLGJV05], the authors introduce a change of variables given by the $2n \times 2n$ matrix $M(\theta)$ constructed by juxtaposing $DK(\theta)$ and $J(K(\theta))DK(\theta)N(\theta)$ as in (22).

$$(22) \quad M(\theta) := \begin{pmatrix} DK(\theta) & J(K(\theta))^{-1}DK(\theta)N(\theta) \end{pmatrix},$$

that transforms the derivative Df into

$$M(\theta + \omega)^{-1}Df(K(\theta))M(\theta) = C(\theta) + B(\theta)$$

with

$$(23) \quad C(\theta) := \begin{pmatrix} I_n & S(\theta) \\ 0 & I_n \end{pmatrix},$$

and

$$\|B\|_{m-2r-1} \leq C\nu^{-2} \|M^{-1}\|_{m-1} \|e\|_m.$$

Since B is linear in the error e , then we can solve the modified equation

$$(24) \quad \begin{pmatrix} I_n & S(\theta) \\ 0 & I_n \end{pmatrix} M^{-1}(\theta)\Delta(\theta) - M^{-1}(\theta+\omega)\Delta(\theta+\omega) = -M^{-1}(\theta+\omega)e(\theta).$$

Notice that equation (24) differs from the Newton step equation by a term $BM^{-1}\Delta$ which is quadratic in e so the modified Newton Method (24) gives rise to a quadratically convergent scheme.

Moreover, equation (24) can be solved in two steps. We are therefore led to the following algorithm.

Algorithm 5.2. The iterative step is constructed as follows:

1) Compute

$$\begin{aligned} e(\theta) &= f \circ K - K \circ T_\omega, \\ N(\theta) &= (DK(\theta)^T DK(\theta))^{-1}, \\ M(\theta) &= (DK(\theta) \quad J^{-1}(K(\theta))DK(\theta)N(\theta)), \\ &M^{-1}(\theta), \\ &\text{and} \\ E(\theta) &= M^{-1}(\theta)e(\theta). \end{aligned}$$

2) Find a normalized function W_1 (i.e. $\text{avg}\{W_1\}_\theta = 0$) solving the equation

$$W_2(\theta) - W_2(\theta + \omega) = E_2(\theta)$$

We can choose $\mathcal{T} \in \mathbb{R}^n$ such that

$$\text{avg}\{E_1\}_\theta = \text{avg}\{S(\cdot)(E_2(\cdot) + \mathcal{T})\}_\theta$$

3) We solve for W_2 from

$$W_1(\theta) - W_1(\theta + \omega) = E_1(\theta) - S(\theta)(E_1(\theta) + \mathcal{T})$$

and set $\text{avg}\{W_1\}_\theta = 0$.

4) Set $\Delta(\theta) = M(\theta)W(\theta)$ and

$$\tilde{K}(\theta) = K(\theta) + \Delta(\theta)$$

\tilde{K} is the improved solution.

5.4. Estimates for the Quasi-Newton Method. In this section we provide estimates for the iterative step described in Algorithm 5.2. The form of the estimates we will prove will be typical of the Nash-Moser strategy. We will show that the new error will be bounded (in a less smooth norm).

Actually, we will follow the formulation of Theorem A.1 and we will describe the Algorithm 5.2 by a linear operator η that produces the correction Δ out of the true error e . That is

$$(25) \quad \Delta = \eta[K]e$$

According to the strategy of Theorem A.1 we will check that

- 1) The operator η can be defined for all K in a ball.
- 2) We will provide estimates for η .
- 3) We will show that η is an approximate left inverse for the derivative of the functional.

As is discussed in [dLGJV05], an approximate solution K of (11) with error e defined in (21). Define S , M , and C by (16), (22), and (23), respectively, and let us define \mathcal{E} as

$$(26) \quad \mathcal{E}(\theta) := Df(K(\theta))M(\theta) - M(\theta + \omega)C(\theta).$$

and we notice that

$$B = M^{-1} \circ T_\omega \mathcal{E}$$

so

$$\|B\|_{m-2\tau-1} \leq C\nu^{-2} \|M^{-1}\|_{m-1} \|e\|_m$$

Lemma 5.3. *Let $m > \frac{n}{2} + 2\tau + 1$, $F[K] \in H^m$ and $\eta : H^m \rightarrow H^{m-2\tau}$ the operator constructed in Algorithm (5.2).*

Then the previous estimates imply that

$$\|\eta[K]F[K]\|_{m-2\tau-1} \leq C\nu^{-2} \|M\|_{m-1} \|M^{-1}\|_{m-2\tau-1} \|F[K]\|_{m-1}$$

We will also need estimates on $DF[K]\eta[K]$. This estimates establish that $\eta[K]$ is an approximate left inverse of $DF[K]$ as we show in the following lemma.

Lemma 5.4. *Let $m > \frac{n}{2} + 2\tau + 1$, $F[K] \in H^m$, and $F[K]$, $\eta[K]$ defined above.*

Then we have the estimates

$$(27) \quad \begin{aligned} & \| (DF[K]\eta[K] - \text{Id})F[K] \|_{m-2\tau-1} \\ & \leq C\nu^{-2} \|M\|_{m-1}^2 \|M^{-1}\|_{m-2\tau-1} \|F[K]\|_{m-1} \|F[K]\|_m \end{aligned}$$

Proof. We have

$$\begin{aligned}
(28) \quad & \| (DF[K]\eta[K] - \text{Id})F[K] \|_{m-2\tau-1} \\
& \leq \| DF\eta[k]F[K] + M \circ T_\omega BM^{-1}\eta[K]F[K] \\
& \quad - M \circ T_\omega BM^{-1}\eta[K]F[K] - F[K] \|_{m-2\tau-1} \\
& \leq \| M \circ T_\omega [(C+B)M^{-1}\eta[k]F[K] - (M^{-1}\eta[K]F[K]) \circ T_\omega] \\
& \quad - M \circ T_\omega BM^{-1}\eta[K]F[K] - F[K] \|_{m-2\tau-1} \\
& \leq \| M \circ T_\omega BM^{-1}(\eta[K]F[K]) \circ T_\omega \|_{m-2\tau-1} \\
& \leq C\nu^{-3} \| M \|_{m-1}^2 \| M^{-1} \|_{m-2\tau-1} \| F[K] \|_{m-1} \| F[K] \|_m
\end{aligned}$$

which completes the estimates for the approximate inverse.

The final result follows from an application of Theorem A.1. In the context of Theorem A.1 we consider the previous estimates with $\alpha = 2\tau - 1$ and the estimates of theorem 3.

6. THE CRITERION OF BREAKDOWN FOR MODELS IN STATISTICAL MECHANICS

In this section we present a full mathematical justification of a criterion for the breakdown of analyticity in models coming from statistical mechanics. This includes as particular cases the breakdown of KAM tori for twist mappings. In section 6.1, we introduce the models considered. In section 6.6, we state the theorem that justifies the criterion for these models.

As we anticipated, the proof of this statement is based on an abstract Nash-Moser implicit function theorem (see Theorem A.1). The statement of Theorem 6.1 asserts that if the Sobolev norms of an approximate solution are small enough then there is a true solution. Thus, the existence of a true solution is validated. The algorithm which is the basis of the Newton step (and which is a practical algorithm for numerical computation) is detailed in section 6.7. The estimates used for the step are in 6.8 and the convergence is established using theorem A.1 from the appendix.

6.1. Models considered. We will consider one dimensional systems. At each integer, there is one site, whose state is described by one real variable. Hence, the configuration of the system is characterized by sequence of real values (equivalently a function $x : \mathbb{Z} \rightarrow \mathbb{R}$). Following [Rue99], the physical properties of a model are determined by an energy which is a formal sum of the energy of every group of particles (we allow multibody interactions).

In this paper, we will be concerned with the existence of equilibrium states (see Definition 6.3) with density $1/\omega$.

We will assume that the interaction is invariant under translations. Hence, we will consider models whose formal energy is of the form:

$$(29) \quad \mathcal{S}(\{x_n\}) = \sum_{L \in \mathbb{N}} \sum_{k \in \mathbb{Z}} H_L(x_k, \dots, x_{k+L})$$

This sum is purely formal, but there are well defined ways of making sense of several quantities of interest. We will furthermore make the following assumptions in our models.

i) The following periodicity condition holds.

$$(30) \quad H_L(x_k, \dots, x_{k+L}) = H_L(x_k + 1, \dots, x_{k+L} + 1)$$

The property (30) is a rather weak periodicity condition. It is implied by the stronger property

$$(31) \quad H_L(x_k, \dots, x_{k+L}) = H_L(x_k + \ell_0, \dots, x_{k+L} + \ell_L)$$

for all $\ell_i \in \mathbb{Z}$. The latter property (31) is natural when the variables x_i are angles. For example, spin variables. The weaker property (30) has appeared in many situations. It is natural when considering twist maps of the annulus [MF94a] or monotone recurrences [Ang90].

ii) We will also require a decay condition for the criterion to hold. In section 6.8, we present the detailed description of the decay condition and in 3 we state its relevance for the persistence of quasi-periodic solutions.

6.2. Some examples of models. Models of the form (29) include as particular cases, several models which have been proposed in the literature and which are worth to keep in mind.

- If we consider the case when $H_L \equiv 0$ for $L \geq 2$ and

$$(32) \quad \partial_1 \partial_2 H_1(x, y) \leq -c < 0.$$

Then models of the form (29) appear as variational principles for twist mappings. In this case, the physical meaning of \mathcal{S} is an action while the assumption (32) is then the twist condition.

- A common example of twist maps that follows the description of the point above is the Frenkel-Kontorova model. The Frenkel-Kontorova is obtained by taking $H_0(t) = \lambda V(t)$, where λ is a coupling constant and $V(t)$ is periodic function – a popular one is $V(\theta) = -\frac{\varepsilon}{4\pi^2} \cos(2\pi\theta)$, $H_1(x, y) = \frac{1}{2}|x - y - a|^2$, and

$H_L \equiv 0$ for $L \geq 2$. This models have appeared in many context is physics (e.g. as models of deposition [ALD83], models of dislocations [FK39]), and in dynamical systems as twist maps, [Mei92, MF94a].

- If Frenkel-Kontorova models are considered as models of dislocations, some more realistic models include longer range interactions [CDLFM07].

An interesting toy model which we refer as the extended Frenkel-Kontorova model corresponds to taking H_0, H_1 as above, but we take, for $k \geq 2$

$$(33) \quad H_k(x_0, \dots, x_k) = \frac{A_k}{2}(x_0 - x_k)^2$$

The decay condition needed to apply the theorem will be translated in a decay condition in the coefficients A_k .

We also note that for certain careful choices of A_k in (33) (in particular, $A_k = 0$ for $k > R$), the equilibrium equations of this model appear as multi-step order $2R$ integration methods for ODE's.

- The XY model of magnetism corresponds to taking $H_0(t) = B \cos(2\pi t)$, where B is the external magnetic field. $H_1(x, y) = J \cos(2\pi(x-y))$ and $H_L \equiv 0$ for $L \geq 2$. The physical meaning of the x in the XY model that $S = (\cos(2\pi x), \sin(2\pi x))$ is the spin variable at site i . [BB07, p. 600] considers possible long range interactions that are relevant for the model. Computations of the coefficients of these interactions is are discussed in [RS63].
- In [Ang90], one can find a discussion of monotone recurrences. These models correspond to taking $H_L = 0$ for $L \geq R$ and assuming the monotonicity properties

$$\partial_i \partial_j H_J \leq 0 \quad \text{for } i \neq j,$$

and

$$\partial_i \partial_{i+1} H_L \leq C < 0.$$

One good example of monotone recurrences is the equilibrium equation of the Extended Frenkel-Kontorova model.

- Models in materials science with non-local interactions. See[Bat06] and references there.

6.3. Equilibrium equations. Equilibrium configurations, by definition are solutions of the Euler-Lagrange equations indicated formally as

$$(34) \quad \partial_{x_i} \mathcal{S}(\{x_n\}) = 0$$

The physical meaning of the equilibrium equations is that the total force on each of the sites exerted from the other ones vanish.

The equilibrium states have a direct physical relevance (they are sometime called meta-stable states, instantons). In dynamical systems, when \mathcal{S} has the physical interpretation of an action, equilibrium states correspond to orbits of a dynamical system.

We note that under convexity properties on the action, the equilibria parameterized by a smooth ‘‘hull function’’ (see section 6.4) are ground states. Since the methods described here apply to several models which do not satisfy convexity (e.g. the XY model). we will not emphasize this point.

For models of the form (29) the Euler-Lagrange equations are:

$$(35) \quad \sum_{L \in \mathbb{N}} \sum_{j=0}^L \partial_j H_L(x_{k-j}, \dots, x_{k-j+L}) = 0 \quad \forall k \in \mathbb{Z}$$

We call attention that, in contrast with the sums defining \mathcal{S} which are merely formal, the sums involved in equilibrium equations (35) are meant to converge.

A practical case of equilibria that has attracted a great deal of attention is ground states [Mat82, Ban89, MF94b] (also known as Class A minimizers) we note that under convexity assumptions, using Hilbert integrals all critical points given by a continuous hull functions are ground states. The Frenkel-Kontorova and twist mappings satisfy this assumptions.

6.4. Plane-like configurations and hull functions. We are interested in equilibrium configurations $\{x_n\}$ that can be written as

$$(36) \quad x_n = h(n\omega)$$

for $\omega \in \mathbb{R} \setminus \mathbb{Q}$ and where h satisfies the periodicity condition

$$(37) \quad h(x + e) = h(x) + e \quad \forall e \in \mathbb{Z}$$

and is analytic.

The function h is often called the *hull function*. The periodicity condition (37) means that h can be considered as a map of the circle to itself. We will use the notation

$$h(\theta) = \theta + u(\theta).$$

Where u is a periodic function.

6.5. Equilibrium equations in terms of hull functions. For configurations of the form (36), the equilibrium equations become:

$$\begin{aligned}
(38) \quad E[u](\theta) &\equiv \sum_L \sum_{j=0}^L \partial_j H_L(\theta - j\omega + u(\theta - j\omega), \dots, \\
&\quad \theta + u(\theta), \dots, \theta + (L - j)\omega + u(\theta + (L - j)\omega)) \\
&= 0
\end{aligned}$$

6.6. Statement of an *a posteriori* theorem for statistical mechanics models.

Theorem 6.1. *Let $m > \frac{n}{2} + 2\tau$ and $H_L \in C^{m+34\tau}$ be translation invariant interactions as in (29) satisfying the periodicity condition (30). Let $\omega \in \mathbb{R}$. Let $h = \text{Id} + u$, with $u \in H^{m+32\tau}$, $\text{avg}\{u\}_\theta = 0$ be a diffeomorphism of \mathbb{T} . Assume:*

H1) ω is Diophantine, i.e., for some $\nu > 0$, $\tau > 0$

$$(39) \quad |p\omega - q| \geq \nu|q|^{-\tau} \quad \forall p, q \in \mathbb{Z}$$

H2) The interactions $H_L \in C^{m+34\tau}$.

Denote

$$\begin{aligned}
M_L &= K_m \|H_L\|_{C^{m+3}} \|(\text{Id} + u')\|_m^2 \\
a &= \sum_{L \geq 2} M_L L^4
\end{aligned}$$

H3) Assume that the inverses indicated below exist and that:

$$\|\mathcal{C}_{0,1,1}^{-1}\|_m \leq T.$$

$$\left(\text{avg}\{\mathcal{C}_{0,1,1}^{-1}\}_\theta\right)^{-1} \leq U.$$

The following bounds measure the non-degeneracy of the problem.

- a1) $\|(\text{Id} + u')\|_m \leq N^+$.
- a2) $\|(\text{Id} + u')^{-1}\|_m \leq N^-$.
- b) $\|E[u]\|_{m-2\tau} \leq \varepsilon$.

Assume furthermore that the above upper bounds satisfy the following relations:

- i) Let $T(1 + a) < A$, $UT(1 + a) < B$
- ii) $\varepsilon \leq \varepsilon^*(N^-, N^+, \nu, \tau, a, T, A, B)$ where ε^* is a function which we will make explicit along the proof. The function ε^* makes quantitative the relation between the smallness conditions and the non-degeneracy conditions.

Then, there exists a periodic function $u^* \in H^m$ such that

$$(40) \quad E[u^*] = 0$$

Moreover

$$\|u - u^*\|_m \leq C\nu^{-2}(N^+)^2\varepsilon$$

The function u^* is the only function in a neighborhood of u in H^m satisfying (40) and $\text{avg}\{u^*\}_\theta = 0$.

Remark 6.1. In [dlL08], it is shown that if H_L are analytic and satisfy analogs of H2) and H3) and i) with analytic norms in place of C^{m+3} norms then, if $m > m_0$ with m_0 depending only on τ , then any solution of the equilibrium equations in H^m is, in fact, analytic.

Consider the case when H1), H2), and H3) are satisfied. The statement of the theorem asserts that if there is a numerical solution and its Sobolev norm H^r is not too large, there is a true solution nearby. Furthermore, there is an open set of parameters with invariant solutions. Hence, if the solutions cease to exist, the Sobolev norms of the numerically computed solutions have to blow up.

Remark 6.2. In the special case of twist mappings with Diophantine rotation numbers, the non-degeneracy conditions, H1), H2), and H3), are trivially satisfied. Therefore, the only thing that has to be checked is that for ε small enough, the Sobolev norms of the approximate solution, u , are finite.

6.7. Quasi-Newton method for statistical mechanics models.

In this section we describe an iterative procedure (a quasi-Newton method) to improve approximate solutions.

This method (similar to that in [dlL08]) is the basis of very practical algorithms and it is the key to the proof of Theorem 6.1 which we use to justify the criterion. The improvement $u + v$ of an approximate solution u is given by solving for v from the following equation

$$(41) \quad h'(\theta)(DE[u]v)(\theta) - v(\theta)(DE[u]h')(\theta) = -h'(\theta)E[u](\theta).$$

Note that equation (41) differs from the Newton step equation by the term $v(\theta)(DE[u]h')(\theta)$. Using the identity

$$(42) \quad \frac{d}{d\theta}E[u](\theta) = DE[u]h'(\theta).$$

We see that this neglected term is quadratic in $E[u]$ so that adding a term of this form to a standard Newton method will give rise to a quadratically convergent iterative scheme given that we can solve for v from equation (41). The advantage of (41) comes from the fact that the

left hand side can be factored into a sequence of invertible operators. For a detailed exposition of this factorization we refer the reader to [dlL08]. Here we give a brief summary.

Introducing the operator

$$[\mathcal{L}_l f](\theta) = f(\theta + l\omega) - f(\theta) .$$

and the new variable w related to v by $v(\theta) = h'(\theta)w(\theta)$, the equation (41) transforms into:

$$(43) \quad \mathcal{L}_1[(\mathcal{C}_{0,1,1} + \mathcal{G})\mathcal{L}_{-1}w] = -h'E[u].$$

where

$$\mathcal{C}_{i,j,L} = \partial_i \partial_j H_L \circ \gamma_L(\theta - j\omega) h'(\theta) h'(\theta - (i-j)\omega)$$

with

$$\gamma_L(\theta) = (h(\theta), h(\theta + \omega), \dots, h(\theta + L\omega))$$

and

$$\mathcal{G} = \sum_{L \leq 2} \sum_{i > j} \mathcal{L}_1^{-1} \mathcal{L}_{i-j} \mathcal{C}_{i,j,L} \mathcal{L}_{j-i} \mathcal{L}_{-1}^{-1}$$

We note that the operators $\mathcal{L}_{\pm 1}$ are invertible on functions with average 0. That is, given a function ξ with average 0, we can solve for φ satisfying

$$(44) \quad \varphi(\theta \pm \omega) - \varphi(\theta) = \xi(\theta)$$

Thus, equation (43) can be solved following the next algorithm:

Algorithm 6.2. a) Check that $\text{avg} \{h'E[u]\}_\theta = 0$.

b) Find a normalized function φ (i.e. $\text{avg} \{\varphi\}_\theta = 0$) solving the equation

$$(45) \quad \mathcal{L}_1 \varphi = -h'E[u]$$

Therefore, if φ is a solution for (45) then for any $\mathcal{T} \in \mathbb{R}$ the equation $\mathcal{L}_1(\varphi + \mathcal{T}) = h'E[u]$ holds. In particular, we choose \mathcal{T} such that

$$\text{avg} \{(\mathcal{C} + \mathcal{G})^{-1}(\varphi + \mathcal{T})\}_\theta = 0.$$

c) We solve for w from

$$(46) \quad \mathcal{L}_{-1}w = (\mathcal{C} + \mathcal{G})^{-1}(\varphi + \mathcal{T})$$

d) Finally we obtain the improved solution

$$\tilde{u}(\theta) = u(\theta) + h'(\theta)w(\theta)$$

6.8. Estimates for the Quasi-Newton Method. The goal of this section is to provide precise estimates for the iterative step described in Section 6.7. Throughout this section we will assume that $\omega \in \mathbb{R}$ satisfies the Diophantine condition given in Definition 4.4.

The following lemma is proven in [dlL08]

Lemma 6.3. *For every $m > 0$ we have:*

$$(47) \quad \begin{aligned} \|\mathcal{L}_\ell \mathcal{L}_{\pm 1}^{-1}\|_m &\leq |\ell| \\ \|\mathcal{L}_{\pm 1}^{-1} \mathcal{L}_\ell\|_m &\leq |\ell| \end{aligned}$$

From these estimates we get the following

$$\begin{aligned} \|\mathcal{G}\|_m &\leq \sum_{L \geq 2} \sum_{j < i}^L \|\mathcal{L}_1^{-1} \mathcal{L}_{j-i} \mathcal{C}_{i,j,L} \mathcal{L}_{i-j} \mathcal{L}_{-1}^{-1}\|_m \\ &\leq \mathcal{C} \sum_{L \geq 2} L^4 M_L = a \end{aligned}$$

where

$$M_L = K_1 \|H_L\|_{C^{m+3}} \|\text{Id} + u'\|_m^2$$

and K_1 is the constant of (1) depending only on m .

Then if $T(1+a) < 1$ we get

$$\|(\mathcal{C} + \mathcal{G})^{-1}\|_m < \frac{T}{1 - Ta} < 1$$

Similarly we get estimates for \mathcal{T} since

$$(\text{avg} \{C^{-1}\}_\theta) \mathcal{T} + (\text{avg} \{(\mathcal{C} + \mathcal{G})^{-1} - C^{-1}\}_\theta) \mathcal{T} = \text{avg} \{(\mathcal{C} + \mathcal{G})^{-1} \varphi\}_\theta$$

The second term in the left hand side can be treated as a perturbation of the first term. Therefore

$$|\mathcal{T}| \leq U/(1 - 2UTa) \|\varphi\|_m \leq 2U \|\varphi\|_m$$

The operator $\eta[u]$ is the operator obtained by applying the procedure 6.2.

To apply the abstract implicit function theorem we will need the following estimates on the approximate inverse η . The estimates obtained from the construction of the operator η are given in the following lemma.

Consider $r \in \mathbb{N}$.

Lemma 6.4. *Let $m > \frac{n}{2} + 2\tau$, $E[u] \in H^m$, and $\eta : H^m \rightarrow H^{m-2\tau}$ the operator constructed in Algorithm (6.2).*

Then we have the following estimates on η

$$(48) \quad \|\eta[u]E[u]\|_{m-2\tau} \leq C\nu^{-2}(N^+)^2 \|E[u]\|_m.$$

We will also need estimates on $DE[u]\eta[u]$.

Lemma 6.5. *Let $m > \frac{n}{2} + 2\tau$, $E[u] \in H^m$, and $E[u]$, and $\eta[u]$ defined above.*

Then we have the estimates

$$(49) \quad \|(DE[u]\eta[u] - \text{Id})E[u]\|_{m-2\tau} \leq C\nu^{-2}(N^+)^2N^-\|E[u]\|_{m-2\tau-1}\|E[u]\|_m$$

Proof. Let $\psi = DE[u]\eta[u]E[u] - E[u]$, then we have that

$$(50) \quad \begin{aligned} \psi &= DE[u]\eta[u]E[u] + (-h')^{-1} \cdot \eta[u]E[u] \cdot DE[u]h' \\ &\quad - (-h')^{-1} \cdot \eta[u]E[u] \cdot DE[u]h' - E[u] \\ &= (-h')^{-1} \cdot (h'DE[u]\eta[u]E[u] - \eta[u]E[u] \cdot DE[u]h') \\ &\quad + (h')^{-1} \cdot \eta[u]E[u] \cdot DE[u]h' - E[u] \\ &= (h')^{-1} \cdot \eta[u]E[u] \cdot DE[u]h' \end{aligned}$$

So we have that

$$(51) \quad \begin{aligned} &\|(DE[u]\eta[u] - \text{Id})E[u]\|_{m-2\tau} \\ &\leq \|(h')^{-1} \cdot \eta[u]E[u] \cdot DE[u]h'\|_{m-2\tau} \\ &\leq C\nu^{-2}(N^+)^2N^-\|E[u]\|_{m-2\tau-1}\|E[u]\|_m, \end{aligned}$$

which completes the estimates for the approximate inverse.

The final result follows from an application of Theorem A.1. In the context of Theorem A.1 we consider the previous estimates with $\alpha = 2\tau$ and the estimates of Theorem 3.

APPENDIX A. AN ABSTRACT NASH-MOSER IMPLICIT FUNCTION THEOREM

In this appendix we prove Theorem A.1, an abstract Nash-Moser implicit function theorem that is very well suited for the proof of Theorem 6.1. We hope that this theorem can have other applications.

In contrast with the elementary implicit function theorems, which assume that the derivative of the functional considered is invertible, the Nash-Moser implicit function theorems can cope with derivatives which are not boundedly invertible from one space to itself. In our applications this arises because the linearized equation involves solving equations with small divisors. It has become standard to think of the problem as a functional equation acting on a scale of Banach spaces, so that the linearization is boundedly invertible from one space to another (with some appropriate quantitative bounds).

The main technique is to combine the Newton step – which loses derivatives – with some smoothing that restores them. It is remarkable that, when the inverses of the linearization have a bounded order, the

whole procedure converges. This has become a basic tool of nonlinear analysis.

The theorem A.1 is very close to the main theorem in [Sch60] (see also the exposition in [Sch69]) but we allow an extra term in the remainder as in [Zeh75], we impose the extra condition that the approximate inverse. We also remark that it suffices to estimate the approximate inverse in the range of the operator. As pointed out in [Zeh75] this extra term, allows to deal very comfortably with equations with a *group structure*. In particular with conjugacy equations. Even if our problem is not a conjugacy problem (except in the case of twist maps), it is close enough to it so that it fits in the scheme. One feature of Theorem A.1 which is very important for our purposes is that Theorem A.1 does not assume that the initial system is close to integrable. The main hypothesis is that the initial guess satisfies the equation very approximately (as well as some other explicit non-degeneracy conditions. We call these theorems *a posteriori* following the notation that one uses in numerical analysis.

Compared with the scheme in [Zeh75], it has the advantage that only use one smoothing and not a double smoothing. So that we do not need to assume that the initial approximation is analytic. The theorem we present applies to all the cases discussed in [Zeh76]. Hence we can obtain the results there without requiring that the initial approximation is analytic, nevertheless, the differentiability loss is more severe than in [Zeh76].

The proof we present follows very closely [Sch60]. In particular, we have followed the choices of [Sch60] in the loss of regularity. Clearly, these choices are far from optimal. In particular, we have assumed that the functional and the approximate inverse loose α derivatives. This is natural for PDE applications, but in our case the functional does not loose any derivatives.

In the abstract set up, we will assume that there is a family of Banach spaces endowed with smoothing operators. The non-linear operator will satisfy some assumptions.

In our applications the scale of spaces will be the Sobolev spaces, and we will denote the scale of spaces by H^m . Nevertheless Theorem A.1 works for general scales of spaces and indeed, the scheme of the proof can also produce results with analytic regularity.

We will consider scales of Banach spaces \mathcal{X}^r such that $\mathcal{X}^r \subset \mathcal{X}^{r'}$ whenever $r' \leq r$ and the inclusions are continuous.

A.1. Smoothing operators.

Definition A.1. *Given a scale of spaces, we say that $\{S_t\}_{t \in \mathbb{R}^+}$ is a family of smoothing operators when*

i)

$$\lim_{t \rightarrow \infty} \|(S_t - \text{Id})u\|_0 = 0$$

ii)

$$\|S_t u\|_m \leq C t^{m-n} \|u\|_n$$

iii)

$$\|(\text{Id} - S_t)u\|_m \leq C t^{-n} \|u\|_{n+m}$$

In the concrete case of Sobolev spaces, the smoothing operators S_t are defined for $t > 1$ as follows

$$(52) \quad \widehat{(S_t u)}_k = e^{-|k|/t} \hat{u}_k$$

Note that $S_t u$ is analytic.

Lemma A.2. *The operators S_t defined in (52) are smoothing operators in the sense of Definition A.1.*

Proof. Notice that for $0 \leq m, n < \infty$

$$(53) \quad \begin{aligned} \|S_t u\|_m^2 &= \sum e^{-2|k|/t} (1 + |k|^2)^m |u_k|^2 \\ &= \sum e^{-2|k|/t} (1 + |k|^2)^{m-n} (1 + |k|^2)^n |u_k|^2 \\ &\leq \sum e^{-2|k|/t} t^{2m-2n} (1 + \frac{|k|^2}{t^2})^{m-n} (1 + |k|^2)^n |u_k|^2 \\ &\leq C t^{2(m-n)} \|u\|_n^2 \end{aligned}$$

We also have that

$$(54) \quad \begin{aligned} \|(S_t - \text{Id})u\|_m^2 &= \sum (e^{-|k|/t} - 1)^2 (1 + |k|^2)^m |u_k|^2 \\ &\leq \sum \frac{(e^{-|k|/t} - 1)^2}{\left(1 + \frac{|k|^2}{t^2}\right)^n} t^{-2n} (1 + |k|^2)^{m+n} |u_k|^2 \\ &\leq C_n t^{-2n} \|u\|_{m+n}^2 \end{aligned}$$

with

$$C_n = \sup_x \frac{(e^{-x} - 1)^2}{(1 + x^2)^n}.$$

One important consequence of the existence of smoothing operators are interpolation inequalities [Zeh75].

Lemma A.3. *Let \mathcal{X}^r be a scale of Banach spaces with smoothing operators. For any $0 \leq n \leq m$, $0 \leq \theta \leq 1$, denoting*

$$l = (1 - \theta)n + \theta m$$

we have for any $u \in \mathcal{X}^m$:

$$\|u\|_l \leq C_{n,m} \|u\|_n^{1-\alpha} \|u\|_m^\alpha$$

In the case of Sobolev spaces, these are well-known interpolation inequalities.

A.2. Formulation of Theorem A.1. In this section, we formulate and prove the abstract implicit function theorem TheoremA.1. Following standard practice in KAM theory, we use the letter C to denote arbitrary constants that depend only on the uniform assumptions of the theorem. In particular, the meaning of C can change from line to line.

Theorem A.1. *Let $m > \alpha$ and \mathcal{X}^r for $m \leq r \leq m + 17\alpha$ be a scale of Banach spaces with smoothing operators. Let \mathcal{B}_r be the unit ball in \mathcal{X}^r , $\tilde{\mathcal{B}}_r = u_0 + \mathcal{B}_r$ the unit ball translated by $u_0 \in \mathcal{X}^r$, and $\mathcal{B}(\mathcal{X}^r, \mathcal{X}^{r-\alpha})$ is the space of bounded linear operators from \mathcal{X}^r to $\mathcal{X}^{r-\alpha}$. Consider a map*

$$\mathcal{F} : \tilde{\mathcal{B}}_r \rightarrow \mathcal{X}^{r-\alpha}$$

and

$$\eta : \tilde{\mathcal{B}}_r \rightarrow \mathcal{B}(\mathcal{X}^r, \mathcal{X}^{r-\alpha})$$

satisfying:

- i) $\mathcal{F}(\tilde{\mathcal{B}}_r \cap \mathcal{X}^r) \subset \mathcal{X}^{r-\alpha}$ for $m \leq r \leq m + 17\alpha$.
- ii) $\mathcal{F}|_{\tilde{\mathcal{B}}_m \cap \mathcal{X}^r} : \tilde{\mathcal{B}}_m \cap \mathcal{X}^r \rightarrow \mathcal{X}^{r-\alpha}$ has two continuous Fréchet derivatives, both bounded by M , for $m \leq r \leq m + 17\alpha$.
- iii) $\|\eta[u]z\|_{r-\alpha} \leq C\|z\|_r$, $u \in \tilde{\mathcal{B}}_r$, $z \in \mathcal{X}$, for $r = m - \alpha, m + 16\alpha$.
- iv) $\|(D\mathcal{F}[u]\eta[u] - \text{Id})z\|_{r-\alpha} \leq C\|\mathcal{F}[u]\|_r\|z\|_r$, $u \in \tilde{\mathcal{B}}_r$, $z \in \mathcal{X}^r$, for $r = m$
- v) $\|\mathcal{F}[u]\|_{m+16\alpha} \leq C(1 + \|u\|_{m+17\alpha})$, $u \in \tilde{\mathcal{B}}_m$

Then if $\|\mathcal{F}[u_0]\|_{m-\alpha}$ is sufficiently small, there exists $u^* \in \mathcal{X}^m$ such that $\mathcal{F}[u^*] = 0$. Moreover,

$$\|u - u^*\|_m < C\|\mathcal{F}[u_0]\|_{m-\alpha}$$

Remark A.2. Note that conditions iii) and iv) can be replaced by the weaker conditions

- iii)' $\|\eta[u]\mathcal{F}[u]\|_{r-\alpha} \leq C\|\mathcal{F}[u]\|_r$, $u \in \tilde{\mathcal{B}}_r$, for $r = m - \alpha, m + 16\alpha$.
- iv)' $\|(D\mathcal{F}[u]\eta[u] - \text{Id})\mathcal{F}[u]\|_{r-\alpha} \leq C\|\mathcal{F}[u]\|_r^2$, $u \in \tilde{\mathcal{B}}_r$, for $r = m$.

Indeed in both of our applications the definition of the approximate inverse requires that some average of z is small which is true for functions in the range but not in general.

A.3. Proof of Theorem A.1. The proof is based on an iterative procedure combining the ideas of [Sch60, Zeh75]. Given a function $u \in \mathcal{X}^{m+13\alpha}$ so that $\|\mathcal{F}[u]\|_{m-\alpha}$ is sufficiently small compared with the other properties of the function, the iterative procedure constructs another function \tilde{u}

Let $\kappa > 1$, $\beta, \mu, \delta > 0$, $0 < \nu < 1$ be real numbers to be specified later. We will need that they satisfy a finite set of inequalities among them and with the quantities appearing in the assumptions of the problem.

We construct a sequence $\{u_n\}_{n \geq 0}$ by taking

$$(55) \quad u_{n+1} = u_n - S_{t_n} \eta[u_n] \mathcal{F}[u_n]$$

where $t_n = e^{\beta \kappa^n}$. We will prove that this sequence satisfies

(p1;n)

$$(u_n - u_0) \in \mathcal{B}_m$$

(p2;n)

$$\|\mathcal{F}[u_n]\|_{m-\alpha} \leq \nu e^{-\mu \alpha \beta \kappa^n}$$

(p3;n)

$$1 + \|u_n\|_{m+16\alpha} \leq \nu e^{\delta \alpha \beta \kappa^n}$$

Suppose that conditions (p1; j), (p2; j), and (p3; j) are true for $j < n$. We start by establishing (p1; n).

Notice that (p2; n - 1) implies that

$$\begin{aligned} \|u_{n-1} - u_n\|_m &= \|S_{t_{n-1}} \eta[u_{n-1}] \mathcal{F}[u_{n-1}]\|_m \leq C e^{2\alpha \beta \kappa^{n-1}} \|\eta[u_{n-1}] \mathcal{F}[u_{n-1}]\|_{m-2\alpha} \\ &\leq C \nu e^{\alpha \beta \kappa^{n-1}(2-\mu)} \end{aligned}$$

Then if $\mu > 2$, $\{u_n\} \subset \mathcal{X}^m$ converges to some $u \in \mathcal{X}^m$.

Now, to prove (p1; n), we notice that

$$(56) \quad \begin{aligned} \|u_n - u_0\|_m &\leq C \nu \sum_{j=1}^{\infty} e^{\alpha \beta \kappa^j (2-\mu)} \\ &\leq C \nu \sum_{j=1}^{\infty} e^{\alpha \beta j (\kappa-1) (2-\mu)} \\ &\leq C \nu \frac{e^{\alpha \beta (\kappa-1) (2-\mu)}}{1 - e^{\alpha \beta (\kappa-1) (2-\mu)}} \end{aligned}$$

Therefore, $\|u_n - u_0\|_m \leq C \nu$ for $\mu > 2$ and β large enough.

Then we can prove (p2; n) by writing the following inequality.

$$\begin{aligned}
(57) \quad \|\mathcal{F}[u_n]\|_{m-\alpha} &\leq \|\mathcal{F}[u_n] - \mathcal{F}[u_{n-1}] + D\mathcal{F}[u_{n-1}]S_{t_{n-1}}\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-\alpha} \\
&\quad + \|(\text{Id} - D\mathcal{F}[u_{n-1}]\eta[u_{n-1}])\mathcal{F}[u_{n-1}]\|_{m-\alpha} \\
&\quad + \|D\mathcal{F}[u_{n-1}](\text{Id} - S_{t_{n-1}})\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-\alpha}.
\end{aligned}$$

The right hand side of the inequality is obtained by means of adding and subtracting terms and using (55).

We estimate the first term of (57) using assumption *iii*) and the quadratic remainder of Taylor's theorem.

$$\begin{aligned}
(58) \quad &\|\mathcal{F}[u_n] - \mathcal{F}[u_{n-1}] + D\mathcal{F}[u_{n-1}]S_{t_{n-1}}\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-\alpha} \\
&\leq C\|S_{t_{n-1}}\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_m^2 \\
&\leq Ce^{2\alpha\beta\kappa^{n-1}}\|\eta[u_n]\mathcal{F}[u_n]\|_{m-2\alpha}^2 \\
&\leq C\nu^2 e^{2\alpha\beta\kappa^{n-1}(2-\mu)}
\end{aligned}$$

For the second term of (57) by assumption *iv*) we get

$$(59) \quad \|(D\mathcal{F}[u_{n-1}]\eta[u_{n-1}] - \text{Id})\mathcal{F}[u_{n-1}]\|_{m-\alpha} \leq C\|\mathcal{F}[u_{n-1}]\|_m^2.$$

We can estimate the quadratic term, $\|\mathcal{F}[u_{n-1}]\|_m^2$, using interpolation inequalities and induction hypotheses ($p2; n-1$) and ($p3; n-1$).

$$\begin{aligned}
(60) \quad \|\mathcal{F}[u_{n-1}]\|_m^2 &\leq C\|\mathcal{F}[u_{n-1}]\|_{m-\alpha}^{36/17}\|\mathcal{F}[u_{m-1}]\|_{m+12\alpha}^{2/17} \\
&\leq C\|\mathcal{F}[u_{n-1}]\|_{m-\alpha}^{36/17}(1 + \|u_{n-1}\|_{m+13\alpha})^{2/17} \\
&\leq C\nu^2 e^{\alpha\beta\kappa^{n-1}(-\frac{36\mu}{17} + \frac{2\delta}{17})}
\end{aligned}$$

For the third term of (57), we use the properties of the smoothing operators and the fact that the Fréchet derivative, $D\mathcal{F}[u]$, is bounded.

$$\begin{aligned}
(61) \quad &\|D\mathcal{F}[u_{n-1}](\text{Id} - S_{t_{n-1}})\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-\alpha} \\
&\leq C\|(\text{Id} - S_{t_{n-1}})\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_m \\
&\leq Ct^{-15\alpha}\|\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m+15\alpha} \\
&\leq Ct^{-15\alpha}\|\mathcal{F}[u_{n-1}]\|_{m+16\alpha} \\
&\leq C\nu e^{-15\alpha\beta\kappa^{n-1}}(1 + \|u_{n-1}\|_{m+17\alpha}) \\
&\leq C\nu e^{\alpha\beta\kappa^{n-1}(\delta-15)}
\end{aligned}$$

The desired inequality ($p2; n$) is satisfied if

$$C(\nu^2 e^{2\alpha\beta\kappa^{n-1}(2-\mu)} + \nu^2 e^{\alpha\beta\kappa^{n-1}(\frac{2\delta}{17} - \frac{36\mu}{17})} + \nu e^{\alpha\beta\kappa^{n-1}(\delta-15)}) \leq \nu e^{-\mu\alpha\beta\kappa^n}$$

or equivalently by the condition

$$(62) \quad C(\nu e^{-\alpha\beta\kappa^{n-1}(2(\mu-2)-\mu\kappa)} + \nu e^{-\alpha\beta\kappa^{n-1}(-\frac{2\delta}{17} + \frac{36\mu}{17} - \mu\kappa)} + e^{-\alpha\beta\kappa^{n-1}(15-\delta-\mu\kappa)}) \leq 1.$$

Condition (62) is true whenever ν is small enough and

$$(63) \quad \begin{aligned} \mu(2 - \kappa) &> 4, \\ \mu(36 - 17\kappa) &> 2\delta, \\ 15 - \mu\kappa &> \delta, \end{aligned}$$

and β is sufficiently large. This establishes $(p2; n)$.

Finally we note that

$$(64) \quad \begin{aligned} 1 + \|u_n\|_{m+17\alpha} &\leq 1 + \sum_{j=0}^{n-1} \|S_{t_j} \eta[u_j] \mathcal{F}[u_j]\|_{m+17\alpha} \\ &\leq 1 + C \sum_{j=0}^{n-1} e^{2\alpha\beta\kappa^j} \|\eta[u_j] \mathcal{F}[u_j]\|_{m+15\alpha} \\ &\leq 1 + C \sum_{j=0}^{n-1} e^{2\alpha\beta\kappa^j} \|\mathcal{F}[u_j]\|_{m+16\alpha} \\ &\leq 1 + C \sum_{j=0}^{n-1} e^{2\alpha\beta\kappa^j} (1 + \|u_j\|_{m+17\alpha}) \\ &\leq 1 + C \sum_{j=0}^{n-1} e^{\alpha\beta(2+\delta)\kappa^j}. \end{aligned}$$

Thus

$$(65) \quad (1 + \|u_n\|_{m+13\alpha}) e^{-\delta\alpha\beta\kappa^n} \leq e^{-\delta\alpha\beta\kappa^n} + C \sum_{j=0}^{n-1} e^{\alpha\beta\kappa^j(2+\delta-\kappa\delta)}$$

To have $(p3; n)$ we need that (65) is less than 1. If $\delta > \frac{2}{\kappa-1}$ the right side of (65) will be less than 1 for sufficiently large β .

If we consider $\kappa = 4/3$, $\delta = 6$, and $\mu = 61/10$ then (63) and $\delta > \frac{2}{\kappa-1}$ are satisfied at the same time. To complete the induction, we fix β large enough so that (65) and (62) are satisfied.

Finally we consider with our choices of β and μ , and fix ν to be

$$(66) \quad \nu = \|\mathcal{F}[u_0]\|_{m-\alpha} e^{\alpha\beta\mu}.$$

From this choice of ν , together with (56) we have that

$$\|u^* - u_0\|_m \leq C\nu \frac{e^{\alpha\beta(\kappa-1)(2-\mu)}}{1 - e^{\alpha\beta(\kappa-1)(2-\mu)}} \leq C_{\mu,\alpha,\beta,\kappa} \|\mathcal{F}[u_0]\|_{m-\alpha},$$

which completes the proof.

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DEPT. OF MATHEMATICS, 1 UNIVERSITY STATION C1200, AUSTIN TX 78712-0257

E-mail address: rcalleja@math.utexas.edu

DEPT. OF MATHEMATICS, 1 UNIVERSITY STATION C1200, AUSTIN TX 78712-0257

E-mail address: llave@math.utexas.edu