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Existence and persistence of invariant objects in dynamical systems and mathematical physics

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Existence and persistence of invariant objects in dynamical systems and mathematical physics

by

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To my parents.

To Claudia.

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Existence and persistence of invariant objects in dynamical systems and mathematical physics

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In this dissertation we present four papers as chapters. In Chapter 2, we extended the techniques used for the Klein-Gordon Chain by Iooss, Kirchgässner, James, and Sire, to chains with non-nearest neighbor interactions. We look for travelling waves by reducing the Klein-Gordon chain with second nearest neighbor interaction to an advance-delay equation. Then we reduce the equation to a finite dimensional center manifold for some parameter regimes. By using the normal form expansion on the center manifold we were able to prove the existence of three different types of travelling solutions for the Klein Gordon Chain: periodic, quasi-periodic and homoclinic to periodic orbits with exponentially small amplitude.

In Chapter 3 we include numerical methods for computing quasi-periodic solutions. We developed very efficient algorithms to compute smooth quasi-periodic equilibrium states of models in 1-D statistical mechanics models allowing non-nearest neighbor interactions. If we discretize a hull function using

N Fourier coefficients, the algorithms require $O(N)$ storage and a Newton step for the equilibrium equation requires only $O(N \log(N))$ arithmetic operations. This numerical methods give rise to a criterion for the breakdown of quasi-periodic solutions. This criterion is presented in Chapter 4.

In Chapter 5, we justify rigorously the criterion in Chapter 4. The justification of the criterion uses both Numerical KAM algorithms and rigorous results. The hypotheses of the theorem concern bounds on the Sobolev norms of a hull function and can be verified rigorously by the computer. The argument works with small modifications in all cases where there is an *a posteriori* KAM theorem.

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Chapter 1

Introduction

In this dissertation we present four papers completed in the Department of Mathematics in the University of Texas at Austin. Each paper is organized as a chapter of the dissertation. Chapter 2 is based on a paper with Prof. Y. Sire, which was submitted to Nonlinearity in October 2008 and is now undergoing revision. Chapter 3, Chapter 4, and Chapter 5 are based on papers with Rafael de la Llave. Chapter 3 is based on a paper that has been accepted for publication in Nonlinearity and will appear soon. Chapter 4 based on a paper recently submitted to Journal of Physics A. Chapter 5 is based on a preprint that is undergoing final revisions before submission. In the following we include summaries of the chapters.

The aim of Chapter 2 is to provide a construction of travelling waves in an extended one-dimensional lattice model with non nearest neighbor interactions. These models, coming mainly from solid state physics, are known to play an important role in the mechanisms of propagation of energy. We focus on an extended version of the Klein-Gordon chains, i.e. each particle is embedded into an anharmonic potential and linearly coupled to their first and second neighbors. The technique we use is a reduction to a center mani-

fold that goes back to [202, 108, 204, 106] and relies on the reduction of this infinite-dimensional problem to a finite-dimensional one. New phenomena appear due to the extended interactions. We find propagating solutions on the lattice which were not present for models involving coupling with only the nearest neighbors.

In Chapter 3 we develop fast algorithms to compute quasi-periodic equilibrium states of one dimensional models in statistical mechanics. The models considered include as particular cases, Frenkel-Kontorova models, possibly with long range interactions, Heisenberg XY models, possibly with long-rage interactions as well as problems from dynamical systems such as twist mappings and monotone recurrences. In the dynamical cases, the quasi-periodic solutions are KAM tori.

The algorithms developed are highly efficient. If we discretize a quasi-periodic function using N Fourier coefficients, the algorithms introduced here require $O(N)$ storage and a Newton step for the equilibrium equation requires only $O(N \log(N))$ arithmetic operations. These algorithms are also backed up by rigorous "a posteriori estimates" that give conditions that ensure that approximate solutions correspond to true ones.

We have implemented the algorithms and present comparisons of timings, accuracy with other algorithms.

More substantially, we use the algorithms to study the *analyticity breakdown* transition, which for twist mappings becomes the breakdown of

KAM tori.

We use this method to explore the analyticity breakdown in some Frenkel-Kontorova models with extended interactions. In some ranges of parameters, we find that the breakdown presents scaling relations that, up to the accuracy of our calculations are the same as those for the standard map.

We also present results that indicate that, when the interactions decrease very slowly, the breakdown of analyticity is quantitatively very different.

In Chapter 4 we consider one dimensional systems of particles interacting and seek quasi-periodic equilibrium states. Standard arguments show that if there are continuous families of ground states, the system can have large scale motion, if the family of ground states is discontinuous, the system is pinned down.

We show that there are fast and efficient algorithms that can compute all the continuous families of ground states even close to the boundary of analyticity. We also show that the boundary of analyticity can be computed by running the algorithm and monitoring the solution computed.

We implemented these algorithms on several models. We found that there are regions where the boundary is smooth and the breakdown satisfies scaling relations. In other regions, the scalings seem to be interrupted and restart again.

In Chapter 5 we formulate and justify rigorously a numerically efficient

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) an 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.

Chapter 2

Travelling waves in discrete nonlinear systems with non-nearest neighbor interactions

2.1 Introduction

The goal of this work is to study the existence of special solutions for extended lattice models. We focus here on the existence of travelling wave solutions.

The models under consideration are discrete in space and continuous in time. Particularly, we focus on a non-static version of the so-called extended Frenkel-Kontorova model described in [36, 35].

More precisely, we consider a chain of particles $(x_n)_{n\in\mathbb{Z}}$, each one being embedded into a nonlinear potential V, analytic in a neighborhood of 0 (and such that $V'(0) = 0, V''(0) > 0$) and coupled to the first and second nearest neighbors. The equations of motion of such a system write

$$\ddot{x}_n + V'(x_n) = \gamma\Big[(x_{n+1} + x_{n-1} - 2x_n) + A(x_{n+2} + x_{n-2} - 2x_n)\Big] \quad n \in \mathbb{Z} \quad (2.1)$$

where $\gamma, A > 0$ are coupling constants.

In this paper, we focus on solutions of (2.1) satisfying

$$x_n(t) = \varphi(n - t/T) \quad (2.2)$$

for a fixed time $T \in \mathbb{R}^*$ and a smooth function φ.

A lot of litterature has been devoted to discrete models like (2.1). In the case $A = 0$ in (2.1), MacKay and Aubry [144] construct breather solutions (i.e. spatially localized time-periodic solutions for low coupling γ). As far as propagating solutions are concerned, the case $A = 0$ has been considered in [106] for travelling wave solutions. In [88, 84] several authors use variational techniques (via concentration compactness) for the problem (2.1) with $A = 0$ and for the so-called Fermi-Pasta-Ulam lattice, i.e. discrete models with non linear coupling (see [82]). One of the authors together with Guillaume James generalized the approach initiated in [106] to pulsating travelling waves in the works [202, 108, 204] for $A = 0$ in (2.1).

In the present work, we pursue this generalization by considering the existence of travelling waves for (2.1) when $A \neq 0$. Considering non-nearest neighbor interactions is reminiscent of taking into account non local effects in the propagation of energy. It is also interesting to notice that the continuous limits (at least at the formal level) depend on the sign of the coupling coefficient A. Here, we will focus on the case $A > 0$ but the computations sketched in the last section of this paper show that one can get a different behaviour when $A < 0$ is allowed. In the paper [36], one of the authors and de la Llave considered the static version of (2.1), i.e.

$$V'(x_n) = \gamma\Big[(x_{n+1} + x_{n-1} - 2x_n) + A(x_{n+2} + x_{n-2} - 2x_n)\Big].$$

The previous system defines a $4-$dimensional map and reduces to a

2−dimensional one when $A = 0$. The limit $A = 0$ is in some sense highly singular and considering non-nearest neighbor interactions considerably enlarges the range of solutions one can consider.

We focus here on small amplitude solutions of (2.1) for several parameter regimes (A, γ, T) and describe which type of solutions bifurcate from the equilibrium 0. Besides extending the theory already developped in references [202, 108, 204, 106], our purpose is to put in light which kind of phenomenon occurs when the coupling is no longer to the first neighbors but to first and second neighbors. We show that in this case the structure of the simplest bifurcations of travelling waves are already more complicated than in [106]. We prove that generically solitary waves (i.e. localized solutions on the lattice) do not exist. Instead, the generic (in some suitable sense) solutions which appear are superpositions of a solitary wave and exponentially small tails.

The method of construction consists in reducing the system (2.1)-(2.2) to a finite dimensional center manifold (for some parameter regimes) which allows to capture all the dynamics of bounded small amplitude solutions. Reduction theorems can be found for instance in [46], [216] (see the Appendix of the present paper where the abstract reduction theorem we use is formulated).

We now describe the results we obtain. Searching for a travelling wave solution of (2.1) amounts to find a function φ such that

$$\ddot{\varphi} + T^2 V'(\varphi) = T^2 \gamma \Big\{ \varphi(.+1) + \varphi(.-1) - 2\varphi + A(\varphi(.+2) + \varphi(.-2) - 2\varphi) \Big\} \quad (2.3)$$

and

$$x_n(t) = \varphi(\xi) = \varphi(n - t/T).$$

2.2 Formulation of the problem

Recall the model under consideration

$$\ddot{x}_n + V'(x_n) = \gamma\Big[x_{n+1} + x_{n-1} - 2x_n + A(x_{n+2} + x_{n-2} - 2x_n)\Big] \quad n \in \mathbb{Z}. \quad (2.4)$$

We consider solutions of (2.4) such that

$$x_n(t) = \varphi(n - t/T)$$

where $T > 0$ is a parameter (one can choose $T > 0$ since the equation (2.4) is invariant under time reversibility). The function φ satisfies the advance-delay equation

$$\begin{aligned}\ddot{\varphi}(\xi) + T^2 V'(\varphi(\xi)) = \gamma T^2\Big\{&\varphi(\xi+1) + \varphi(\xi-1) - 2\varphi(\xi) \\ &+ A(\varphi(\xi+2) + \varphi(\xi-2) - 2\varphi(\xi))\Big\}\end{aligned}$$

where $\xi = n - t/T$.

In order to apply center manifold reduction, we introduce a new variable $v \in [-2, 2]$ which allows to write (2.2) as an evolutionary problem.

We then introduce

$$U(\xi)(v) = (\varphi(\xi), \dot{\varphi}(\xi), \Phi(v, \xi))$$

where $\Phi(v,\xi)=\varphi(\xi+v)$. We denote δ_a the trace operators

$$\delta_a\Phi(t,v)=\Phi(t,a).$$

We end up with the following equation

$$\partial_\xi U=\mathcal{L}_{A,T,\gamma}U+\mathcal{N}_T(U) \tag{2.5}$$

where the linear operator is given by

$$\mathcal{L}_{A,T,\gamma}=\begin{pmatrix} 0 & 1 & 0 \\ T^2[-1-2\gamma(1+A)] & 0 & \gamma T^2(\delta_1+\delta_{-1})+\gamma T^2A(\delta_2+\delta_{-2}) \\ 0 & 0 & \partial_v \end{pmatrix} \tag{2.6}$$

and the nonlinear one by

$$\mathcal{N}_T(U)=\begin{pmatrix} 0 \\ T^2(a\varphi^2+b\varphi^3)+h.o.t. \\ 0 \end{pmatrix} \tag{2.7}$$

where

$$V(x)=\frac{1}{2}x^2-\frac{a}{3}x^3-\frac{b}{4}x^4+\text{h.o.t.}$$

We introduce the following Banach spaces

$$\mathbb{H}=\mathbb{R}^2\times C^0([-2,2],\mathbb{R}) \tag{2.8}$$

and

$$\mathbb{D}=\left\{U\in\mathbb{R}^2\times C^1([-2,2],\mathbb{R})/\Phi(0)=\varphi\right\}. \tag{2.9}$$

The operator $\mathcal{L}_{A,T,\gamma}$ maps $\mathbb{D}$ into $\mathbb{H}$ continuously and the nonlinearity $\mathcal{N}_T : \mathbb{D} \to \mathbb{D}$ is analytic (in a neighborhood of 0) with $\mathcal{N}_T(U) = O(\|U\|^2_{\mathbb{D}})$ as $\|U\|_{\mathbb{D}} \to 0$.

We observe that the symmetry R on $\mathbb{H}$ defined by

$$R(\varphi, \psi, \Phi(v)) = (\varphi, -\psi, \Phi(-v, \xi))$$

satisfies $(\mathcal{L}_{A,T,\gamma} + \mathcal{N}_T) \circ R = -R \circ (\mathcal{L}_{A,T,\gamma} + \mathcal{N}_T)$. Therefore, if U is a solution of the evolution equation (2.5) then $RU(-.)$ is also a solution, i.e. the system is reversible under R. This is reminiscent of the time reversibility of the equation.

2.3 Statement of main results

Our main results are described in the following theorems.

Let Δ_1 be the set of parameters $(A, T, \gamma) \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+$ so that the center spectrum of (2.6) cosists of one simple pair of simple eigenvalues $\pm ip^*$.

Theorem 2.3.1. (Periodic waves)

For every $(A, T, \gamma) \in \Delta_1$ and for U near the origin in $\mathbb{D}$, the evolution equation (2.5) reduces to a two-dimensional reversible smooth vector field.

Moreover, the set of solutions near 0 of (2.5) constitutes a one-parameter family of periodic orbits, bifurcating from 0.

Let Δ_0 be the set of parameters $(A, T, \gamma) \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+$ so that the center spectrum of (2.6) cosists of one pair of double non semi-simple

eigenvalues , $\pm ip_k$, $k = 1, ..., p$, and one pair of simple eigenvalues , $\pm ip_0$.

Theorem 2.3.2. (Waves with exponentially small tails) For every (A, T, γ) close to $(A_0, T_0, \gamma_0) \in \Delta_2$ (except some exceptional points corresponding to strong resonances) there are small amplitude travelling waves of (2.3). These travelling waves are solutions homoclinic to exponentially small periodic orbits whose size is of order $O(e^{-C/d^{1/2}})$ where d is the distance from (A, T, γ) to the bifurcation surface.

The travelling waves exist provided that the following inequality is fullfilled

$$s_0 = \frac{T_0^2(2aK_1 + 4a^2 + 3b)}{1 - T_0^2\gamma_0(\cos(q_0) + 4A_0\cos(2q_0))} < 0$$

where

$$K_1 = \frac{aT_0^2}{T_0^2(1 + 2\gamma_0(1 + A_0)) - 4q_0^2 - 2T_0^2\gamma_0\cos(2q_0) - 2T_0^2\gamma_0 A_0\cos(4q_0)}.$$

The parameters a and b are such that $a = \frac{-V^{(3)}(0)}{2}$ and $b = \frac{-V^{(4)}(0)}{6}$ and $q_0 > 0$ is the imaginary part of the double non semi-simple eigenvalue of the linear operator around 0 associated to (2.3) for $T = T_0$, $\gamma = \gamma_0$ and $A = A_0$.

Remark 2.3.1. It has to be noticed that the method we use here can be adapted to systems involving couplings to third or even farther neighbors, paying the price of additional technicalities in the computations. Furthermore, our method also allows to construct pulsating travelling fronts for (2.1), i.e. solutions satisfying

$$x_n(t) = x_{n+p}(t + T),$$

for a given $p > 1$ (the case $p = 1$ corresponding to the travelling waves studied in the present paper).

2.4 Spectral analysis

As described in Theorem 2.8.1 (see the Appendix), one of the main issue in the applicability of the reduction to a center-manifold technique is to get precise informations on the spectrum of the linear operator $\mathfrak{L}_{A,T,\gamma}$.

From $\mathbb{D}$ into $\mathbb{H}$, the operator $\mathfrak{L}_{A,T,\gamma}$ is closed with compact resolvent. Its spectrum is then discrete with isolated eigenvalues with finite multiplicity.

We consider the following eigenproblem

$$\mathfrak{L}_{A,T,\gamma}\hat{U} = \sigma\hat{U}$$

where $\sigma \in \mathbb{C}$. This leads to the following dispersion relation

$$N(\sigma, T, A, \gamma) = \sigma^2 + T^2 - 2T^2\gamma(\cosh(\sigma) - 1) - 2AT^2\gamma(\cosh(2\sigma) - 1) = 0. \quad (2.10)$$

Simple eigenvalues of $\mathfrak{L}_{A,T,\gamma}$ are simple roots of $N(\sigma, T, A, \gamma)$. Since we are mainly interested in the center spectrum, we will consider $\sigma = iq$ and $q > 0$ (notice that if σ is an eigenvalue so is $-\sigma$). This leads to

$$N(iq, T, A, \gamma) = -q^2 + T^2 - 2T^2\gamma(\cos(q) - 1) - 2AT^2\gamma(\cos(2q) - 1) = 0. \quad (2.11)$$

The eigenvalue iq is going to be a double eigenvalue if it satisfies (2.11) and $\frac{d}{dq}N(iq, T, A, \gamma) = 0$. Similarly, iq is going to be a triple eigenvalue if it satisfies (2.11), $\frac{d}{dq}N(iq, T, A, \gamma) = 0$ and $\frac{d^2}{dq^2}N(iq, T, A, \gamma) = 0$. For eigenvalues of

multiplicity 4, the condition $\frac{d^3}{dq^3}N(iq, T, A, \gamma) = 0$ has to be satisfied aswell. Notice that since we are dealing with a 3-parameter problem, we do not have higher order eigenvalues.

In order to apply Theorem 2.8.1 it is important to have a clear picture of the spectrum of $\mathcal{L}_{A,T,\gamma}$. This is done in the following lemmas. First it is easy to check that the center spectrum is separated from the hyperbolic one.

Lemma 2.4.1. For all $(T, A, \gamma) \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+$, there exists p_0 such that all eigenvalues $\sigma = p + iq$ for $p \neq 0$ satisfy $|p| \geq p_0$.

The proof of Lemma 2.4.1 is very similar to the proof of Lemma 1 in [106] so we will omit it.

We first consider simple eigenvalues. The object of the following lemma is to describe the spectrum of $\mathcal{L}_{A,T,\gamma}$ at low coupling A and time T, γ being fixed.

Lemma 2.4.2. For every $\gamma > 0$, there exist $A_0 > 0$ and $T_0 > 0$ such that for all $(A, T) \in (0, A_0) \times (0, T_0)$, the center spectrum of $\mathcal{L}_{A,T,\gamma}$ consists of one pair of simple eigenvalues $\pm iq^*$.

Proof. Consider $A = 0$ then the roots $q > 0$ of the dispersion relation $N(iq, T, 0, \gamma) = 0$ are the values of q so that for a given T the following holds

$$T^2 = \frac{q^2}{1 + 4\gamma \sin^2(q/2)}. \tag{2.12}$$

Now, define the function

$$f_\gamma(q) = \frac{q^2}{1 + 4\gamma \sin^2(q/2)}.$$

For every $\gamma > 0$, the function $f_\gamma(q)$ is stricly increasing on $(0, \pi)$ and therefore $1-1$ from $(0, \pi)$ into $(f_\gamma(0) = 0, f_\gamma(\pi))$. Consequently, choosing $T_0 = \sqrt{f_\gamma(\pi)}$, for all $T \in (0, T_0)$, there exists a unique q^* such that

$$q^* = f_\gamma^{-1}(T^2).$$

By applying the implicit function theorem we get the existence of a curve $A(T)$ so that $N(iq^*(A,T), T, A(T), \gamma) = 0$ for T and A small enough, γ being fixed.

□

We consider now the case of double eigenvalues. The imaginary part q has to satisfy the two following equations

$$N(iq, T, A, \gamma) = -q^2 + T^2 - 2T^2\gamma(\cos(q) - 1) - 2AT^2\gamma(\cos(2q) - 1) = 0, \quad (2.13)$$

$$\frac{d}{dq}N(iq, T, A, \gamma) = -2q + 2T^2\gamma\sin(q) + 4T^2A\gamma\sin(2q) = 0. \quad (2.14)$$

The occurrence of double eigenvalues is important for our purpose. Indeed, we are interested in solutions of (2.4) connecting 0 at $\pm\infty$ (homoclinic solutions to 0). We then have to consider bifurcations in the parameter space (T, A, γ) such that the spectrum of $\mathcal{L}_{A,T,\gamma}$ consists of a pair of weakly coupled hyperbolic eigenvalues. For some values (A, T, γ), these two pairs of hyperbolic eigenvalues are going to collide on the imaginary axis, yielding a pair of double non semi-simple eigenvalues. The next lemma locates in the parameter plane such curves on which the spectrum has this structure.

Lemma 2.4.3. Fix $\gamma > 0$ and consider the parametrized curve $\Gamma : \Omega_\gamma \mapsto \mathbb{R}^+ \times \mathbb{R}^+$ given by

$$\begin{aligned} T_\gamma(q) &= \left(\frac{q^2 - q\tan(q)}{1+4\gamma\sin^2(q/2)-\gamma\sin(q)\tan(q)}\right)^{1/2} \\ A_\gamma(q) &= \frac{1}{2\gamma T_\gamma(q)^2}\left(\frac{q - T_\gamma(q)^2\gamma\sin(q)}{\sin(2q)}\right). \end{aligned} \tag{2.15}$$

Then there exists a zero Lebesgue measure set $\tilde{\Omega}$ in $\mathbb{R}^+ \times \mathbb{R}^+$ and a subset $\Omega \subset \Gamma(\Omega_\gamma)$ such that for all $(T, A) \in \Omega \backslash \tilde{\Omega}$, the center spectrum of $\mathcal{L}_{A,T,\gamma}$ consists in a pair of double non semi-simple eigenvalues and a finite number of pairs of simple eigenvalues.

Proof. We are looking for double eigenvalues of $\mathcal{L}_{A,T,\gamma}$ so we look for roots of (2.13) and (2.14). Solving $2\gamma T^2 A$ from (2.14) leads to

$$2\gamma T^2 A = \frac{q - T^2\sin(q)}{2\sin(q)\cos(q)}. \tag{2.16}$$

Plugging this expression back into equation (2.13), this gives an expression for T^2, namely

$$T^2 = \frac{q^2 - q\tan(q)}{1 + 4\gamma\sin^2(q/2) - \gamma\sin(q)\tan(q)}.$$

The set Ω_γ is the set of $q \in \mathbb{R}^+$ such that $T^2 > 0$ and $A > 0$. To get the expression for A we simply solve from (2.16).

The set $\tilde{\Omega}$ contains the values of (A, T) such that the spectrum admits triple eigenvalues and several pairs of double eigenvalues. Triple eigenvalues occur at cusp points of the curve Γ (see Figure 1). We also exclude in $\tilde{\Omega}$ the curves in the parameter plane where the simple eigenvalues collide, yielding semi-simple double eigenvalues.

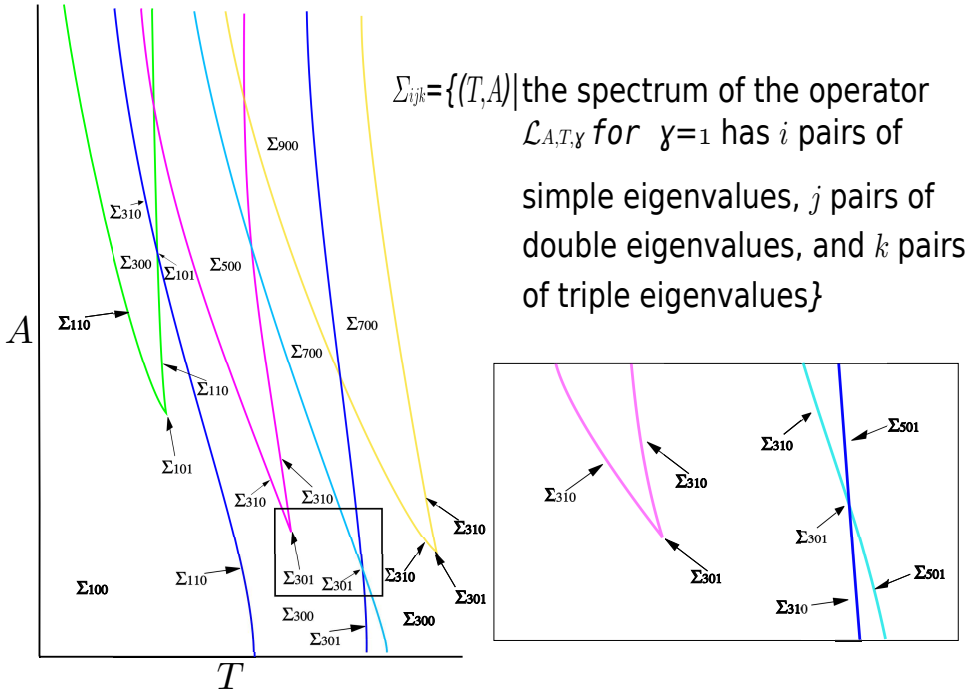

Figure 2.1: Curves parametrized by (2.15) for $\gamma = 1$ on the parameter space (T, A). The different colors represent different branches of the curves.

This set is clearly negligible for the product measure in $\mathbb{R}^2$.

According to Lemma 2.4.2, there exists a region in the parameter plane where the center spectrum of $\mathcal{L}_{A,T,\gamma}$ consists of only one pair of simple eigenvalues. By continuity of the spectrum, we deduce that except on the set $\tilde{\Omega}$, the image of the curve Γ provides the set of parameters for which the spectrum just consists of a pair of double non semi-simple eigenvalues and a finite number of pairs of simple ones.

We refer the reader to Figure 1 where the complete spectrum is given in the parameter plane (T, A) for some $\gamma = \gamma_0$.

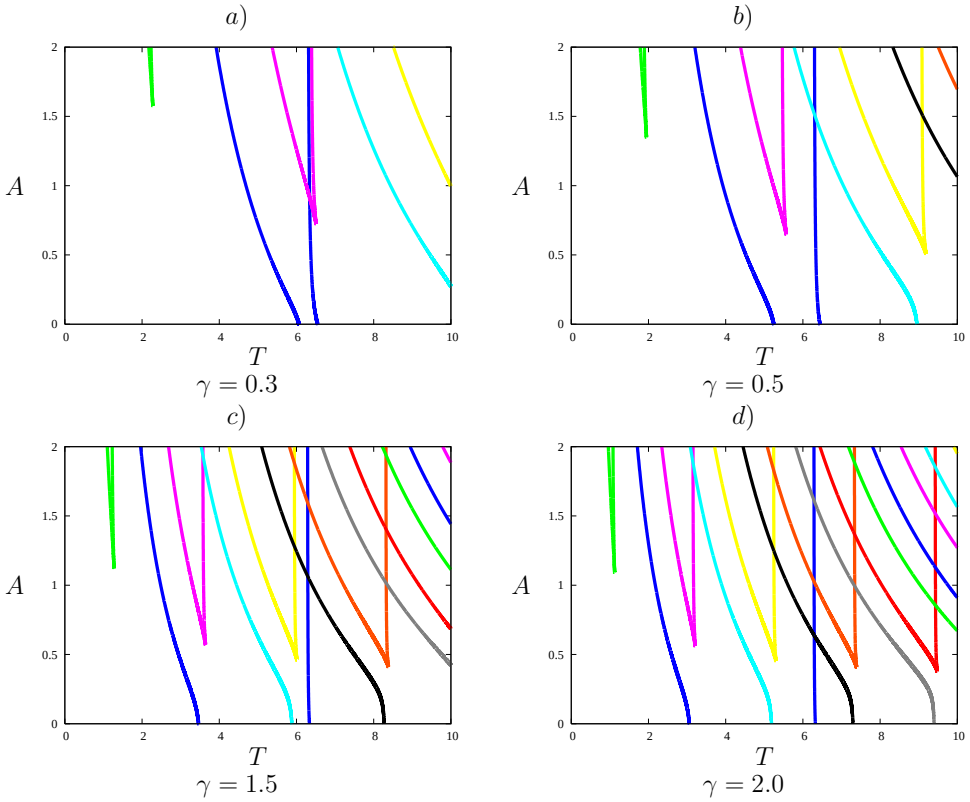

Figure 2.2: Curves parametrized by (2.15) for several values of γ on the parameter space (T, A).

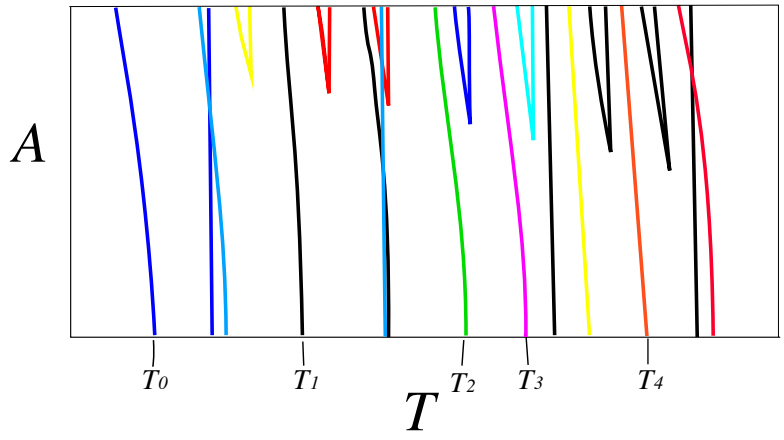

Figure 2.3: Curves parametrized by (2.15) for $\gamma = 1$ on the parameter space (T, A) for low coupling A. The sequence of times $T_0, T_1, ...$ illustrates the statement of lemma 2.4.4.

□

It is important to notice that the bifurcation curve described in the previous lemma involves branches of bifurcations of double eigenvalues which were not present in the works [106, 202, 108]. These new branches are the ones starting from $A = 0$ and they are present for each $\gamma > 0$ (see figures 2). More precisely, by just analyzing the equation $A_\gamma(q) = 0$, one can see that they occur as soon as

$$\gamma T^2 > 1.$$

This is a new feature of coupling to second nearest neighbors and not just to first nearest neighbors. As a consequence, the bifurcation picture is more involved and new solutions appear. Indeed, in the work [106] (i.e. $A = 0$ in our context), one can see that for every $T_0 > 0$, there exists $\gamma_0 > 0$ such

that for all $T < T_0$ and $\gamma < \gamma_0$, the center spectrum of the linear operator consists of *one* pair of simple eigenvalues.

In our context, we have the following lemma, whose proof follows from a continuity argument as a consequence of the two previous lemmata. We refer the reader to Figure 3 also.

Lemma 2.4.4. Fix $\gamma > 0$ and A small enough. Then there exists an increasing sequence of times $\{T_n\}_{n\geq 0}$ such that

- $T_0 > \sqrt{\frac{1}{\gamma}}$
- There exists a sequence $\{\delta_n > 0\}_{n\geq 0}$ such that for every $T \in (T_n, T_n + \delta_n)$ the center spectrum consists of $2n + 3$ pairs of simple eigenvalues.

In order to study bifurcations of travelling waves near 0, we restrict ourselves to the set Δ of A, T and γ in the parameter space such that the center spectrum Σ_c of $\mathcal{L}_{A,T,\gamma}$ has the following structure

$$\Sigma_c = \{\pm iq_0, \pm iq_1, ..., \pm iq_p\}$$

where $\pm iq_0$ is a pair of double non semi-simple eigenvalues and $\pm iq_j$ ($j = 1, ..., p$) are pairs of simple eigenvalues. In this case, the linear space generated by Σ_c is $2p + 4$-dimensional.

As previously mentioned, the reason why we consider this type of bifurcations is that the pair of double non semi-simple eigenvalues gives rise to homoclinic connections for the normal form of the evolution equation (2.5) on

the center manifold. The additional pairs of simple eigenvalues will lead to oscillatory tails.

One can check the following properties.

Lemma 2.4.5. *Fix $(A, \gamma, T) \in \Delta$ and let V_0, V_j for $j = 1, ..., p$ be the eigenvectors for the associated to iq_0 and iq_j respectively. Denote by $\hat{V}_0$ the generalized eigenvector associated to iq_0. The eigenvectors can be chosen in the following way:*

$$V_0 = \begin{pmatrix} 1 \\ iq_0 \\ e^{iq_0 v} \end{pmatrix}, \quad \hat{V}_0 = \begin{pmatrix} 0 \\ 1 \\ ve^{iq_0 v} \end{pmatrix}, \quad \text{and} \quad V_j = \begin{pmatrix} 1 \\ iq_j \\ e^{iq_j v} \end{pmatrix}$$

for $j = 1, ..., p$. Moreover, these eigenvectors satisfy

$$RV_0 = \bar{V}_0, \quad RV_j = \bar{V}_j, \quad R\hat{V}_0 = -\bar{\hat{V}}_0.$$

2.5 Problem on the hyperbolic subspace and reduction to a center manifold

In this section we compute the spectral projection on the hyperbolic subspace (invariant subspace under $\mathcal{L}_{A,T,\gamma}$ corresponding to the hyperbolic spectral part) and prove a regularity result for the associated inhomogeneous linearized equation. This result is a crucial assumption for applying center manifold reduction theory (see Theorem 2.8.1 in the Appendix). Our proof closely follows the method given in [106]. For sake of completeness, we however give the proof in the present case, making sure that the additional coupling term in A is not an obstruction to the solvability.

We call P_0, P_1, ..., P_p respectively the spectral projection on the 4-dimensional invariant subspace associated to $\pm iq_0$ and on the p 2-dimensional subspaces corresponding to $\pm iq_j$, for $j = 1, ..., p$. We also define $P = \sum_{j=0}^{p} P_j$ (spectral projection on the $2p + 4$-dimensional central subspace) and use the notations $\mathbb{D}_h = (\mathbb{I} - P)\mathbb{D}$, $\mathbb{H}_h = (\mathbb{I} - P)\mathbb{H}$, $\mathbb{D}_c = P\mathbb{D}$, $U_h = (\mathbb{I} - P)U$. The affine linearized system on $\mathbb{H}_h$ reads

$$\frac{dU_h}{d\xi} = \mathfrak{L}_{A,T,\gamma} U_h + F_h(\xi) \tag{2.17}$$

where $F(\xi) = (0, f(\xi), 0)^T$ lies in the range of the nonlinear operator (2.7). We shall note $U_h = (\varphi^h, \dot{\varphi}^h, \Phi^h(v))^T$.

Our aim is to check the regularity property of equation (2.17) (see [216], property (ii) p.127 or see the appendix). This property can be stated as follows. We introduce the following Banach space, for a given Banach space Z and $\alpha \in \mathbb{R}^+$:

$$E_j^\alpha(Z) = \left\{ f \in C^j(\mathbb{R}, Z) \ \|f\|_j = \max_{0 \le k \le j} \sup_{t \in \mathbb{R}} e^{-\alpha|t|} |D^k f(t)| < \infty \right\}. \tag{2.18}$$

We have to prove that system (2.17) admits a unique solution U_h in $E_0^\alpha(\mathbb{D}_h) \bigcap E_1^\alpha(\mathbb{H}_h)$ for $0 \le \alpha < \alpha_0$ (for some $\alpha_0 > 0$), the operator $K_h : E_0^\alpha(\mathbb{R}) \to E_0^\alpha(\mathbb{D}_h)$, $f \mapsto U_h$ being bounded.

We do not know *a priori* if the operator $\mathfrak{L}_{A,T,\gamma}$ is sectorial, providing explicit estimates on U_h. Following the method in [106, 204], we compute by hand the solution U_h and provide necessary estimates.

2.5.1 Computation of the spectral projection on the hyperbolic subspace

The spectral projection on the central subspace is defined by the Dunford integral

$$P = \frac{1}{2i\pi}\int_C (\sigma\mathbb{I} - \mathfrak{L}_{A,T,\gamma})^{-1} dC, \tag{2.19}$$

where C is a regular curve surrounding $\pm iq_0, \pm iq_1, ..., \pm iq_p$. The spectral projection on the hyperbolic subspace is $P_h = \mathbb{I} - P$.

We shall use the following result for computing P_h.

Lemma 2.5.1. *Let $h(z) = \frac{f(z)}{g(z)}$ be a function of $z \in \mathbb{C}$. Assume the function $f(z)$ is differentiable at $z = z_0$ and the function $g(z)$ admits a double zero at $z = z_0$. Then the residue of h at $z = z_0$ is given by*

$$Res(h, z_0) = \frac{2f'(z_0)g''(z_0) - \frac{2}{3}f(z_0)g'''(z_0)}{g''(z_0)^2}. \tag{2.20}$$

Proof. We can assume that $g(z) = (z - z_0)^2\varphi(z)$, with $\varphi(z_0) \neq 0$.

Then the residue will be given by the following limit

$$Res(h, z_0) = \lim_{z\to z_0}((z - z_0)^2 h(z_0))' = \lim_{z\to z_0}\frac{f'(z)\varphi(z) - f(z)\varphi'(z)}{\varphi^2(z)}$$

We obtain the result by computing the limit. □

In the following lemma, we compute the spectral projection on the hyperbolic subspace of a vector F lying in the range of the nonlinear operator (2.7).

Lemma 2.5.2. *Let $F \in \mathbb{D}$ be a vector of the type $F = (0, f, 0)^T$. Then the projection of F on the hyperbolic subspace reads*

$$F_h = (0, k_1 f, k_2(v) f)^T, \tag{2.21}$$

where $k_1 \in \mathbb{R}$ and $k_2 \in C^\infty([-2, 2])$ depend on A, γ and T.

Proof. We first compute the resolvent of $\mathcal{L}_{A,T,\gamma}$. One has to solve $(\sigma \mathbb{I} - \mathcal{L}_{A,T,\gamma})U = F$ for $U = (u_1, u_2, u_3)^T$, which yields the system

$$\sigma u_1 = u_2 \tag{2.22}$$

$$\beta_1 u_1 - \gamma T^2[(u_3(1) + u_3(-1)) + A(u_3(2) + u_3(-2))] = f \tag{2.23}$$

$$u_3 = u_1 e^{\sigma v} \tag{2.24}$$

for $\beta_1 = T^2(1 + 2\gamma(1 + A)) + \sigma^2$. We have then that

$$u_1 = \frac{f}{N(\sigma, T, A, \gamma)}.$$

Now we compute the spectral projection P_j. Since $\sigma_j = iq_j$, for $j = 1, ..., p$, are simple roots of the dispersion relation, one has

$$Res(u_1, iq_j) = \frac{f}{-2q_j + 2\gamma T^2 \sin(q_j) + 4A\gamma T^2 \sin(2q_j)},$$

Denoting $(P_1 F)_i$ the ith component of $P_j F$, we get consequently

$$(P_j F)_1 = Res(u_1, iq_j) + Res(u_1, -iq_j) = 0,$$

In the same spirit

$$(P_j F)_2 = \frac{-2q_j f}{-2q_j + 2\gamma T^2 \sin(q_j) + 4A\gamma T^2 \sin(2q_j)},$$

$$(P_jF)_3 = \frac{2\cos(q_jv)f}{-2q_j + 2\gamma T^2\sin(q_j) + 4A\gamma T^2\sin(2q_j)},$$

which completes the computation of the projections P_jF. For computing the spectral projection P_0 associated to the double eigenvalues $\pm iq_0$, we use formula (2.20). These computations lead to equation (2.21). □

2.5.2 Resolution of the affine equation for bounded functions of t

We first solve (2.17) in the spaces E_j^α with $\alpha = 0$, i.e. we consider bounded functions of t (note that $E_j^0(\mathbb{H}) = C_b^j(\mathbb{H})$). Fixing $\alpha = 0$ will allow us to take the Fourier transform in time of the system in the space of tempered distributions $S'(\mathbb{R})$.

From (2.17), we directly deduce

$$\begin{aligned}\Phi^h(t,v) &= \varphi^h(t+v) + \int_0^v k_2(s)f(t+v-s)ds \\ &= \varphi^h(t+v) + \int_t^{t+v} k_2(t+v-s)f(s)ds,\end{aligned} \tag{2.25}$$

(this expression comes from the two last equations of the affine linear system and from conditions $\Phi(0,t) = \varphi(t)$).

From the previous equations and the fact that k_2 and its derivatives are bounded functions of v, we deduce that

$$\|\Phi^h\|_{E_0^0(C^1[-2,2])} \leq \|\varphi^h\|_{E_1^0} + C\|f\|_{E_0^0}. \tag{2.26}$$

We now have to estimate φ^h and $\dot{\varphi}^h$. Taking the Fourier transform in time of the system (2.17) in the tempered distributional space $S'(\mathbb{R})$, we have

$$(ik - \mathcal{L}_{A,T,\gamma})\hat{U}_h = \hat{F}_h. \tag{2.27}$$

We deduce

$$\hat{\dot{\varphi}}^h = ik\hat{\varphi}^h,$$
$$\hat{\dot{\varphi}}^h = e^{ikv}\hat{\varphi}^h + \hat{f}\int_0^v e^{ik(v-s)}k(s)ds.$$

For $\hat{\varphi}^h$, we have

$$N(ik, T, A, \gamma)\hat{\varphi}^h = \hat{f}. \tag{2.28}$$

Then from (2.28) we define the function $\hat{G}$ as

$$\hat{\varphi}^h = \hat{G}\hat{f}.$$

The operator $(ik - \mathfrak{L}^h_{A,T,\gamma})^{-1}$ ($\mathfrak{L}^h_{A,T,\gamma}$ denoting the restriction of $\mathfrak{L}_{A,T,\gamma}$ to the hyperbolic space) is analytic in a strip around the real axis. We deduce that $\hat{G}$ is an analytic function in the same strip. Moreover, $\hat{G}$ behaves like $O(\frac{1}{k^2})$ as $k \to \pm\infty$ due to the fact that $N(ik, A, T, \gamma) = O(k^2)$ as $k \to \pm\infty$. The fact that the dispersion relation behaves like k^2 is important in our context. Here, even if the coupling term is more complicated, involving the second nearest neighbors, the perturbation is still $O(1)$ in terms of k.

Since $N(iq_j, A, T, \gamma) = 0$, $N'(iq_0, A, T, \gamma) = 0$ and $N'(iq_j, A, T, \gamma)$ and $N''(iq_0, A, T, \gamma)$ do not vanish, equation (2.28) yields

$$\hat{\varphi^h} = \hat{G}\hat{f} + b_0^+\delta'_{iq_0} + b_0^-\delta'_{-iq_0} + \sum_{j=1}^{p}\left(a_j^+\delta_{iq_j} + a_j^-\delta_{-iq_j}\right) \tag{2.29}$$

Furthermore, $k \to (1+|k|^2)^{1/2}\hat{G}$ belongs to $L^2(\mathbb{R})$. Therefore, using the inverse Fourier Transform and lemma 3 p.448 of [106], there exists a function $G \in H^1_\delta(\mathbb{R})$ (i.e $e^{\delta|t|}G \in H^1(\mathbb{R})$, $\delta > 0$ small enough) such that $\hat{G}$ is the unique Fourier transform of G. We have the following estimates

$$\begin{aligned} \|\frac{dG}{dt} * f\|_{C^0_b} &= \sup_{t\in\mathbb{R}} |\int_{\mathbb{R}} \frac{dG}{dt}(t-s)f(s)ds| \\ &\leq C(\delta)\|f\|_{C^0_b}\|G\|_{H^1_\delta(\mathbb{R})}. \end{aligned} \tag{2.30}$$

Now we make the solution of (2.17) explicit. We set $\tilde{U}_h = (\tilde{u}^h_1, \tilde{u}^h_2, , \tilde{u}^h_3)^T$ and

$$\begin{aligned} \tilde{u}^h_1 &= G * f, \\ \tilde{u}^h_2 &= \frac{d\tilde{u}^h_1}{dt}, \\ \tilde{u}^h_3(t,v) &= \tilde{u}^h_1(t+v) + \int_0^v k_2(s)f(t+v-s) + k_8(s)\,ds, \end{aligned}$$

By construction, $\tilde{u}^h$ satisfies (2.17) and $P\hat{\tilde{U}}_h = 0$ (hence $P\tilde{U}_h = 0$) for $f \in E^\alpha_0(\mathbb{R})$ with $\alpha < 0$ ($\hat{f}_i$ are analytic functions in a strip around the real axis). Since the computations are formally the same for $\alpha = 0$, we have $P\hat{\tilde{U}}_h = 0$ for $\alpha = 0$, hence $P\tilde{U}_h = 0$ for $\alpha = 0$.

Moreover, we have the estimate

$$\|\tilde{U}_h\|_{C^0_b(\mathbb{D}_h)\bigcap C^1_b(\mathbb{H}_h)} \leq C\|f\|_{C^0_b(\mathbb{R})} \tag{2.31}$$

due to estimates (2.26), (2.30) (with analogous estimates on H_2). For $\alpha = 0$, we obtain u^h by adding to $\tilde{u}^h$ the inverse Fourier transforms of Dirac measures,

i.e

$$\begin{aligned} u_1^h &= \tilde{u}_1^h + \sum_{j=1}^{p}(a_j^+ e^{iq_1 t} + a_j^- e^{-iq_1 t}) \\ &\quad +(a_0^+ + itb_0^+)e^{iq_0 t} + (a_0^- - itb_0^-)e^{-iq_0 t}, \end{aligned} \tag{2.32}$$

$$\begin{aligned} u_2^h &= \tilde{u}_2^h + \sum_{j=1}^{p}(c_j^+ e^{iq_j t} + c_j^- e^{-iq_j t}) \\ &\quad +(c_0^+ + itd_0^+)e^{iq_0 t} + (c_0^- - itd_0^-)e^{-iq_0 t}. \end{aligned} \tag{2.33}$$

Since $P\tilde{U}_h = 0$, we have $PU_h = 0$ if and only if

$$a_j^\pm = c_j^\pm = b_0^\pm = a_0^\pm = d_0^\pm = 0 \quad \text{for } j = 1, ..., p. \tag{2.34}$$

It follows that $U_h = \tilde{U}_h$. Finally, we have proved the following

Lemma 2.5.3. *Assume $F = (0, f, 0)^T$ and $f \in C_b^0(\mathbb{R})$. Then the affine linear system (2.17) has a unique bounded solution $U_h \in C_b^0(\mathbb{D}_h) \bigcap C_b^1(\mathbb{H}_h)$ and the operator $K_h : C_b^0(\mathbb{R}) \to C_b^0(\mathbb{D}_h)$, $f \mapsto U_h$ is bounded.*

2.5.3 Affine equation in exponentially weighted spaces

The problem now is to extend lemma 2.5.3 to the case $f \in E_0^\alpha(\mathbb{R})$, with $\alpha > 0$ sufficiently close to 0. This has been done in [106] by constructing a suitable distribution space, but the following lemma gives an alternative proof (see [170]).

Lemma 2.5.4. *Consider Banach spaces $\mathbb{D}$,$\mathbb{Y}$ and $\mathbb{X}$ such that: $\mathbb{D} \hookrightarrow \mathbb{Y} \hookrightarrow \mathbb{X}$. Let L be a closed linear operator in $\mathbb{X}$, of domain $\mathbb{D}$, such that the equation*

$$\frac{dU}{dt} = LU + f \tag{2.35}$$

admits for any fixed $f \in C_b^0(\mathbb{Y})$ *a unique solution*

$$U = Kf$$

in $C_b^0(\mathbb{D}) \bigcap C_b^1(\mathbb{X})$*, with in addition* $K \in \mathfrak{L}(C_b^0(\mathbb{Y}), C_b^0(\mathbb{D}))$*. Then there exists* $\alpha_0 > 0$ *such that if* $0 \leq \alpha < \alpha_0$*, for all* $f \in E_0^\alpha(\mathbb{Y})$ *the system (2.35) admits a unique solution in* $E_0^\alpha(\mathbb{D}) \bigcap E_1^\alpha(\mathbb{X})$ *with*

$$\|U\|_{E_0^\alpha(\mathbb{D})} \leq C(\alpha)\|f\|_{E_0^\alpha(\mathbb{Y})}. \tag{2.36}$$

Applying this result to our problem yields the following result.

Proposition 2.5.5. There exists $\alpha_0 > 0$ such that for all $F = (0, f, 0)^T$ with $f \in E_0^\alpha(\mathbb{R})$ and $\alpha \in [0, \alpha_0]$, the affine linear system (2.17) has a unique solution $U_h \in E_0^\alpha(\mathbb{D}_h) \bigcap E_1^\alpha(\mathbb{H}_h)$. Moreover, the operator $K_h : E_0^\alpha(\mathbb{R}) \to E_0^\alpha(\mathbb{D}_h)$, $f \mapsto U_h$ is bounded (uniformly in $\alpha \in [0, \alpha_0]$).

Remark 2.5.6. It has to be remarked that the previous argument is also valid if the system involves more general linear coupling terms (to the third or farther neighbors). Indeed, the perturbation in the dispersion relation still involves $O(1)$ terms in k and as a consequence $N(ik, A, T, \gamma)$ is still $O(k^2)$. Hence the regularity argument with the kernel G still holds.

However, for the case of pulsating travelling waves, as it was pointed out in [108, 202], one has to be more careful. Indeed, one can use for instance the alternative argument developed in [202] to overcome the fact that the dispersion relation does not have the suitable behaviour.

2.6 Normal form computations

This section is devoted to the computation of the normal form after reduction to a center manifold. Normal form theory (see for instance [105]) ensures that there exists a change of variables $U_c = \tilde{U}_c + \tilde{P}_{\gamma,T}(\tilde{U}_c)$ (here $U_c = PU$ an $\tilde{P}$ is close to the identity). The simplifies the reduced equation on the center manifold. In this section, we provide this normal form at order 3.

2.6.1 Normal forms

The linear operator $\mathfrak{L}_{A,T,\gamma}$ restricted to the $(2p+4)$-dimensional subspace $\mathbb{D}_c$ has the following structure in the basis $(V_0, \hat{V}_0, V_1, ..., V_p, \bar{V}_0, \bar{\hat{V}}_0, \bar{V}_1, ..., \bar{V}_p)$ of eigenvectors in Lemma 2.4.5

$$\mathfrak{L}_c = \begin{pmatrix} J_1 & & & \\ & \Lambda & & \\ & & J_2 & \\ & & & \Lambda' \end{pmatrix}$$

where

$$J_1 = \begin{pmatrix} iq_0 & 1 \\ 0 & iq_0 \end{pmatrix}, \qquad J_2 = \begin{pmatrix} -iq_0 & 1 \\ 0 & -iq_0 \end{pmatrix},$$
$$\Lambda = \begin{pmatrix} iq_1 & & \\ & \ddots & \\ & & iq_p \end{pmatrix}, \quad \Lambda' = \begin{pmatrix} -iq_1 & & \\ & \ddots & \\ & & -iq_p \end{pmatrix}. \tag{2.37}$$

To compute the normal form, we exclude points of Δ which are close to points where $sq_0 + \sum_{j=1}^{p} r_j q_j = 0$ for $s, r_j \in \mathbb{Z}$ and $0 < |s| + \sum_{j=1}^{p} |r_j| \leq 4$ which correspond to strong resonances. We denote this new set by Δ_0. The normal form computation is very similar to [106], to which we refer for details.

In what follows we set $\tilde{U}_c = \mathcal{A}V_0 + \mathcal{B}\hat{V}_0 + \sum_{j=1}^{p} \mathcal{C}_j V_j + \bar{\mathcal{A}}\bar{V}_0 + \bar{\mathcal{B}}\hat{\bar{V}}_0 + \sum_{j=1}^{p} \bar{\mathcal{C}}_j \bar{V}_j$. The normal form of the evolution equation (2.5) restricted to the center space up to order 3 is given in the following lemma.

Lemma 2.6.1. *The normal form of the reduced equation at order 3 reads*

$$\begin{aligned}
\frac{d\mathcal{A}}{d\xi} &= iq_0\mathcal{A} + \mathcal{B} + i\mathcal{A}\mathcal{P} + O((|\mathcal{A}| + |\mathcal{B}| + \sum_{j=1}^{p} |\mathcal{C}_j|)^4), \\
\frac{d\mathcal{B}}{d\xi} &= iq_0\mathcal{B} + i\mathcal{B}\mathcal{P} + \mathcal{A}\mathcal{S} + O((|\mathcal{A}| + |\mathcal{B}| + \sum_{j=1}^{p} |\mathcal{C}_j|)^4), \\
\frac{d\mathcal{C}_j}{d\xi} &= iq_j\mathcal{C}_j + i\mathcal{C}_j\mathcal{Q}_j + O((|\mathcal{A}| + |\mathcal{B}| + \sum_{j=1}^{p} |\mathcal{C}_j|)^4) \quad \textit{for } j = 1, ..., p.
\end{aligned} \tag{2.38}$$

where $\mathcal{P}, \mathcal{S}, \mathcal{Q}_k$ are polynomials of the variables $u_0 = \mathcal{A}\bar{\mathcal{A}}, v_0 = i(\mathcal{A}\bar{\mathcal{B}} - \bar{\mathcal{A}}\mathcal{B}), u_j = \mathcal{C}_j\bar{\mathcal{C}}_j$, with real coefficients depending smoothly on the parameters (T, A, γ) in the neigborhood of Δ. Furthermore, we have

$$\begin{aligned}
\mathcal{P}(u_0, v_0, u_1, ..., u_p) &= p_0'(A, T, \gamma) + \sum_{j=0}^{p} p_j u_j + p_{p+1} v_0 \\
\mathcal{S}(u_0, v_0, u_1, ..., u_p) &= s_0'(A, T, \gamma) + \sum_{j=0}^{p} s_j u_j + s_{p+1} v_0 \\
\mathcal{Q}_k(u_0, v_0, u_1, ..., u_p) &= \tilde{q}_{0,k}'(A, T, \gamma) + \sum_{l=0}^{p} \tilde{q}_{l,k} u_l + \tilde{q}_{p+1,k} v_0
\end{aligned} \tag{2.39}$$

where $p_0', s_0', \tilde{q}_{0j}'$ vanish on Δ_0.

The truncated normal form (obtained by neglecting terms of orders 4 and higher) is integrable with the following first integrals

$$\begin{gathered}
A\bar{B} - \bar{A}B, \\
|B|^2 - \int_0^{|A|^2} \mathcal{S}(x, |C|^2, |D|^2, i(A\bar{B} - \bar{A}B))dx, \\
|C_j|^2, \text{for } j = 1, ..., p.
\end{gathered} \tag{2.40}$$

The existence of homoclinic orbits is linked to the sign on the coefficiont s_0 in the polynomial $\mathcal{S}$. We consider values of the parameters A and T so that $s_0'(A,T) > 0$. The following section is devoted to the computation of s_0.

2.6.2 Computation of the coefficient s_0

First we expand the evolution equation (2.5) as follows

$$\begin{gathered}\frac{dU}{d\xi} = \mathcal{L}^{(0)}U + (A-A_0)\mathcal{L}^{(1)}U + (T-T_0)\mathcal{L}^{(2)}U + (\gamma-\gamma_0)\mathcal{L}^{(3)}U + \\ M_2(U,U) + M_3(U,U,U) + ...\end{gathered} \tag{2.41}$$

where $\mathcal{L}^{(0)}$ is the linear operator $\mathcal{L}_{A,T,\gamma}$ for $(A_0,T_0,\gamma_0) \in \Delta_0$,

$$\mathcal{L}^{(1)} = \gamma T^2 \begin{pmatrix} 0 \\ -2\varphi + \Phi(2) + \Phi(-2) \\ 0 \end{pmatrix},$$

$$\mathcal{L}^{(2)} = 2T \begin{pmatrix} 0 \\ (-1-2\gamma(1+A))\varphi + \gamma(\Phi(1)+\Phi(-1)) + \gamma A(\Phi(2)+\Phi(-2)) \\ 0 \end{pmatrix},$$

$$\mathcal{L}^{(3)} = T^2 \begin{pmatrix} 0 \\ -2(1+A)\varphi + (\Phi(1)+\Phi(-1)) + A(\Phi(2)+\Phi(-2)) \\ 0 \end{pmatrix},$$

$$M_2(U,U) = aT^2 \begin{pmatrix} 0 \\ \varphi^2 \\ 0 \end{pmatrix},$$

and

$$M_3(U,U,U) = bT^2 \begin{pmatrix} 0 \\ \varphi^3 \\ 0 \end{pmatrix},$$

We now expand the solution U around (A_0,T_0,γ_0) in the following way

$$\begin{gathered}U = \mathcal{A}V_0 + \mathcal{B}\hat{V}_0 + \sum_{j=1}^{p} \mathcal{C}_j V_j + \bar{\mathcal{A}}\bar{V}_0 + \bar{\mathcal{B}}\bar{\hat{V}}_0 + \sum_{j=1}^{p} \bar{\mathcal{C}}_j \bar{V}_j + \\ \sum (A-A_0)^m (T-T_0)^n (\gamma-\gamma_0)^l \mathcal{A}^{r_0}\mathcal{B}^{\hat{r_0}} C_1^{r_1} C_2^{r_2} ... C_p^{r_p} \\ \bar{\mathcal{A}}^{s_0}\bar{\mathcal{B}}^{\hat{s_0}} \bar{C}_1^{s_1} \bar{C}_2^{s_2} ... \bar{C}_p^{s_p} \phi^{(m,n,l)}_{r_0 \hat{r_0} r_1 ... r_p s_0 \hat{s_0} s_1 ... s_p}\end{gathered} \tag{2.42}$$

Then we use the use the expression of the normal form and the expanssion (2.41) to find the terms of order $\mathcal{A}^2, |\mathcal{A}|^2, \mathcal{A}|\mathcal{A}|^2$ by identification. We get the expressions (we omit the index $(m,n,l)=(0,0,0)$ in the notations)

$$\begin{aligned} (2iq_0 - \mathcal{L}_{A_0,T_0,\gamma_0})\phi_{20\ldots000\ldots0} &= M_2(V_0,V_0), \\ -\mathcal{L}_{A_0,T_0,\gamma_0}\phi_{10\ldots010\ldots0} &= 2M_2(V_0,\bar{V}_0), \\ s_0\hat{V}_0 + ip_0V_0 + (iq_0 - \mathcal{L}_{A_0,T_0,\gamma_0})\phi_{20\ldots010\ldots0} &= 2M_2(\bar{V}_0,\phi_{20\ldots000\ldots0}) \\ &\quad +2M_2(V_0,\phi_{10\ldots010\ldots0}) \\ &\quad +3M_3(V_0,V_0,\bar{V}_0). \end{aligned} \tag{2.43}$$

This leads to

$$\begin{aligned} \phi_{20\ldots000\ldots0} &= K_1 \begin{pmatrix} 1 \\ 2iq_0 \\ e^{2iq_0v} \end{pmatrix} \\ \phi_{10\ldots010\ldots0} &= 2a \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \\ \phi_{20\ldots010\ldots0} &= \varphi \begin{pmatrix} 1 \\ iq_0 \\ e^{iq_0v} \end{pmatrix} + ip_0 \begin{pmatrix} 0 \\ 1 \\ ve^{iq_0v} \end{pmatrix} + \frac{s_0}{2} \begin{pmatrix} 0 \\ 0 \\ v^2e^{iq_0v} \end{pmatrix} \end{aligned} \tag{2.44}$$

with p_0 and φ still unknown and

$$K_1 = \frac{aT_0^2}{T_0^2(1+2\gamma(1+A_0)) - 4q_0^2 - 2T_0^2\gamma\cos(2q_0) - 2T_0^2\gamma A_0\cos(4q_0)} \tag{2.45}$$

$$[1 - \gamma_0T_0^2\cos(q_0) - 4A_0\gamma_0T_0^2\cos(2q_0)]s_0 = T_0^2(2aK_1 + 4a^2 + 3b) \tag{2.46}$$

The other coefficients can be computed in a similar way.

2.7 Small amplitude solutions of the evolution equation (2.5)

This section is devoted to the study of the small amplitude solutions of (2.1) after reduction to a center manifold. This relies mainly on the study of the normal form given below

$$\begin{aligned}
\frac{d\mathcal{A}}{d\xi} &= iq_0\mathcal{A} + \mathcal{B} + i\mathcal{A}\mathcal{P} + O((|\mathcal{A}| + |\mathcal{B}| + \sum_{j=1}^{p} |\mathcal{C}_j|)^4), \\
\frac{d\mathcal{B}}{d\xi} &= iq_0\mathcal{B} + i\mathcal{B}\mathcal{P} + \mathcal{A}\mathcal{S} + O((|\mathcal{A}| + |\mathcal{B}| + \sum_{j=1}^{p} |\mathcal{C}_j|)^4), \\
\frac{d\mathcal{C}_j}{d\xi} &= iq_j\mathcal{C}_j + i\mathcal{C}_j\mathcal{Q}_j + O((|\mathcal{A}| + |\mathcal{B}| + \sum_{j=1}^{p} |\mathcal{C}_j|)^4) \quad \text{for } j = 1, ..., p.
\end{aligned} \tag{2.47}$$

Depending on the parameter regime, we study several types of solutions for equation (2.5): periodic, quasi-periodic and homoclinic solutions.

2.7.1 Periodic solutions of the evolution equation (2.5)

Consider Δ_1 as the set of parameters for which the center spectrum consists of one pair of simple eigenvalues $\pm iq^*$. By the spectral theory in Section 2.4, this set is non empty. The theory developped in Section 2.5 applies (it is a particular case when the total projection P is just the projection P_* onto the 2-dimensional invariant subspace associated to $\pm iq^*$). Therefore, one gets the following reduction theorem since the analysis in Section 2.5 shows that the assumptions of Theorem 2.8.1 in the Appendix are satisfied.

Theorem 2.7.1. Fix $(A_0, T_0, \gamma_0) \in \Delta_1$ and $k \geq 1$. There exists a neighborhood $\mathcal{U} \times \mathcal{V}$ of $(0, A_0, T_0, \gamma_0)$ in $\mathbb{D} \times \mathbb{R}^3$ and a map $\psi \in C_b^k(\mathbb{D}_c \times \mathbb{R}^3, \mathbb{D}_h)$ such that the following properties hold for all $(A, T, \gamma) \in \mathcal{V}$ (with $\psi(0, A, T, \gamma) = 0, D\psi(0, A_0, T_0, \gamma_0) = 0$).

- If $U : \mathbb{R} \to \mathbb{D}$ solves (2.5) and $U(t) \in \mathcal{U}\ \forall t \in \mathbb{R}$ then $U_h(t) = \psi(U_c(t), A, T, \gamma)$

for all $t \in \mathbb{R}$ and U_c is a solution of

$$\frac{dU_c}{dt} = \mathcal{L}_{A_0,T_0,\gamma_0} U_c + P_* \mathcal{N}_T(U_c + \psi(U_c, A, T, \gamma)). \tag{2.48}$$

- If $U_c : \mathbb{R} \to \mathbb{D}_c$ is a solution of (2.48) with $U_c \in \mathcal{U}_c = P_* \mathcal{U}$ $\forall t \in \mathbb{R}$, then $U = U_c + \psi(U_c, A, T, \gamma)$ is a solution of (2.5).

- The map $\psi(., A, T, \gamma)$ commutes with R. Moreover, the reduced system (2.48) is reversible under R.

The normal form (2.47) then reduces in this case to

$$\frac{d\mathcal{C}_*}{d\xi} = iq_* \mathcal{C}_* + i\mathcal{C}_* \mathcal{Q}_* + O(|\mathcal{C}_*|^4)$$

together with the conjugate equation.

We now apply the center Devaney-Lyapunov theorem to get the following result

Theorem 2.7.2. For every $(A, T, \gamma) \in \Delta_1$ and for U near the origin in $\mathbb{D}$, the evolution equation (2.5) reduces to a two-dimensional reversible smooth vector field.

Moreover, the set of solutions near 0 of (2.5) constitutes a one-parameter family of periodic orbits, bifurcating from 0.

As a corollary of the previous theorem, one gets Theorem 2.3.1.

2.7.2 Quasi-periodic solutions of (2.5)

We are now interested in quasi-periodic motions for equation (2.5). Let Δ_2 be the set of parameters for which the center spectrum consists of a finite number of pairs of simple eigenvalues $\pm iq_k$ for $k = 1, ..., p$ with $p > 1$. Once again, Section 2.4 shows that this set is non empty. We have the following reduction theorem where $P = \sum_{k=1}^{p} P_k$ is the total projection with the same notation as in Section 2.5.

Theorem 2.7.3. Fix $(A_0, T_0, \gamma_0) \in \Delta_2$ and $k \geq 1$. There exists a neighborhood $\mathcal{U} \times \mathcal{V}$ of $(0, A_0, T_0, \gamma_0)$ in $\mathbb{D} \times \mathbb{R}^3$ and a map $\psi \in C_b^k(\mathbb{D}_c \times \mathbb{R}^3, \mathbb{D}_h)$ such that the following properties hold for all $(A, T, \gamma) \in \mathcal{V}$ (with $\psi(0, A, T, \gamma) = 0, D\psi(0, A_0, T_0, \gamma_0) = 0$).

- If $U : \mathbb{R} \to \mathbb{D}$ solves (2.5) and $U(t) \in \mathcal{U}\ \forall t \in \mathbb{R}$ then $U_h(t) = \psi(U_c(t), A, T, \gamma)$ for all $t \in \mathbb{R}$ and U_c is a solution of

$$\frac{dU_c}{dt} = \mathcal{L}_{A_0,T_0,\gamma_0} U_c + P\mathcal{N}_T(U_c + \psi(U_c, A, T, \gamma)). \tag{2.49}$$

- If $U_c : \mathbb{R} \to \mathbb{D}_c$ is a solution of (2.49) with $U_c \in \mathcal{U}_c = P\mathcal{U}\ \forall t \in \mathbb{R}$, then $U = U_c + \psi(U_c, A, T, \gamma)$ is a solution of (2.5).

- The map $\psi(., A, T, \gamma)$ commutes with R. Moreover, the reduced system (2.49) is reversible under R.

In this case, the normal form (2.47) writes

$$\frac{d\mathcal{C}_j}{d\xi} = iq_j\mathcal{C}_j + i\mathcal{C}_j\Omega_j + O((\sum_{k=1}^{p}|\mathcal{C}_k|)^4) \quad \text{for } j = 1, ..., p \tag{2.50}$$

together with the conjugate equations.

Considering the standard (almost-complex) symplectic structure J in $\mathbb{R}^{2p}$ (up to some complexification), it is then easy to see that the previous system (2.50) inheritates an Hamiltonian structure $H = H_0 + \mathcal{R}$, where H_0 is integrable (in the Arnold-Liouville sense) and $\mathcal{R}$ stands for higher order terms.

In order to apply a KAM theorem to ensure the existence of invariant $p-dimensional$ tori (we refer to [58] for an account on KAM theorems), one has to check several assumptions. The phase space is foliated by invariant tori for the unperturbed system (i.e. getting rid of high order terms in (2.50), $\mathcal{R} = 0$), which are given by

$$q_1\mathbb{S}^1 \times \cdots \times q_p\mathbb{S}^1 \times \{a\}^p,$$

provided that $(q_1, ..., q_p)$ is Diophantine in $\mathbb{R}^p$, $a \in \mathbb{R}$ and where $q_j\mathbb{S}^1$ stands for the torus $\mathbb{R}/(q_j\mathbb{Z})$. To be able to apply the standard KAM theorem in our context, one has to check: first, some regularity and smallness assumptions on the underlying Hamiltonian H and second, the twist condition. Our Hamiltonian H is not analytic since it comes from the reduction to a center manifold, which are not analytic manifolds. However, it is a well-known fact in KAM theory that one can overcome this difficulty by introducing suitable smoothing operators (see for instance [58]). The smallness assumption

amounts to control the remainder $\mathcal{R}$ in a suitable norm. This can be done by shrinking a little bit the amplitude of our solutions. The most intricate assumption to check is the twist condition. In our context, according to the form of the Hamiltonian H this amounts to check the invertibility of a matrix involving the coefficients $\tilde{q}_{l,j}$ of the normal form (2.47).

We are not going to state a result since it involves lengthy computations but one can say that generically, there exists an open set of parameters such that system (2.5) admits invariant tori of dimension p.

2.7.3 Homoclinic solutions of (2.5)

We now concentrate on homoclinic solutions (possibly to 0) for system (2.5). In this case, these solutions for the truncated normal form for $C_j = 0$ $(j = 1, ..., p)$ are given by, provided $s_0(A_0, T_0, \gamma_0) < 0$ and $s_0'(A, T, \gamma) > 0$

$$\mathcal{A}(\xi) = r_0(\xi)e^{i(q_0\xi+\psi(\xi)+\theta)}, \quad \mathcal{B}(\xi) = r_1(\xi)e^{i(q_0\xi+\psi(\xi)+\theta)}, \tag{2.51}$$

where

$$\begin{aligned} r_0(\xi) &= \sqrt{\tfrac{2s_0}{-s_0'}}\operatorname{sech}(\xi\sqrt{s_0}) \\ r_1(\xi) &= \frac{dr_0(\xi)}{d\xi} \\ \psi(\xi) &= p_0\xi - \frac{2p_0'\sqrt{s_0}}{s_0'}\tanh(\xi\sqrt{s_0'}) \end{aligned} \tag{2.52}$$

This orbits are reversible under R if one chooses θ equal to 0 or π. We first state the reduction theorem. Let Δ_0 be the set of parameters introduced in Section 2.4. We have

Theorem 2.7.4. Fix $(A_0, T_0, \gamma_0) \in \Delta_0$ and $k \geq 1$. There exists a neighborhood $\mathcal{U} \times \mathcal{V}$ of $(0, A_0, T_0, \gamma_0)$ in $\mathbb{D} \times \mathbb{R}^3$ and a map $\psi \in C_b^k(\mathbb{D}_c \times \mathbb{R}^3, \mathbb{D}_h)$ such that the following properties hold for all $(A, T, \gamma) \in \mathcal{V}$ (with $\psi(0, A, T, \gamma) = 0, D\psi(0, A_0, T_0, \gamma_0) = 0$).

- If $U : \mathbb{R} \to \mathbb{D}$ solves (2.5) and $U(t) \in \mathcal{U}\ \forall t \in \mathbb{R}$ then $U_h(t) = \psi(U_c(t), A, T, \gamma)$ for all $t \in \mathbb{R}$ and U_c is a solution of

$$\frac{dU_c}{dt} = \mathcal{L}_{A_0,T_0,\gamma_0} U_c + P\mathcal{N}_T(U_c + \psi(U_c, A, T, \gamma)). \tag{2.53}$$

- If $U_c : \mathbb{R} \to \mathbb{D}_c$ is a solution of (2.53) with $U_c \in \mathcal{U}_c = P\mathcal{U}\ \forall t \in \mathbb{R}$, then $U = U_c + \psi(U_c, A, T, \gamma)$ is a solution of (2.5).

- The map $\psi(., A, T, \gamma)$ commutes with R. Moreover, the reduced system (2.53) is reversible under R.

On the center manifold, the normal form is given by Lemma 2.6.1. The question is now to study the persistence of the solution given by equations (2.51). Several regimes of parameters have to be considered.

We choose $(A, T, \gamma) \approx (A_0, T_0, \gamma_0)$ ($(A_0, T_0, \gamma_0) \in \Delta_0$), in such a way that the linearized operator $\mathcal{L}_{A,T,\gamma}$ has four symmetric eigenvalues close to $\pm i q_0$ and having non zero real parts ($s_0'(A, T, \gamma) > 0$). We will assume that (A, T, γ) is such that Δ_0 contains only one pair of eigenvalues (see Section 2.4) and that $s_0(A, T, \gamma) < 0$. Roughly speaking, (A, T, γ) is close to the *first* tongue in the parameter plane (see Figure 1). We are now in position to

apply the results by Lombardi (see [133], [107]): homoclinic solutions to 0 do not persist for the full normal form (2.47). Instead, solutions homoclinic to exponentially small periodic orbits whose size is of order $O(e^{-C/d^{1/2}})$ where d is the distance from (A, T, γ) to the bifurcation surface.

This allows to get the following theorem

Theorem 2.7.5. Let (A, T, γ) be close to $(A_0, T_0, \gamma_0) \in \Delta_0$ (except of some exceptional points corresponding for instance to strong resonances) such that the center spectrum consists of one pair of double non semi-simple eigenvalues and one pair of simple eigenvalues.

Then the evolution equation (2.5) is reducible to a 6 dimensional vector-field for U close to the origin in $\mathbb{D}$ and there are travelling waves which are the superposition of a localized wave with an exponentially small periodic tail provided that the coefficient depending only on constants of the problem satisfies $s_0(A_0, T_0, \gamma_0) < 0$.

The previous theorem implies Theorem 2.3.2. In the previous situation where the center spectrum consists of one pair of double non semi-simple and only one pair of simple eigenvalues, one can give a complete result thanks to Lombardi's results. However, in our case (see Section 2.4), even at low coupling A there are some regions in the parameter plane for which the center spectrum consists of one pair of double non semi-simple eigenvalue and *several* pairs of simple eigenvalues. In this context, a complete theory is not yet available. The structure of the possible oscillatory tails is more involved in this case.

As in [108, 202], one can conjecture the persistence of homoclinic connections to higher dimensional tori.

2.8 Formal Multiscale expansions

This section is devoted to a multi-scale expansion yielding a continuous approximation of the lattice equation (2.1). This type of analysis has been done by Remoissenet (from a formal point of view) in [191] and justified in [92] in the case $A = 0$.

In this section, we use the approach of Remoissenet to get our continuous approximation for $A > 0$. However, it could be justified rigourously using the methods developped in [92]. The whole point consists in searching for a solution of (2.1) in the form of modulated plane waves. We write a solution of (2.1) as

$$x_n(t) = F_{1n}(t)e^{i\theta_n} + c.c. + \varepsilon \left[F_{0n}(t) + F_{2n}(t)e^{2i\theta_n} + c.c.\right] \tag{2.54}$$

with $\theta_n = q_0(n - t/T_0)$. We use a continuum approximation for the functions F_{jn} (replacing $F_{jn}(t)$ by $F_j(t, x)$). Making use of a multi-scale expansion as in [191], we end up with the following nonlinear Schrödinger equation (NLS) given by

$$iF_{1s} + PF_{1ZZ} + Q|F_1|^2F_1 = 0, \tag{2.55}$$

where s, Z are slow variables (s stands for a time variable and Z for a spatial variable). The previous equation (2.55) is obtained by plugging (2.54)

into (2.1) and identifying up to order ε^2 and the coefficients P and Q are given by the formulas

$$P = \frac{\gamma_0 T_0}{q_0}\left(\cos(q_0) + 4A\cos(2q_0) - \frac{\gamma_0 T_0^2}{q_0^2}(\sin(q_0) + 2A\sin(2q_0))^2\right) \tag{2.56}$$

and

$$Q = \frac{T_0}{2q_0}\left(4a^2 - \frac{2a^2}{3 + 16\gamma_0(\sin^4(q_0/2) + A\sin^4(q_0))} + 3b\right). \tag{2.57}$$

Now, using the dispersion relations (2.13) and (2.14), we notice that

$$\begin{aligned} &T_0^2(3 + 16\gamma_0(\sin^4(q_0/2) + A\sin^4(q_0))) \\ &\quad = T_0^2(-1 - 2\gamma_0(1 + A_0)) + 4q_0^2 + 2\gamma_0 T_0^2\cos(2q_0) + 2A\gamma_0 T_0^2\cos(4q_0) \end{aligned} \tag{2.58}$$

and

$$\begin{aligned} \gamma_0 T_0^2(\cos(q_0) + 4A_0\cos(2q_0) - &\frac{\gamma_0 T_0^2}{q_0^2}(\sin(q_0) + 2A\sin(2q_0))^2) \\ &= (\gamma_0 T_0^2(\cos(q_0) + 4A_0\cos(q_0)) - 1). \end{aligned} \tag{2.59}$$

So, we can express P and Q in the following way

$$P = \frac{1}{q_0 T_0}\left(\gamma_0 T_0^2(\cos(q_0) + 4A_0\cos(q_0)) - 1\right) \tag{2.60}$$

and

$$Q = \frac{T_0}{2q_0}\left(4a^2 + 2aK_1 + 3b\right) \tag{2.61}$$

where K_1 is given by the expression (2.45).

The existence of solitons in NLS for the specific wave number $\frac{q_0}{2}$ relies on the condition $PQ > 0$. Using the expressions (2.60) and (2.61), one can see that this condition is equivalent to have $s_0 < 0$ where s_0 is given by (2.46).

It has to be noticed and this is an important feature of the model, that the previous computations work for $A > 0$. The case $A < 0$ has also a physical meaning. It corresponds to anti-ferromagnetic interactions. In this case, an easy computation shows that the continuous approximation is no longer NLS but an elliptic equation involving a 4th derivative operator. We believe that the case $A < 0$ deserves more investigation and we postpone it to future work.

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Appendix: reduction to a center manifold theorem

We recall here the theorem we use to reduce to a center manifold. We state it as it is written in [216].

Let X, Y and Z be three Banach spaces with X continuously embedded in Y and Y continuously embedded in Z. Let $A \in \mathcal{L}(X, Z)$ and $g \in C^k(X, Y)$

for some $k \geq 1$. We consider the following differential equation

$$\dot{x} = Ax + g(x). \tag{2.62}$$

Before stating the theorem, we introduce some definitions and notations. Let E and F be two Banach spaces, $V \subset E$ an open subset, $k \in \mathbb{N}$ and $\eta \geq 0$. Then we define

$$C_b^k = \left\{ w \in C^k(V, F) \,|\, |w|_{j,V} = \sup_{x \in V} \|D^j w(x)\| < \infty,\, 0 \leq j \leq k \right\}$$

and

$$BC^\eta(\mathbb{R}, E) = \left\{ w \in C^0(\mathbb{R}, E) \,|\, \|w\|_\eta = \sup_{t \in \mathbb{R}} e^{-\eta|t|} \|w(t)\|_E < \infty \right\}.$$

Theorem 2.8.1. Assume that

- The function $g \in C^k(X, Y)$ for some $k \geq 1$ and $g(0) = 0$, $Dg(0) = 0$.
- There exists a continuous projection $\pi_c \in \mathcal{L}(Z, X)$ onto a finite-dimensional subspace $Z_c = X_c \subset X$ such that for all $x \in X$

  $$A\pi_c x = \pi_c A x$$

  and such that if we set

  $$Z_h = (I - \pi_c)Z, \;\; X_h = (I - \pi_c)X, \;\; Y_h = (I - \pi_c)Y,$$

  $$A_c = A|_{X_c} \in \mathcal{L}(X_c), \;\; A_h = A|_{X_h} \in \mathcal{L}(X_h, Z_h),$$

  then the following holds:

1. The spectrum of A_c is on the imaginary axis

2. There exists some $\beta > 0$ such that for each $\eta \in [0, \beta)$ and for each $f \in BC^\eta(\mathbb{R}, Y_h)$ the affine problem

$$\dot{x}_h = A_h x_h + f(t)$$

has a unique solution $x_h = K_h f$ where

$$K_h \in \mathcal{L}(BC^\eta(\mathbb{R}, Y_h), BC^\eta(\mathbb{R}, X_h))$$

for each $\eta \in [0, \beta)$ and

$$\|K_h\|_\eta \leq \gamma(\eta)$$

for all $\eta \in [0, \beta)$ and some continuous curve γ.

Then there exists a neighborhood Ω of the origin in X and a mapping $\psi \in C_b^k(X_c, X_h)$ with $\psi(0) = 0$ and $D\psi(0) = 0$ such that

$$\mathcal{M} = \{x_c + \psi(x_c) \,|\, x_c \in X_c\}$$

is a local center manifold for (2.62).

Chapter 3

Fast numerical computation of quasi-periodic equilibrium states in 1-D statistical mechanics, including twist maps

3.1 Introduction

The goal of this paper is to develop efficient algorithms to compute smooth quasi-periodic equilibrium states of models in 1-D statistical mechanics.

The class of models we consider (described in Section 4.2) is very general. The models we consider include as a particular case twist mappings of an annulus, but they include several other models which do not have a dynamical interpretation.

When the model describes a twist mapping, the equilibrium states are orbits of the map. Hence our algorithm includes, as particular cases, the computation of KAM tori for twist maps. The computation of KAM tori for twist mappings has been studied extensively in [149, 137, 185, 126, 14]. Other particular cases of the models considered are the Frenkel-Kontorova models of deposition of materials and of dislocations [14, 30], as well as some long range variants [39], the XY models of magnetism and their long range variants

[167, 26], models of spin waves, and monotone recurrences [11].

The models we consider describe sites in a 1-D lattice whose internal state is given by a single number. Hence, the state of the system is given by a sequence x_i of numbers. Each site interacts with all the others. The interactions we consider can be multi-body but, as customary in Statistical Mechanics, we will assume that the interactions decay fast enough with the distance (power law decay with a power bigger than 4 is enough).

We will also assume that the interactions are invariant under translation and that they satisfy some mild periodicity conditions (they are automatic when the x_i have the physical interpretation of an angle, such as in spin waves).

We seek quasi-periodic equilibria. That is, we seek equilibrium configurations of the form $x_i = h(\omega i)$ with $h(t+1) = h(t) + 1$. Equilibrium configurations means that the total forces in each of the sites vanish or, equivalently that the derivative of the energy with respect to the state of all the particles vanishes.

These quasi-periodic equilibrium configurations have been extensively studied in twist mappings and Frenkel-Kontorova models. In particular, we call attention to [14]. In that paper, it is showed that many important physical properties of the materials described by a Frenkel-Kontorova model depend on whether the function h is analytic or has discontinuities. Both alternatives happen for different values of the parameter of the model which are, apparently arbitrarily close. A great deal of effort has been devoted understanding this

breakdown of analyticity transition. For the case of nearest neighbor interactions, this breakdown of analyticity is equivalent to the problem of breakdown of KAM tori and the onset of large scale stochasticity. See [168, 165] for reviews written with two different viewpoints.

The goal of this paper is to implement very efficient numerical methods for the computation of quasi-periodic equilibria and then, use them to study the breakdown of analyticity and generate precise mathematical conjectures.

The main strategy is that we derive a functional equation for h which is equivalent to the fact that the configuration $x_i = h(\omega i)$ is in equilibrium and then consider Newton methods for this equation. Since $h(t) - t$ is periodic, it is natural to discretize h using Fourier coefficients.

If we discretize h using N Fourier coefficients, a straightforward implementation of Newton method (which we will later call the *"large matrix method"* will require storage of $O(N^2)$ terms for the $N \times N$ matrix of the discretized derivative and $O(N^3)$ operations for a Newton step. The methods implemented here require only $O(N)$ storage and $O(N \log(N))$ operations for one Newton step. Perhaps, relatedly, they seem to be less prone to round-off error than the straightforward implementation of Newton method. Using the fast methods, we can use $N \approx 10^4$ in a modest desktop computer with an Intel Core 2 Duo processor at $2.40GHz$ and have Newton steps that take $\approx .1sec$.

We include a discussion of an implementation of the large matrix method in 3.3.1. This serves as a comparison with the more efficient methods which

are the main novelty of this paper. Perhaps more importantly, we note that the large matrix method can be used to study models with rather long range interactions. These long-range models are somewhat similar to the hierarchical models of [75], which experiment phase transitions even if they are one-dimensional. We find empirically that the large matrix method does not have any difficulty finding invariant tori. We call attention to the fact that there is no rigorous study of the existence of quasi-periodic solutions in these very long-range models.

Using the Large Matrix model, we run computations with 256 Fourier modes which take .3 secs per continuation step in a modest desktop computer with an Intel Core 2 Duo processor at $2.40GHz$. Extrapolating the cubic behavior, we see that the fast algorithms introduced here, produce a speed up of a factor of more than 10^4 over the straightforward methods.

Of course, even if Newton methods lead to very accurate solutions, they require rather good initial guesses. We have two alternatives: The first one is to use a continuation method from an integrable case [7], roughly, starting from the integrable case, whose solutions are known, we use the accurate solutions of for some parameters as initial approximations for the computation of solutions of a slightly different parameter.

A second alternative, in the models considered are ferromagnetic (or twist in the language of dynamical systems), comes from the fact that the quasi-periodic equilibria are minimizers of a variational principle which we develop in section 3.2.5. In these cases, we compute the minimizer using a

minimization algorithm and then, polish the computation using the Newton method.

For models such as the XY-model which do not have a convex variational principle, the main method to obtain good guesses is to use continuation from the integrable case.

We also note that the computations presented here are backed by rigorous results. In [60] it is shown that, given one approximate solution of the equilibrium equations, if the solution is approximate enough compared with some quality numbers computable out of the approximate solution (some non-degeneracy assumptions and some appropriate norms of the approximate solution) then, there is a true solution close to the approximate solution. Furthermore, the solution is unique in a small neighborhood.

As a first application of the method, in Section 3.5, we undertake a study of breakdown of analyticity transition. This transition is of great importance for the applications of the models. Since the analyticity of not of the quasi-periodic solutions determines several physical properties such as stickiness (in the Frenkel-Kontorova model) or global transport (in twist-maps).

From the numerical point of view, the computation is rather delicate since the goal is to compute invariant tori when the parameters of the model are as close as possible to the parameter values for which the tori cease to exist. As the parameters get close to the breakdown, the truncated solutions have large norms. At the same time, the truncated equations have many spurious

solutions which are artifacts of the discretization.

The methods developed in this paper are very well suited for these delicate calculations. Given the efficiency of the calculation, we can use a higher order truncation of the Fourier series. At the same time, the rigorous validation results allow us to be confident that the succesfull computations correspond to true effects and allow us to exclude the spurious solutions.

As a byproduct of the validation of the calculations, we obtain a direct way to compute the analyticity transition. As we approach the breakdown of the analytic solutions, the norms of the function have to blow up. This gives a criterion for the breakdown of analyticity which is independent of the criterion of [95] and which is applicable to extended models.

In this paper, we report some explorations of the breakdown of KAM tori in twist mappings, Frenkel-Kontorova models with long range interactions and and XY models. The results that we found is that, there are regions in the parameter space where all these models have breakdowns with some scaling behavior.

The scaling behavior found in these models is, up to the error of the computations reported here, is very similar to the scaling exponents found in twist mappings [149, 137, 122]. Since some of the models studied here cannot be interpreted as a dynamical systems, this suggests that there should be formulations of renormalization group for models of statistical models which are not dynamical systems.

Remark 3.1.1. The speedup of the methods presented here comes from several identities that are derived from the variational structure of the models. This is very different from other recent algorithms for Hamiltonian systems [104]. The algorithms presented in this paper apply for systems that do not have an interpretation as a dynamical system – much less as a Hamiltonian one –. On the other hand, the algorithms of [104] apply to systems such as non-twist mappings that have a Hamiltonian structure but not a variational one.

Remark 3.1.2. In the case that the interactions satisfy some convexity properties – which are not needed by the KAM method – there are variational methods that allow to produce quasi-periodic solutions. In the case of nearest neighbor interactions, this is the celebrated Aubry-Mather theory [153, 151, 165, 14]. Extensions to systems with long range interactions (and to higher dimensional lattices, and existence of other multiple critical points) were obtained in [11, 38, 67, 68],

The above mentioned variational methods can produce solutions in which the hull function is discontinuous. From the technical point of view, we note that the variational method requires less differentiability from the interactions. The algorithms in this paper apply to models such as the XY model for which the the convexity properties of Aubry-Mather are not satisfied.

Remark 3.1.3. We note that the methods presented here do not depend on the system being close to integrable. The paper [40, 43] use a perturbative series expansion to produce an approximate solution. Since power series expansions only converge in complex disks, they are affected by the closest singularities.

Continuation methods do not have this problem. Some comparisons bewteen Newton methods were done in [65, 64]. Some early applications of continuation methods appear in [190, 57].

3.2 Statistical mechanics models in 1-D and their equilibrium configurations

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 giving a sequence of real values (equivalently a function $x : \mathbb{Z} \to \mathbb{R}$).

As is standard in Statistical Mechanics, [192] the interaction among the particles of the system is described by assigning an energy to each finite subset of sites. The total energy of a configuration of the system is the sum of all the possible energies. As it is well known, this sum is purely formal, but there are well defined ways of making sense of several quantities of interest.

We will assume that:

(H1) The interaction is invariant under translations. Hence, we will consider models whose formal energy is of the form:

$$\mathcal{S}(\{x_n\}) = \sum_{L \in \mathbb{N}} \sum_{k \in \mathbb{Z}} H_L(x_k, ..., x_{k+L}) \tag{3.1}$$

(H2) The following periodicity condition holds.

$$H_L(x_k, ..., x_{k+L}) = H_L(x_k + 1, \ldots, x_{k+L} + 1) \tag{3.2}$$

The property (5.30) is a rather weak periodicity condition. It is implied by the stronger property

$$H_L(x_k, ..., x_{k+L}) = H_L(x_k + \ell_0, \ldots, x_{k+L} + \ell_L) \tag{3.3}$$

for all $\ell_i \in \mathbb{Z}$. The latter property (5.31) is natural when the variables x_i are angles. For example, spin variables. The weaker property (5.30) has appeared in many situations. It is natural when considering twist maps of the annulus [165] or monotone recurrences [11].

(H3) H_L decays "fast enough" with L.

The paper [60] contains a precise formulation of decay conditions which leads to a rigorous theorem. Even if it is clear that some decay is needed (e.g. to make sense of the equilibrium equations (5.35)), we prefer to omit a precise statement Indeed, in section 3.3.1 we consider models which do not satisfy the conditions of [60] and find that some numerical methods work well. We think that this deserves future investigation.

These will be all the assumptions on the model. Later, we will introduce some assumptions on the relations of the model with respect to the approximate solutions we are considering and assume that the frequency ω satisfies the Diophantine properties that are standard in KAM theory.

3.2.1 Some examples of models

Models of the form (5.29) include as particular cases, several models which have been proposed in the literature and which are worth to keep in mind.

- The Frenkel-Kontorova model corresponds to taking $H_0(t) = \lambda V(t)$, where λ is an arbitrary 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 in physics (e.g. as models of deposition [14], models of dislocations [83]), and in dynamical systems as twist maps, [168, 165].

- If Frenkel-Kontorova models are considered as models of dislocations, some more realistic models include longer range interactions [39].

  An interesting toy model which we refer as the extended Frenkel-Kontorova model (see Section 3.4.2) corresponds to taking H_0, H_1 as above, but we take, for $k \geq 2$

  $$H_k(x_0, \ldots, x_k) = \frac{A_k}{2}(x_0 - x_k)^2 \tag{3.4}$$

  One case, that we will consider later is $A_k = ak^{-\alpha}$, $k \geq 2$. These models are very similar to the hierarchical models of [75].

- 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.

Note that in the Heisenberg models it is very natural to consider interactions with longer range since the spin interactions extend for several sites. Indeed [26, p. 600] considers adding terms of the form $a_k s_i \cdot s_{i+k}$, $b_k(s_i \cdot s_{i+k})^2$, $c_{j,k,l}[(s_i \cdot s_{i+j}) \cdot (s_{i+k} \cdot s_{i+l}) + (s_{i+j} \cdot s_{i+k}) \cdot (s_{i+k} \cdot s_i) - (s_i \cdot s_{i+k}) \cdot (s_{i+j} \cdot s_{i+l})$. The coefficients a, b, c above are expected to decrease exponentially, Computations of these coefficients are discussed in [189]. Models including these terms fit well into the models discussed in this paper.

- In Dynamical Systems, models of the form (5.29) appear as variational principles for twist mappings (again $H_L \equiv 0$ for $L \geq 2$). In this case, the physical meaning of $\mathcal{S}$ is an action. Under the assumption that $\partial_1 \partial_2 H_1(x, y) \leq -c < 0$, the critical points of the action are the orbits of a twist map.

- In [11], one can find a discussion of monotone recurrences. The models that can be considered as dynamical systems are finite range. Hence we can just consider that $H_L \equiv 0$ for $L \neq R$. The monotonicity comes from $\partial_i \partial_j H_J \leq 0$ 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.

  For certain choices of A_k in (5.33) (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.

3.2.2 The equilibrium equations

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

$$\partial_{x_i} \mathcal{S}(\{x_n\}) = 0 \tag{3.5}$$

The physical meaning of the equilibrium equations is that the total force on each of the sites exerted from the other ones vanish (remember that the forces are the derivative of all the total energy with respect to the position). In the case that the physical meaning of $\mathcal{S}$ is an action, the equilibrium solutions are the orbits of the dynamical system.

Equilibrium solutions are very important for the physical properties of the model. For example, the ground states of the system – which dominate the low temperature behavior – are equilibrium solutions. Many of the thermodynamic properties of the system are affected by the abundance of these equilibrium solutions. On the more technical side, there are asymptotic expansions (the *instanton expansions*) which give the properties of the model in terms of the critical points.

For models of the form (5.29) the Euler-Lagrange equations are:

$$\sum_{L\in\mathbb{N}} \sum_{j=0}^{L} \partial_j H_L(x_{k-j}, ..., x_{k-j+L}) = 0 \quad \forall k \in \mathbb{Z} \tag{3.6}$$

We call attention that, in contrast with the sums defining $\mathcal{S}$ which are merely formal, the sums involved in equilibrium equations (5.35) are meant to

converge.

For example, for the Frenkel-Kontorova model, the extended Frenkel-Kontorova model and the XY model the equilibrium equations are respectively:

$$\begin{aligned} & x_{i+1} + x_{i-1} - 2x_i + \lambda V'(x_i) = 0 \\ & \sum_{k=1} A_k(x_{i+k} + x_{i-k} - 2x_i) + \lambda V'(x_i) = 0 \\ & J\left[\sin(2\pi(x_{i+1} - x_i)) - \sin(2\pi(x_i - x_{i-1}))\right] + B\sin(2\pi x_i) = 0 \end{aligned} \tag{3.7}$$

Remark 3.2.1. The equilibrium equations can be considered as a dynamical systems but this point of view has limitations.

The equation of equilibrium for the Frenkel-Kontorova model can be considered as a dynamical system in 2 dimensions. It suffices to consider the state of the system given by (x_i, x_{i-1}). Then, the equations (3.7), allow to determine (x_{i+1}, x_i). Indeed, this dynamical system is the well known area preserving standard map.

In the extended FK model, when $A_k = 0$ $j > R$, We can also consider it as a dynamical system in $2R$ dimensional space. It suffices to consider the state of a system given by $(x_{i+R-1}, \ldots, x_{i-R})$. Then, the equilibrium equations (3.7), allow to determine the next state. This is a symplectic dynamical system [217]. Note however that, changing A_{R+1} from zero to a small quantity, even if a small perturbation from the physical point of view, and from the point of veiw of the formalism discussed here, is a very drastic perturbation from the dynamical systems point of view. This arbitrarily small changes even change the dimension of the phase space. Some of the terms in the evolution include factors $1/A_{R+1}$.

Of course, when all the A_k are different from zero, but converging to zero, the interpretation as a dynamical system is not possible.

For the XY model, if we want to consider (3.7) as defining a dynamical system, we need to extricate x_{i+1} from the equilibrium equations. This requires that $|\sin(2\pi(x_i - x_{i-1})) - B/J \sin(2\pi x_i)| < 1$. Unfortunately, this condition is not invariant under the dynamical system so that the nature of the phase space of this system is rather problematic and certainly dependes on the parameters.

3.2.3 Plane-like configurations and hull functions

We are interested in equilibrium configurations $\{x_n\}$ that can be written as

$$x_n = h(n\omega) \tag{3.8}$$

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

$$h(x + e) = h(x) + e \quad \forall e \in \mathbb{Z} \tag{3.9}$$

and is analytic.

The function h is often called the *hull function*. The periodicity condition (5.37) means that h can be considered as a map of the circle to itself. We will use the notation

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

Were u is a periodic function.

(H4) We will require that ω satisfies a Diophantine condition, which is standard in KAM theory.

We recall that ω is Diophantine if for some $\kappa, \tau > 0$ we have that

$$|p\omega - q| \geq \kappa |q|^{-\tau} \qquad \forall p \in \mathbb{Z} - \{0\}, \quad q \in \mathbb{Z} \tag{3.10}$$

3.2.4 Equilibrium equations in terms of hull functions

For configurations of the form (5.36), the equilibrium equations become:

$$\begin{aligned} E[u](\theta) \equiv & \sum_{L} \sum_{j=0}^{L} \partial_j H_L(\theta - j\omega + u(\theta - j\omega), \ldots, \\ & \theta + u(\theta), \ldots, \theta + (L-j)\omega + u(\theta + (L-j)\omega)) \\ = & 0 \end{aligned} \tag{3.11}$$

3.2.5 Percival Variational Principle

It is easy to see that (5.38) is the Euler-Lagrange equation associated to the functional $\mathcal{P}$ given by the expression

$$\mathcal{P}[u] = \int_0^1 \sum_{L} \frac{1}{L} H_L(\theta + u(\theta), ..., \theta + L\omega + u(\theta + L\omega)). \tag{3.12}$$

This is an extension to the functional introduced in [185, 186].

In the case that $\mathcal{P}$ satisfies some convexity properties, implied by the ferromagnetism (or the twist), the minimizers of the problem satisfy very interesting properties [153, 14] and, in particular, they will be described by a hull function. Unfortunately, the regularity of the minimizer may depend on the parameter.

We can compute minimizers of $\mathcal{P}$ using minimization algorithms such as conjugate gradient methods. These minimizers can be used as first approximations for the Newton methods developed. If the system is not ferromagnetic, then properties of minimizers – or even their existence – is not clear.

A standard problem of minimization problems is that, when the computations of the functional has an error ϵ (truncation and round-off), the minimizers can only be computed with a precision $C\epsilon^{1/2}$, since any functions which are closer than that will give indistinguishable values of the functional. A good algorithm is to polish the minimizers taking them as an initial guess for a Newton method. This produces solutions which are accurate up to the truncation and roundoff error.

3.3 Algorithms for the solution of equilibrium solutions for hull functions

The algorithms considered come from discretizations of Newton and Quasi-Newton methods. In this section we discuss some advantages and disadvantages of each method considered.

3.3.1 Straightforward Newton method

The Newton step consists in, given u, replace it by $u+v$ where v satisfies the equation

$$E'[u]v(\theta) = -E[u](\theta). \tag{3.13}$$

The numerical Newton method consists in discretizing (3.13). If we discretize functions using N Fourier modes, $E'[u]$ is an $N \times N$ matrix. We note that $E'[u]$ is typically a dense matrix so its inversion can be performed with $O(N^3)$ operations and its storage is $O(N^2)$.

We will refer to this method as "The large matrix method".

3.3.2 Quasi-Newton method

The Quasi-Newton method is based in the algorithms developed in [60]. Given u, the improved solution is $u + v$ where v is obtained solving

$$h'(\theta)(E'[u]v)(\theta) - v(\theta)(E'[u]h')(\theta) = -h'(\theta)E[u](\theta). \tag{3.14}$$

Note that the equation (5.41) differs from the Newton step equation (3.13) by the term $v(\theta)(E'[u]h')(\theta)$. Using the identity

$$\frac{d}{d\theta}E[u](\theta) = E'[u]h'(\theta) \tag{3.15}$$

we see that (3.13) and (5.41) differ by a term whose norm can be controlled by $||E||\,||v|| \approx ||E||^2$. Hence, the iterative method based on solving (5.41) will also be quadratically convergent.

The advantage of (5.41) comes from the fact that it can can be solved very efficiently because the left hand side can be factored into a sequence of simple operators. For a detailed exposition of this factorization and estimates we refer the reader to [60]. Here we summarize what we need.

Introducing the operator

$$[\Delta_l f](\theta) \;\; = \;\; f(\theta + l\omega) - f(\theta) \;\; .$$

and the new variable w related to v by $v(\theta) = h'(\theta)w(\theta)$, the equation (5.41) transforms into:

$$\Delta_1[(\mathcal{C}_{0,1,1} + \mathcal{G})\Delta_{-1}w] = -h'E[u]. \tag{3.16}$$

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

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

and

$$\mathcal{G} = \sum_{L\leq 2}\sum_{i>j} \Delta_1^{-1}\Delta_{i-j}\mathcal{C}_{i,j,L}\Delta_{j-i}\Delta_{-1}^{-1}$$

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

$$\varphi(\theta \pm \omega) - \varphi(\theta) = \eta(\theta) \tag{3.17}$$

The equation(5.45) can be solved observing that the operators $\Delta_{\pm 1}$ are diagonal in Fourier space. Indeed, the solution is given by:

$$\hat{\varphi}_k = \hat{\eta}_k/(\exp(\pm 2\pi i\omega k) - 1), \quad k \neq 0 \tag{3.18}$$

The average of φ, $\hat{\varphi}_0$ is arbitrary. The equation (5.45) and its solution (3.18) are very standard in KAM theory. Very detailed estimates can be found in [193] when ω is Diophantine, which is our hypothesis (H4). See also the exposition in [59].

The operator $\mathcal{C}_{0,1,1}$ is invertible. If (H3) is satisfied, then $\mathcal{G}$ is a small perturbation of $\mathcal{C}_{0,1,1}$. Therefore, the operator $(\mathcal{C}_{0,1,1} + \mathcal{G})$ is invertible and the inverse can be found perturbatively.

Thus, equation (5.43) can be solved following the next algorithm:

Algorithm 3.3.1. [1)]

1. Check that $\int_{\mathbb{T}} h' E[u] = 0$.

   Note that (3.15) guarantees that this would be true if the evaluation was exact. Hence, the average gives a measure of the numerical error.

2. Find a normalized function φ (i.e. $\int \varphi = 0$) solving the equation

$$\Delta_1 \varphi = -h' E[u] \tag{3.19}$$

   Therefore, if φ is a solution for (5.46) then for any $\mathcal{T} \in \mathbb{R}$ the equation $\Delta_1(\varphi + \mathcal{T}) = h' E[u]$ holds. In particular, we choose $\mathcal{T}$ such that

$$\int (\mathcal{C} + \mathcal{G})^{-1}(\varphi + \mathcal{T}) = 0.$$

3. We solve for w from

$$\Delta_{-1} w = (\mathcal{C} + \mathcal{G})^{-1}(\varphi + \mathcal{T}) \tag{3.20}$$

4. Finally we obtain the improved solution

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

There are different implementations depending on what discretizations we use for the functions.

We call attention that all the steps are diagonal either in Fourier space or in real space. The steps in Algorithm 2 are of the following form:

- Arithmetic operations among functions, evaluation of some nonlinear functions.
- Computing derivatives
- Solving two small divisors problems

$$\text{Find } \varphi(\theta) \text{ so that } \int_{\mathbb{T}} \varphi d\theta = 0 \text{ and } \Delta_{\pm 1}\varphi = \eta_{\pm}. \tag{3.21}$$

- We also need to find the inverse of the operator $(\mathcal{C}_{0,1,1} + \mathcal{G})$ which is diagonal in real space.

  One algorithm that we used is to compute a few terms of the Neumann Series

$$(\mathcal{C}_{0,1,1} + \mathcal{G})^{-1} = \left(\sum_{n \geq 0} (-\mathcal{C}_{0,1,1}^{-1} \circ \mathcal{G})^n \right) \circ \mathcal{C}_{0,1,1}^{-1} \tag{3.22}$$

  This gives an initial guess for a Conjugate Gradient (CGNE) method [195]. Since these operators are diagonal in real space then the inversion

can be performed in $O(N)$ operations once we have computed the operators. In fact, the main cost of the complete inversion procedure lies in the computation of the elements of $\mathcal{C}_{0,1,1}$ and $\mathcal{G}$.

3.3.3 Methods of computation

Since components of the parameterization of the quasi-periodic orbits are periodic functions of one angle variable θ, it is natural to consider Fourier Series of the form

$$f(\theta) = \sum_{k=-N}^{N} \hat{f}_k e^{2\pi i k\theta} \tag{3.23}$$

$$\hat{f}_k = \bar{\hat{f}}_{-k}. \tag{3.24}$$

where (3.24) comes from the fact that f is real on the real axis. Then, it is clear that we can store a f using either $N+1$ coefficients of the Fourier series or the values of f on a grid of $2N-1$ points.

As we discussed in section 3.3.2, the Newton methods involve some operators that are diagonal in Fourier Spaces (i.e., shifts, sums) and some that are diagonal in real space (i.e., sums, products, divisions, composition with transcendental functions, etc.). Therefore, sometimes it will be convenient to store a periodic function as $N+1$ Fourier coefficients, and sometimes as values on a grid of $2N-1$ points. An alternative to storing the values on a grid could be to compute the operations between periodic functions directly from the Fourier series as described in the next section.

In Sections 3.3.3.2,3.3.3.3, we discuss the operation count and stor-

age cost of implementations using just Fourier series discretizations and in Section 3.3.3.4 we discuss the same issues for discretization on Fourier coefficient/grid. The accuracy and numerical stability will be discussed empirically in Section 3.3.5.

3.3.3.1 Sobolev norms

We define

$$\|f\|_{H^r} = \|D^r f\|_{L^2}. \tag{3.25}$$

Note that (3.25) is a norm on a space of periodic functions with zero average, which is the only case we will consider.

This norm can also be computed by

$$\|f\|_{H^r} = \left(\sum_{k\geq 0}(2\pi k)^r |f_k|^2\right)^{\frac{1}{2}}. \tag{3.26}$$

Renormalization techniques (see section 3.5.3) will make clear that values of r greater than 3 will have to be taken into consideration when we perform computations. Different methods of computation were tested since the H^r norm (3.26) tends to be sensitive to round-off error in the higher frequency terms (see section 3.3.5). Note that (3.26) makes sense even if r is not an integer.

3.3.3.2 Algebraic operations by manipulating Fourier coefficients

Elementary algebraic function (sum, product and product by scalar) can be implemented using formulas for the coefficients of the result in terms

of the coefficients of each of the terms. Of course, addition and subtraction are trivial, multiplication can be computed using Cauchy formula.

$$\widehat{(uv)}_k = \sum_j \hat{u}_j \hat{v}_{k-j} \tag{3.27}$$

Note that the straightforward implementation of (3.27) requires $O(N^2)$ operations. From the practical point of view, evaluations of sums such as (3.27) are very well optimized for almost any computer in the `cdot` function of the BLAS library.

The book [120, p. 525–533] contains several groupings of (3.27) whose operation count is $O(N^\alpha)$ for some $\alpha < 2$. We will not consider these operations in these paper.

There are several possible implementations of division by manipulation of Fourier series. The most straightforward one is to use a Newton method to find v solving $v \cdot u = 1$. Given an approximate solution, a more approximate one will be $\tilde{v} = v + (u \cdot v - 1) \cdot v \cdot v$. As we will see, there are many ways to obtain an approximate solution, so, in practice, one iteration of the Newton method is enough.

3.3.3.3 Computation of the elementary transcendental functions by manipulation of Fourier coefficients

One first idea to compute transcendental functions of a Fourier series is to use a Taylor expansion and the duplication formulas. In [120], one can find an alternative that is more efficient and is also useful in the computation

of Lindstedt series. Let us briefly discuss the method for the exponential and refer to [120] for more details.

We recall that if $P(z)$ is a polynomial, $E(z) \equiv \exp(P(z))$ satisfies $E'(z) = E(z)P'(z)$ so that equating the coefficients of z^n, $n \geq 0$ we obtain:

$$(n+1)E_{n+1} = \sum_{k=0}^{n}(k+1)P_{k+1}E_{n-k} \tag{3.28}$$

which, after initializing with $E_0 - \exp(P(0))$, allows us to compute the coefficients E_n.

Note that the computation of N coefficients requires only $O(N^2)$ operations. The exponential of a Fourier series can be obtained using that it is the sum of two polynomials in $z = \exp(2\pi ix)$ and $\bar{z} = \exp(-2\pi ix)$.

Recursion formulas in [120, p. 418-514] allow us to compute sin, cos, exp of Fourier series in $O(N^2)$ steps by just manipulating Fourier series.

3.3.3.4 Using Fast Fourier Transforms (FFT)

The fastest algorithm for performing algebraic operations or compositions of transcendental functions is the FFT method. We perform this operations by applying inverse FFT to our coefficients, computing the function on each grid point in real space, and the applying inverse FFT. This procedure has a cost of $O(N \log N)$. Therefore, a straightforward implementation of Algorithm 2 takes $O(N \log N)$ operations.

Another advantage of the FFT method is that the interactions between particles do not have to be given in terms of transcendental functions. As

long as we have a method for computing the interactions in a grid of equally spaced points in the torus we can perform FFT. One algorithm that also deserves further exploration is the algorithm USFFT that can perform Fourier transforms in non-equally spaced grids [10, 74]. This seems quite promising for the cases in which the function is rather differentiable.

3.3.4 The efficiency of Algorithm 2

Besides the operations discussed in the above section, we note that shifts, computations of derivatives and solutions of difference equations are $O(N)$ in Fourier space.

We conclude that it is possible to implement Algorithm 2 using only discretizations in N Fourier terms and manipulating Fourier coefficients (or using FFT to compute the derivatives).

We also note that keeping Fourier series discretizations, the storage required for Algorithm 2 is only $O(N)$.

If we use systematically the FFT to evaluate the operators with the least operations, we obtain that a Quasi-Newton step, takes $O(N \log N)$ operations. If we use Cauchy formulas or recursions for the computation of functions, we use $O(N^2)$ operations.

3.3.5 Empirical study of the accuracy of algorithms for manipulating fourier series

In the previous section, we have discussed the issues of storage and operation count. This is, of course, a good indication of the speed and practicality of the algorithms. Of course, nowadays, the standard operation count of theoretical computer science is not a complete indicator of the speed. Memory access is nowadays the slowest part of many computers. Hence, reducing storage so that the problem fits well into the cache is important also for speed.

From the point of view of this paper, accuracy is quite important. Unfortunately, we are very far from having a theoretical understanding of the effect of round-off and truncation. Hence, in this section, we will present an empirical study of the accuracy of different algorithms.

As an example, we will compare empirically product, evaluation of transcendental functions for some functions. We use the Bernoulli polynomials:

$$B_n(\theta) = \frac{1}{(2\pi i)^n} \sum_{k \in \mathbb{Z} - \{0\}} \frac{1}{n^k} e^{2\pi i k \theta} \tag{3.29}$$

The functions B_n admit closed form expressions and their product satisfy identities (see [5]) we can test. Note that, by changing n, we can use B_n as models of functions with different regularities.

A remark about Newton methods One very crucial point for our discussion is that the accuracy of the final result of a Newton method depends only on the accuracy of the evaluation of the functional equation. Provided that

the iterative procedure is sensible, it will converge to an approximate solution which will solve the functional equation up to an accuracy comparable to the accuracy of the evaluation. We note that the rigorous results in [60] show that (provided that the approximate solutions satisfy some non-degeneracy assumptions), there are true solutions.

Hence, when using a Newton method, what seems to be the best is to optimize the accuracy of the evaluation of the functional equation and optimize the speed of the iterative step.

Testing the multiplication of functions Our first test is to check the identity

$$B_n(\theta)B_m(\theta) = \sum_{k=0}^{n+m} \Gamma_{n,m}^k B_k(\theta). \tag{3.30}$$

in different Sobolev norms.

Some representative results for 1500 coefficients are in the following table (More are available in a supplement to this paper).

The conclusion that we obtain is that the direct Cauchy formula (3.27) gives results which are moderately more precise (a factor 2 or 3) than the FFT when the functions are moderately smooth.

An easy improvement of the FFT multiplication is

- Shift the polynomials by $1/2N$ which can be done multiplying the Fourier coefficients by an appropriate phase.

r	n=1	n=2	n=3	n=4	n=5	n=6
0	2.51e-06	5.32e-10	1.70e-13	1.44e-16	5.51e-17	5.19e-17
1	2.36e-02	5.01e-06	1.60e-06	1.36e-12	5.16e-13	4.84e-13
2	2.22e+02		3.59e-06	1.28e-08	4.86e-09	4.55e-09

Table 3.1: H^r semi-norms for the error of the product of Bernoulli polynomials $B_n(\theta)B_4(\theta)$ using the Cauchy formula with 1500 coefficients.

r	n=1	n=2	n=3	n=4	n=5	n=6
0	1.91e-06	1.12e-12	1.29e-13	6.02e-18	6.80e-18	1.37e-17
1	1.80e-02	1.11e-09	1.22e-09	2.70e-14	3.49e-14	6.38e-14
2	1.70e+02	1.05e-05	1.14e-05	2.04e-10	2.71e-10	5.15e-10

Table 3.2: H^r semi-norms for the error of the product of Bernoulli polynomials $B_n(\theta)B_4(\theta)$ using the FFTW.

- Evaluate both in real space, so that we obtain the polynomials evaluated at $2N$ points in real space.
- Multiply them to obtain the product in $2N$ points.
- Compute the FFT to obtain $2N$ coefficients of the product
- Truncate up to order N.

Note that, except for the last step, the procedure – up to round off error – is exact for trigonometric polynomials of degree N. Except for round off error, this should give the same result as Cauchy product.

Composition with elementary functions The FFT method of computing $\sin(f), \cos(f), \exp(f)$ is just to evaluate the function on a grid, evaluate the

f	r	n=1	n=2	n=3	n=4	n=5	n=6
FFT							
sin	0	6.48e-03	8.74e-07	1.15e-10	4.77e-14	4.12e-17	4.97e-17
	1	3.65e+01	5.48e-03	9.17e-07	3.76e-10	1.87e-13	1.98e-13
	2	2.71e+05	4.25e+01	7.67e-03	3.17e-06	1.56e-09	1.55e-09
cos	0	1.93e-03	1.47e-07	4.84e-13	1.59e-15	2.25e-17	2.31e-17
	1	1.52e+01	9.21e-04	2.34e-09	1.25e-11	1.21e-13	1.24e-13
	2	1.30e+05	7.14e+00	2.20e-05	1.06e-07	8.91e-10	9.13e-10
exp	0	5.78e-03	1.05e-06	1.15e-10	4.61e-14	5.70e-17	6.41e-17
	1	3.01e+01	6.56e-03	9.17e-07	3.64e-10	2.95e-13	2.90e-13
	2	2.14e+01	5.09e+01	8.67e-03	3.06e-06	2.30e-09	2.19e-09
FSM							
sin	0	6.62e-03	8.75e-07	1.17e-10	4.80e-14	4.19e-17	4.87e-17
	1	4.32e+01	5.05e-03	9.62e-07	3.20e-10	1.96e-13	1.38e-13
	2	3.58e+05	3.69e+01	8.67e-03	2.39e-06	1.70e-09	9.34e-10
cos	0	1.19e-03	1.47e-07	2.96e-13	1.61e-15	2.32e-17	2.67e-16
	1	7.73e+00	8.52e-04	2.78e-09	1.06e-11	1.24e-13	1.22e-13
	2	5.93e+04	6.21e+00	2.61e-05	7.94e-08	9.06e-10	8.92e-10
exp	0	6.03e-03	1.05e-06	1.17e-10	4.64e-14	1.10e-16	6.47e-17
	1	3.92e+01	6.06e-03	9.62e-07	3.09e-10	3.71e-13	2.42e-13
	2	3.26e+05	4.42e+01	8.67e-03	2.31e-06	2.87e-09	1.72e-09

Table 3.3: H^r norm of the difference between the approximated composition $\widetilde{f(B_n(\theta))}$ and the exact formula $f(B_n(\theta))$ for $f = \sin, \cos, \& \exp$.

function and then, compute the Fourier transform of the resulting grid of points.

The alternative we compare with is the use of recursive formulas involving Fourier coefficients to compute the exponential and trigonometric functions discussed in [120, p. 525-533].

Here, we note that the results are extremely similar by the two methods.

3.4 Numerical results on the computation of quasi-periodic equilibria on several models

In this section we present the results on the computations of several models. We will describe some implementations for some cases and then, explore the limits of validity of the algorithms. The methods allow us to arrive very close to the place where the objects are breaking down and we can obtain several scaling relations near the breakdown.

3.4.1 The XY model

In the XY model x_i are angles describing the orientation of a spin $s_i = (\cos(2\pi x_i), \sin(2\pi x_i))$. The interaction that we consider in this model are interactions with an external field ($B = (\frac{\lambda}{2\pi}, 0)$) and exchange interactions between nearest neighbors. Since the meaning of the interactions are exchange interactions, it makes sense to consider terms which are not just nearest neighbor or, indeed that they are not just two body interactions. See, for example [26, p. 600].

The Euler-Lagrange equations for u are:

$$\begin{aligned} E[u](\theta) &= \sin(2\pi(\omega + u(\theta+\omega) - u(\theta)) \\ &\quad - \sin(2\pi(\omega + u(\theta) - u(\theta-\omega))) \\ &\quad - \tfrac{\lambda}{2\pi}\sin(2\pi(\theta + u(\theta))) = 0 \end{aligned} \tag{3.31}$$

The nearest neighbor interaction operator $\mathcal{C}_{0,1,1}$ appearing in Algorithm 2 is a multiplication operator given by

$$\mathcal{C}_{0,1,1}\eta(\theta) = -\cos(2\pi(\omega + u(\theta) - u(\theta-\omega)))h'(\theta-\omega)h'(\theta)\eta(\theta). \tag{3.32}$$

We notice that we can invert $\mathcal{C}_{0,1,1}$ as long as the argument of the cos is away from $\frac{\pi}{2}$ or $\frac{3\pi}{2}$ and h' is away from zero.

We follow a continuation method starting at the integrable case (i.e. $u = 0$ and for $\lambda_0 = 0$), and then incrementing λ step by step to a predetermined value.

We show some of the $u(\theta) = h(\theta) - \theta$ obtained by the continuation method in figure 3.1.

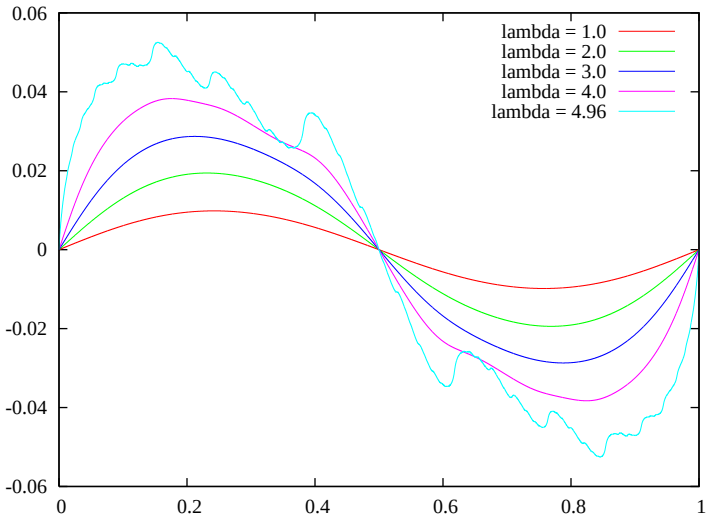

Figure 3.1: $u(\theta)$ for some values of λ.

In figure 3.2, we present the Fourier coefficients computed close to the breakdown ($\varepsilon = 4.97$). For this computation we used $N = 2^{12}$ coefficients. The computation of each one step of the continuation method takes 0.0996 seconds in average in a modest desktop computer with an Intel 2 Duo processor at $2.40GHz$.

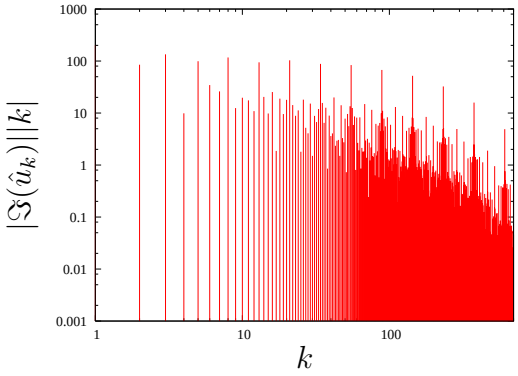

Figure 3.2: Imaginary part of $\hat{u}_k$ times $|k|$ in logarithmic scale versus the subindex k for $\lambda = 4.97$ in model (3.31).

We notice that the amplitude of the function u seems to increase as λ increases. Even at $\lambda = 4.76$, the amplitude of u is still small enough so that the operator $\mathcal{C}_{0,1,1}$ is still invertible.

It is not hard to show that the solutions of the invariance equations for the Heisenberg model are odd. Therefore, the Fourier coefficients will be purely imaginary. This is not built in in the algorithms we use, so that the size of the real part of the Fourier coefficients gives an indication of the effect of the round off and truncation error.

We note in particular that the plot of $\log |\hat{u}_k| k$ as a function of $\log k$ is roughly periodic for several decades. This is the standard signature of scalings that has been found in many critical problems in dynamical systems. For example in [200, 55]. Some more details on scaling behaviors at the breakdown of some of these models will be reported later.

3.4.2 The Frenkel-Kontorova model with extended interactions

In this model we consider the interactions of each particle with the rest of the particles and with the periodic substrate $V(x)$. The energy of these models is given by the formal sum

$$\mathcal{S}(\{x_n\}) = \sum_i \frac{1}{2}(x_i - x_{i+1} - a)^2 + \sum_{k\geq 2} \frac{A_k}{2} \sum_i (x_i - x_{i+k} - b_k)^2 + \sum_i V(x_i) \quad (3.33)$$

The decay of the A_k's depends on the physical model considered. The equilibrium equation is

$$2x_i - x_{i+1} - x_{i-1} + \sum_{k\geq 2} A_k(2x_i - x_{i+k} - x_{i-k}) + V'(x_i) = 0.$$

3.4.2.1 The Frenkel-Kontorova model with first and second nearest neighbor interactions

We consider first and second nearest neighbor interactions. We then the equilibrium equation becomes

$$2x_i - x_{i+1} - x_{i-1} + A(2x_i - x_{i+2} - x_{i-2}) + V'(x_i) = 0 \quad (3.34)$$

where the potential is given by the expression

$$V(\theta) = -\frac{\varepsilon}{4\pi^2}\cos(2\pi\theta) \quad (3.35)$$

Variational principle In the case when the first and second nearest neighbors have positive coefficients finding an invariant torus amounts to minimizing the action given by

$$\mathcal{P}[h] = \int_0^1 \frac{1}{2}(h(\theta) - h(\theta+\omega))^2 + \frac{A}{2}(h(\theta) - h(\theta+2\omega))^2 + V(h(\theta))d\theta \quad (3.36)$$

Then using the fact that a periodic function is translation invariant under integration we can rewrite the action principle in terms of $u(\theta)$ as follows

$$\begin{aligned}\mathcal{P}[u] = \int_0^1 \frac{1}{2}(u(\theta) - u(\theta+\omega))^2 + \frac{A}{2}(u(\theta) - u(\theta+2\omega))^2 d\theta \\ + \int_0^1 V(\theta + u(\theta))d\theta\end{aligned} \quad (3.37)$$

We are looking for a periodic function u that minimizes (3.37). Using Parseval's identity we can write the minimization problem in the following form

$$\begin{aligned}\min_{u\in\mathcal{A}_\rho} \Bigg[\sum_{k\in\mathbb{Z}} \left[(1-\cos(2\pi k\omega)) + A(1-\cos(2\pi k 2\omega))\right] |\hat{u}_k|^2 \\ + \int_0^1 V(\theta + u(\theta))d\theta\Bigg].\end{aligned} \quad (3.38)$$

Problem (3.38) can be solved numerically by truncating the Fourier coefficients and minimizing the resulting functional. We implemented this method for ω equal to the golden mean. In figure 3.3, we plot the minimizers for $\varepsilon = 0.97$ since this value is close to the breakdown of analyticity computed by Greene [95]. We notice that as we move A away from zero the solutions

appear to be more regular for this particular value of ε. This behavior can be understood by observing the decay of the Fourier Series of the minimizers. In the section 3.5, we give a description of this phenomenon.

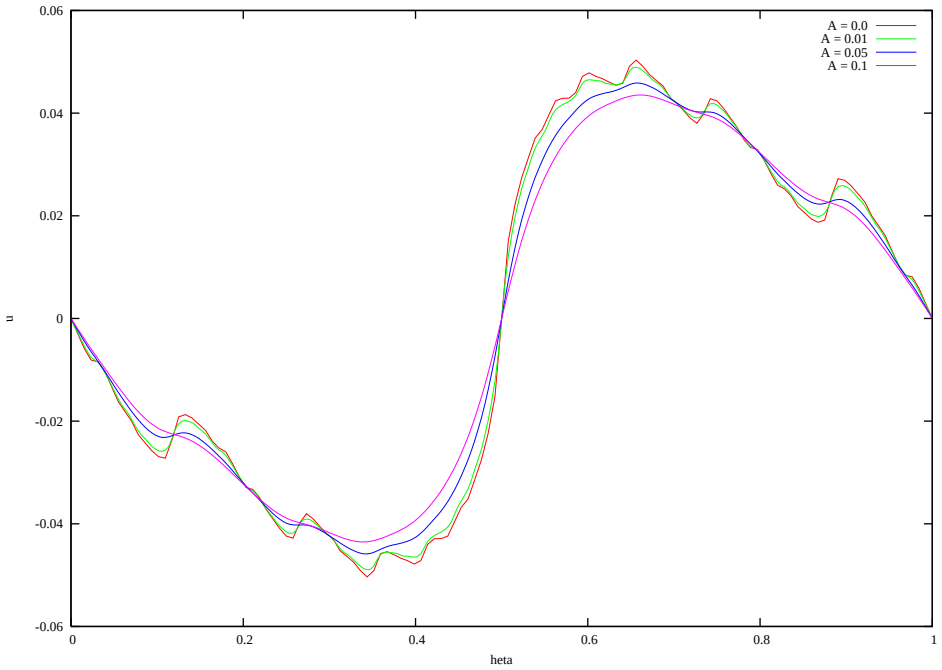

Figure 3.3: Minimizer $u(\theta)$ for $\varepsilon = 0.97$ and different values of A.

The quasi-Newton method For the case of the extended F-K model in equation (5.43) the operators $\mathcal{C}$ and $\mathcal{G}$ simplify to

$$\mathcal{C}\eta(\theta) = -h'(\theta - \omega)h'(\theta)\eta(\theta)$$

and

$$\mathcal{G}\eta(\theta) = -A\left(\Delta_1^{-1}\Delta_2\left[h'(\theta-2\omega)h'(\theta)\Delta_{-2}\Delta_{-1}^{-1}\eta(\theta)\right]\right). \tag{3.39}$$

We note also that as pointed out in [60], the operators $\Delta_{-2}\Delta_{-1}^{-1}$ and $\Delta_1^{-1}\Delta_2$ are easy to compute since

$$\Delta_1^{-1}\Delta_2\gamma(\theta) = \gamma(\theta+\omega) + \gamma(\theta)$$

and

$$\Delta_{-2}\Delta_{-1}^{-1}\xi(\theta) = \xi(\theta-\omega) + \xi(\theta).$$

These computations show that the operators $\mathcal{C}$ and $\mathcal{G}$ are readily computable numerically in this case. The inverse is then obtained computing a few terms of the Neumann series of $(\mathcal{C}+\mathcal{G})^{-1}$ and using the resulting function as a first guess for a Conjugate Gradient iterative method. We have used the CGNE algorithm (see [195, p. 238-240]). This algorithm also allows us to minimize an H^r semi-norm with predetermined r as we iterate. The semi-norms we choose to minimize will be justified when we discuss the renormalization of the system in section 3.5.3.

3.4.2.2 The Frenkel-Kontorova model with long-range interactions

We consider the equilibrum equations for hull functions of the models. Hence, we consider

$$E[u] \equiv \sum_{k=1} A_k[u(\theta + k\omega) + u(\theta - k\omega) - 2u(\theta)] + \lambda V'(\theta + u(\theta)) = 0 \quad (3.40)$$

We notice that $E'[u]$, the derivative of the operator is just given by

$$E'[u]\eta(\theta) = \sum_{k=1} A_k[\eta(\theta + k\omega) + \eta(\theta - k\omega) - 2\eta(\theta)] + V''(\theta + u(\theta))\eta(\theta) \quad (3.41)$$

Hence, the derivative is the sum of a difference operator and a multiplication operator by the function $W(\theta) = V''(\theta + u(\theta))$. The matrix of the difference operator, expressed in Fourier series is diagonal

$$M^d_{ii} = \sum_{k=1} 2A_k(\cos(\omega ik) - 1) \quad (3.42)$$

The matrix of the multiplication by a function U can be read off the Cauchy formula, (3.27),

$$M^m_{i,j} = \widehat{U}_{i-j} \quad (3.43)$$

Notice that M^d_{ii}, the coefficients of the difference operator are independent of the function u so that they can be precomputed once and for all for the algorithm. Indeed, in the case that $A_k = k^\alpha$, whith α integer, these coefficients can be computed explicitly (in the case α even, they agree with the Bernoulli polynomials introduced (3.29)). For example, in the case $\alpha = 2$, which is the

one that we use to illustrate the results the small divisors in the diagonal part, are given by

$$\sum_{k=1}^{\infty} k^{-2}(\cos(2\pi k\theta) - 1) = \frac{\pi^2}{2}\left(\frac{1}{4} - (\theta - 0.5)^2\right) \tag{3.44}$$

The coefficients of the multiplication matrix are computed when we just compute the function $V''(\theta+u(\theta))$ following the approaches in Sections 3.3.3.2,3.3.3.3,3.3.3.4.

Remark 3.4.1. It is amusing to note that near $\theta = 0$, the function (3.44) is asymptotically linear. On the other hand, for the nearest neighbor interation the diagonal terms are $\cos(2\pi\theta) - 1$, which are quadratic. Hence, the small divisors are less severe for the problems with extended interactions than for the standard map.

Remark 3.4.2. The well known small divisor problems cause that the matrices have somewhat large condition numbers ($\approx 10^3$ in the examples. Hence, if one solves the equation with Gaussian elimination, it is extremely important to use pivoting. An alternative that we have found useful is to use the singular value decomposition [93] which is much more numerically stable. The penalty in speed is not very severe (only a factor 2 or 3).

Remark 3.4.3. Since the most expensive step of the algorithm is to compute the inverse of the matrix, we note that it is possible to take several steps without the same inverse. The convergence will not be quadratic, only geometric, but since the steps are much faster, this can be faster.

Another alternative, which also leads to quadratic convergence but re-

quires less updates is the algorithm of [96]

$$\begin{aligned} u_{n+1} &= u_n - \mathcal{J}_n E(u_n), \\ \mathcal{J}_{n+1} &= \mathcal{J}_n - \mathcal{J}_n(\mathrm{Id} - E'(u_{n+1}))\mathcal{J}_n, \end{aligned} \tag{3.45}$$

where $\mathcal{J}_n$ are supposed to be approximate inverses.

Figure 3.4 illustrates several hull functions computed with this method.

In figure 3.5, we present the Fourier coefficients computed close to the breakdown ($\lambda = 2.3375$). For this computation we used $N = 2^{12}$ coefficients.

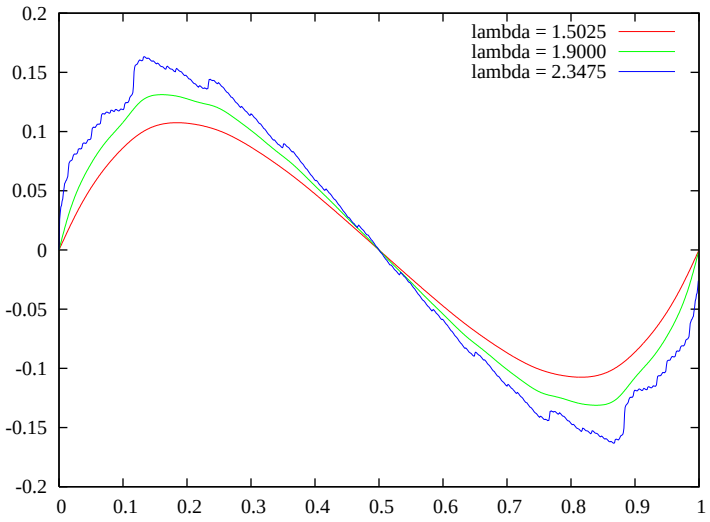

Figure 3.4: $u(\theta)$ for some values of λ.

Even if this figure may look similar to figures 3.2,3.7, we call attention to the fact that in Figure 3.5, the horizontal scale is not logarithmic as in figures 3.2 and 3.7. In the standard map and in the short range models, the scaling keeps some of the features of the small divisors (the big spikes happen at the places where the small divisors are stronger). On the other hand, for

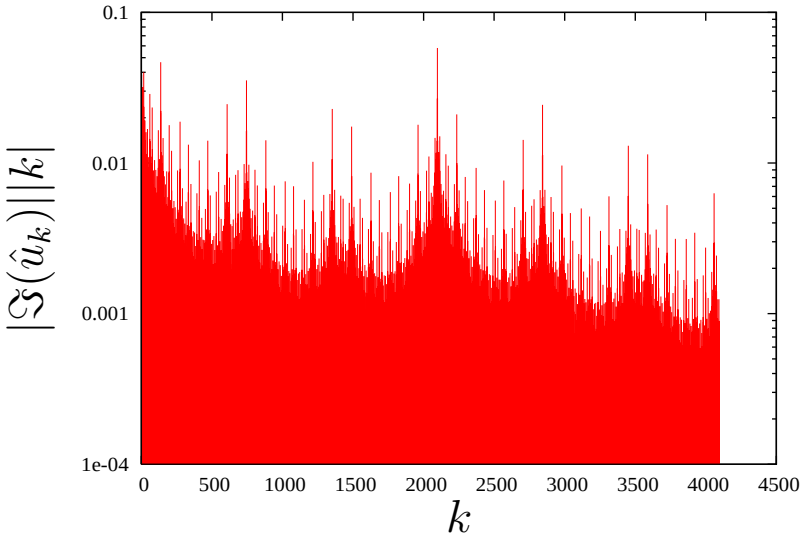

Figure 3.5: Imaginary part of $\hat{u}_k$ times $|k|$ in logarithmic scale versus the subindex k for $\lambda = 2.3375$ in model (3.40).

the long range models, the spikes appear at places that are not determined by the small denominators.

3.5 Studies of the breakdown of analyticity

The methods developed in the earlier section can be used to explore the parameter values for which the solutions of the equilibrium equations cease to be analytic.

In this section, we will try to get as close to possible to the breakdown and explore quantitative features of this phenomena.

One important observation is that the theoretical results of [60, **?**] give us a condition for the analyticity breakdown. Note that the methods described

above in the paper will allow us to produce systematicaly a solution of the truncated equations. The rigorous results of [60] show that if the approximate solution is well behaved, then, there are true solutions in a neighborhood.

It then, follows that, if we get close to the breakdown the smooth norms have to blow up.

Then, the algorithm to identify the boundary, is:

Algorithm 3.5.1. Continue the solutions with respect to parameters, monitoring carefully the truncation error etc.

The empirical boundary of analyticity is identified with the places where some high Sobolev norm becomes rather large.

Notice that, even for twist mappings, this method of computing the analyticity breakdown is different from the method in [95]. Of course, the method above applies also to extended systems.

In Section 3.5.1, we will discover some implementation issues.

In Section 3.5.3 we present a renormalization argument from the theory of twist maps that leads to a quantitative prediction of the way that the Sobolev norms of the solutions blow up as we approach the boundary of analyticity breakdown. We conjecture that, the same scaling behavior happens for systems which are not nearest neighbors.

In Section 3.5.4 we present evidence that the numerical conjectures about scaling are true for several models.

If indeed the conjectures were true, they would allow a computation of the boundary of analyticity breakdown, which is more accurate than Algorithm 3.5.1

Algorithm 3.5.2. Continue the solutions with respect to parameters, monitoring carefully the truncation error etc.

Fit the computed norms to the conjectured scaling relation and obtain the parameters of the transition from the fit.

Of course, Algorithm 3.5.2 can yield more accuracy in the computed transition point, but of course, it depends heavily on the scaling assumption.

We think that the regularities found indicate that there exists a renormalization group for extended models that generalizes the renormalization groups for twist mappings [149, 137, 121].

We think that these regularities deserve a more detailed numerical exploration. Note that, since Algorithm 3.5.1 is independent of scaling, we can explore a wide class of models.

3.5.1 Some remarks about the numerical implementation

Truncation of the solutions to a finite dimensions generates *spurious* solutions. These are solutions of the truncated problem that are not truncations of true solutions of the full problem. It is empirically found that, as the parameters become closer to breakdown, these spurious solutions become more abundant and become harder to distinguish from the true solutions. A

Newton method may lock onto an spurious solution and be lead astray.

The way we use to avoid this spurious solutions is by using adaptive steps in the Newton method. We adjust the step size after performing a test on a new step. The test is summarized as follows

- Shift the new step, $\tilde{u}$, by $1/2N$.
- Evaluate the step and its shift to obtain the step $\tilde{\tilde{u}}$ evaluated at $2N$ points in real space.
- Compute an FFT to obtain $2N$ coefficients.
- Recompute a solution with $2N$ coefficients starting from $\tilde{\tilde{u}}$.
- If it converges we can keep on moving forward with the original step.
- If the solution with twice the coefficients does not converge then we step back and reduce the step size.

3.5.2 Some Preliminary explorations of the breakdown

In figure 3.6, we present some of the values of the H^r semi-norms for the standard map we obtained using the algorithm using adaptive steps described above.

In figure 3.7, we present the Fourier coefficients computed close to the breakdown ($\varepsilon = 0.97$). For this computation we used $N = 2^{12}$ coefficients. The computation of each one step of the continuation method takes 0.0868

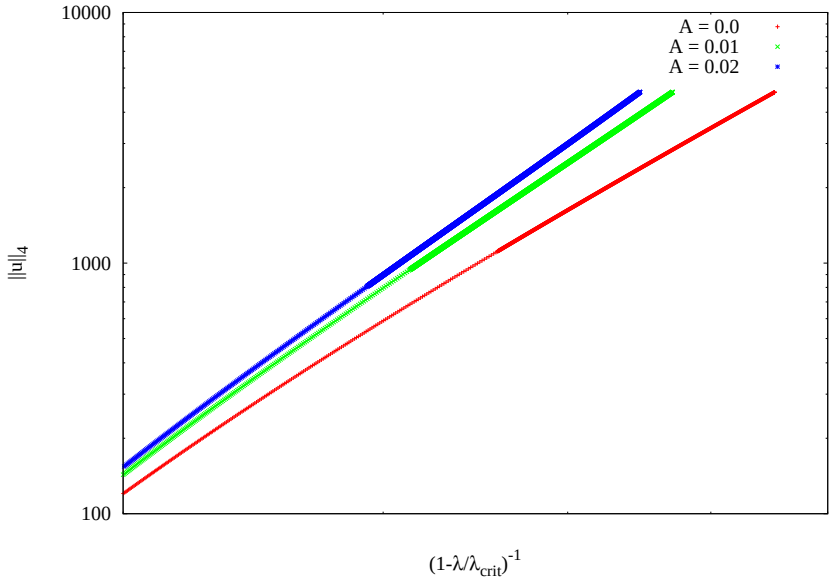

Figure 3.6: $\|u\|_4$ graphed against $(1-\lambda/\lambda_{crit})^{-1}$ in logarithmic scale for fixed A.

seconds in average in a modest desktop computer with an Intel Core 2 Duo processor at $2.40GHz$.

3.5.3 Some predictions from Renormalization theory

As mentioned in Remark 3.2.1, the Frenkel-Kontorova model is equivalent to the standard map. The breakdown of analyticity of the standard map has been extensively studied. In particular, it has been studied using Renormalization group [149, 137, 122].

We want to adapt this renormalization group in such a way that it can be adapted to our problems. We follow [51]. Consider a family of maps T_λ indexed by a parameter λ, with λ_{crit} being the critical parameter at which an-

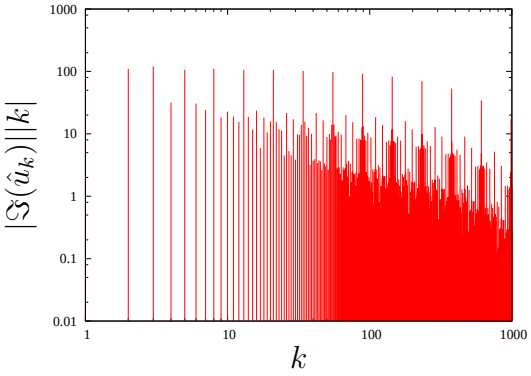

Figure 3.7: Imaginary part of $\hat{u}_k$ times $|k|$ in logarithmic scale versus the subindex k for $\lambda = 0.97$ in the standard map.

alyticity breakdown occurs. The main idea of renormalization is that taking an appropriate iterate of the map and rescaling $\lambda - \lambda_{\text{crit}}$, the problem remains unchanged. The appropriate iterate is given by the convergence of the continued fraction expansion of the rotation. To restore the rotation, we just need to scale the angles.

Hence, we conclude that the following scaling relation holds.

$$u_{\lambda_{\text{crit}}+\delta^{-1}(\lambda-\lambda_{\text{crit}})}(\gamma\theta) \approx u_\lambda(\theta) \tag{3.46}$$

where δ is the expanding eigenvalue of the fixed point of renormalization controlling the transition of analyticity breakdown and γ is the exponent of convergence of the continued fraction of ω.

In the particular case of ω the golden mean, there is a well known fixed point with $\delta \approx 1.6280$ See [149, 137, 3, 122]. The exponential convergence of approximants to the golden mean is well known to be $(\sqrt{(}5)+1)/2 \approx 1.618034$.

The scaling relation leads to several predictions.

P1) The width of the analyticity strip for u_λ, denoted by $\sigma(\lambda)$ has the asymptotic expression:

$$\sigma(\lambda) \approx A|\lambda_{\text{crit}} - \lambda|^{\log\gamma/\log\delta} \tag{3.47}$$

P2) If the Sobolev norm of u_λ blows up, it has the asymptotic expression

$$||D^r u_\lambda||_{L^2} \approx A_r|\lambda_{\text{crit}} - \lambda|^{(\log\delta/\log\gamma)(r-1/2)} \tag{3.48}$$

To deduce (3.47) from (3.46) just observe that reducing the critical parameter by a factor δ, decreases the analyticity radius by a factor γ.

To deduce (3.48) from (3.46), note that $\|D^r u_\lambda(\gamma\cdot)\|_{L^2} = \gamma^{r-\frac{1}{2}}\|D^r u_\varepsilon(\cdot)\|_{L^2}$ and that this is the change induced by scaling the parameter by a factor δ.

Note that, for the golden mean, $\frac{\log(\gamma)}{\log(\delta)} \approx 0.98740$

Remark 3.5.3. The predictions of the scaling relations can be broken up into two parts. A first one is the existence of the scaling relations such as (3.47) or (3.48) and the second one is that the exponents have the values that we are indicating.

If we consider the problem from the point of view of renormalization group and scaling relations, [9, 112], it is natural to conjecture that the same scaling relations happen for models with short range (or decreasing fast enough) interactions. As we have remarked before, the breakdown of analyticity in models with long range interactions is very different.

3.5.4 Numerical verification of the renormalization group predictions

In this section, we present numerical evidence for prediction P2), since it is much easier for our methods. We note that prediction P1) was verified for the Standard map in [23] (as a matter of fact, the work of [23], preceded [51] and motivated the scaling argument). In this paper, we will not be studying prediction P1) for the extended Frenkel-Kontorova model.

In Figure 3.8 we represent the critical value of analyticity breakdown determined fitting the blow up to several norms. As expected, the norm H^3 does not give very reliable results since the H^3 norm is marginal for the problem [101]. On the other hand, the norms that do blowup, indeed all give very compatible results.

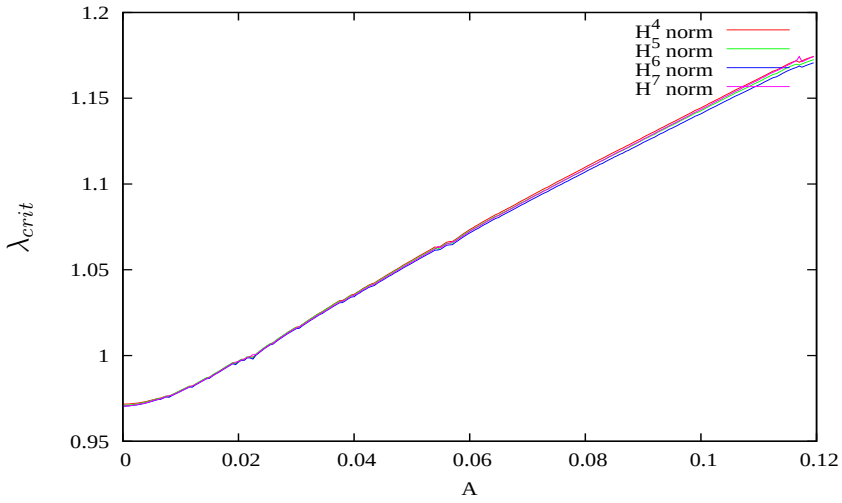

Figure 3.8: The critical value of model (3.38) as a function of the next-nearest coupling parameter

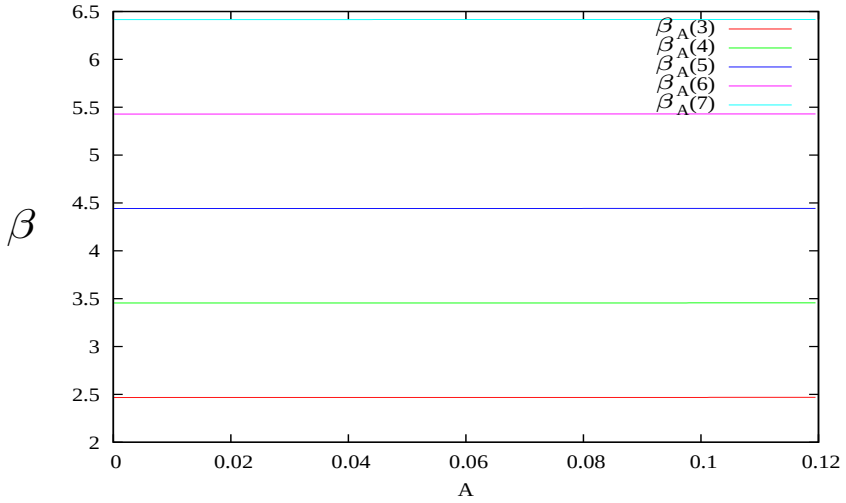

Figure 3.9: A vs. $\beta(r)$ for different values of r

In Figure 3.5.4, we present the values of the blow-up exponent obtained by fitting the relation. Note that they remain almost constant.

In Figure 3.5.4 we present the difference between some of the scaling exponents presented in Figure 3.5.4. Note that they agree very well (more than 3 figures) with the value predicted theoretically.

Acknowledgements

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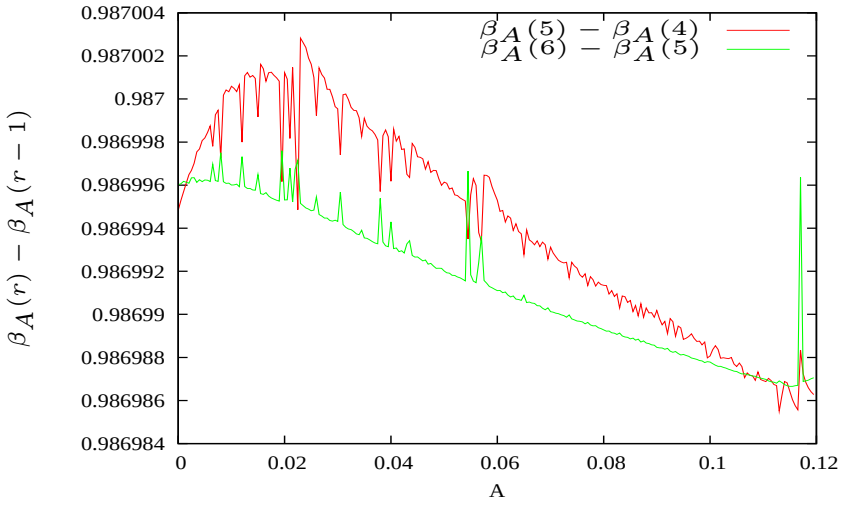


Figure 3.10: Differences between several exponents as a function of A

Chapter 4

Computation of the breakdown of analyticity in statistical mechanics models

4.1 Introduction

The phenomenon of *breakdown of analyticity*, appears in a multitude of physical contexts (See Section 4.2) (dynamical systems, dynamics of fracture, deposition over a substrate, magnetism, quasi-periodic Schrödinger equations etc.) and has a variety of physical implications. It has, therefore been widely studied by a variety of methods from numerical exploration to rigorous mathematical results. See [95, 14, 185, 186, 140, 44, 151] among others.

In general, we are seeking configurations $\{x_n\}_{-\infty}^{\infty}$ which are equilibria of a variational problem (see section 4.2) and which are determined by a hull function. That $x_n = h(n\omega)$ where $h(t+1) = h(t) + 1$. When the system depends on parameters, it is often observed that the function h is smooth for some values of the parameters and it is discontinuous for others. For the values when h is continuous, the system can easily move among equilibria, but when h is discontinuous, the system is pinned down [14].

The goals of this letter is to present an efficient algorithm to compute this transition and to present the results obtained by applying it to Frenkel-

Kontorova models or to Heisenberg XY models of magnetism. These numerical calculations also indicate that in the neighborhood of these transitions, there are scaling relations similar to those of phase transition.

4.2 Models considered

In this letter, we will focus on three models, the Frenkel-Kontorova (FK) models, FK models with long range interactions (EFK) and Heisenberg's XY model of magnetism.

These models describe an array of atoms, indexed by an integer n. The state of the n atom is characterized by a number x_n. The configuration is, therefore, given by a sequence $\{x_n\}$. In the case of the Heisenberg XY model, the physical interpretation of x_n is the orientation of the spin of the n atom. In the original formulation of the FK model [83] x_n was the position of a planar dislocation in a crystal. In [14], the same model was used in the description of deposition over a substratum. Then, x_n is the position of the n deposited atom. Given the above interpretations of the models, it is natural to include interactions that extend beyond nearest neighbors [39, 22, 189, 26].

The Physics of the model is determined by assigning an energy to each

configuration. The energies we will consider are respectively:

$$E_{FK} = \sum_n \frac{1}{2}|x_n - x_{n-1}|^2 + V(x_n) \tag{4.1}$$

$$E_{XY} = \sum_n \cos(2\pi(x_n - x_{n-1})) + B\cos(2\pi x_n) \tag{4.2}$$

$$E_{EFK} = \sum_n \sum_L \frac{1}{2} A_l |x_n - x_{n-l}|^2 + V(x_n) \tag{4.3}$$

In the FK model, the first term models the interactions between nearest neighbors (assumed to be a harmonic oscillator), the second term models the interaction with the substratum given by $V(x_n)$ where $V(t+1) = V(t)$. V will depend on several parameters (coupling constants). We have chosen units of energy and length to normalize the period of V to 1 and the coefficient of the harmonic interaction to $\frac{1}{2}$.

In the XY model the energy is the sum the exchange energy among the next nearest neighbors (it has to be a multiple of the scalar product of the two orientations by rotational invariance) and the interaction with a external magnetic field. Again we choose units of energy to normalize the coefficients.

4.2.1 The equilibrium equations

These systems are in equilibrium when $\partial_{x_n} E = 0$ for all n. One particularly important case of equilibria are ground states, which have smaller energy than any state differing from them in a finite number of sites.

The equilibrium equations are, respectively:

$$2x_n - x_{n-1} - x_{n+1} + V'(x_n) = 0 \tag{4.4}$$

$$\sin(2\pi(x_n - x_{n-1})) + \sin(2\pi(x_{n+1} - x_n)) \tag{4.5}$$

$$B\sin(2\pi x_n) = 0$$

$$\sum_l A_l(2x_n - x_{n-l} - x_{n+l}) + V'(x_n) = 0 \tag{4.6}$$

Introducing the extra variable p_n, (4.4) can be considered as a dynamical system in two dimensions so that $p_{n+1} = p_n + V'(x_n), x_{n+1} = x_n + p_{n+1}$. Therefore, configurations which are critical for E_{FK} are orbits of celebrated standard map.

Note, however that the interpretation of (4.5),(4.6) as dynamical systems is rather difficult since there no general way to obtain x_n as function of $x_{n-1}, x_{n-2}, \ldots, x_{n-L}$.

4.2.2 Configurations given by hull functions

In many of the systems above, it is useful to study equilibrium configurations given by hull functions

$$x_n = h(n\omega) \qquad h(t+1) = h(t) + 1 \tag{4.7}$$

In FK, EFK models, ω is the inverse of the density. The equilibrium

equations can be written in terms of the hull functions as:

$$2h(\theta) - h(\theta - \omega) - h(\theta + \omega) + V'(h(\theta)) = 0 \tag{4.8}$$

$$\sin(2\pi(h(\theta) - h(\theta - \omega)) + \sin(2\pi(h(\theta + \omega) - h(\theta))) \tag{4.9}$$

$$-B\sin(2\pi h(\theta)) = 0$$

$$\sum_l A_l(2h(\theta) - h(\theta - l\omega) - h(\theta + l\omega)) + V'(h(\theta)) = 0 \tag{4.10}$$

It was shown in [14] that all ground states of FK models are given by hull functions. The argument was extended in [38] for EFK models.

The equations (4.8) were shown to have a variational structure [185, 186], but small modifications of the argument show that so do (4.9), (4.10). The paper [185, 186] showed that this variational principle is a very useful computational tool. The paper [153], developed a mathematically rigorous theory of minimizers of the variational principle of [185, 186] which was the beginning of the celebrated Aubry-Mather (AM) theory. See [67, 38], for a thorough treatment of (4.10).

The AM theory guarantees the solutions of equations (4.8), (4.10) for all choices of parameters and all ω. These solutions could be smooth or discontinuous. On the other hand, (4.9) does not satisfy the convexity conditions and there does not seem to be a theory of existence of solutions to (4.9).

4.2.3 The phenomenon of analyticity breakdown

Let h be the solution of (4.8),(4.9), (4.10). If h is continuous, there is a continuous family of critical points and the system can slide from one to other

rather easily. Hence arbitrarily small forces can cause large effects. On the other hand, if h is discontinuous, there are gaps among the states the system is pinned down. The above alternative (pinned down or sliding) depends on the parameters of the system.

The problem we want to address is to compute the regions of parameters where the solution of (4.8),(4.9), (4.10) are smooth or discontinuous.

4.3 Perturbative results

When ω is sufficiently irrational

$$|\omega - p/q| \geq \kappa |q|^{-\tau} \forall p \in \mathbb{Z}, q \in \mathbb{Z} - \{0\} \tag{4.11}$$

there is a perturbative theory for smooth solutions, often known as the KAM (Kolmogorov-Arnold-Moser) theory (see [132] for a review). Extensions to variational problems were obtained in [196, 131] and, for systems with long range interaction in [52, 34]. In contrast with AM theory, the KAM theory requires that the frequencies are sufficiently irrational and that certain quantitative assumptions hold. On the other hand, KAM requires less convexity assumptions.

The core of [52, 34] is an iterative method that, given an approximate solution of (4.8),(4.9),(4.10), produces a significantly more approximate solution (the number of correct figures, roughly doubles).

Given the Fourier coefficients of h obtained by solving either (4.8),(4.9) or (4.10) up to an error e, there is a explicit correction Δ such that

1. $h + \Delta$ reduces the error to $O(e^2)$.

2. Δ is computed from h in $O(N \log N)$ operations using only $O(N)$ storage.

Omitting some technical assumptions of a mathematical nature, the main result of [52, 34] is the following:

Theorem 4.3.1. Consider (4.8),(4.9), (4.10) with V analytic. Assume also that ω satisfies the Diophantine condition (4.11).

Assume that h satisfies the invariance equation up to an error e in place of 0 in the RHS. Assume that for some m large enough, $||e||_m \equiv (\sum_n (1+k^2)^m |\hat{e}_k|^2)^{1/2}$ is sufficiently small compared to $||h||_m$.

Then, the iterative step started in the approximate equation converges to an analytic solution of the invariance equations which is close to the original one.

4.4 Algorithm for the computation of the analyticity breakdown

Theorem 4.3.1 leads immediately to the following algorithm.

Algorithm 4.4.1.

Choose a path in the parameter space

starting in the integrable case.

Initialize the parameters at integrable, h_{ε_0}

Repeat

Increase the parameters along the path

Run the iterative step

If (Iterations do not converge)

Decrease the increment in parameters

Else (Iteration success)

Record the values of the parameters

and the Sobolev norm of sol.

Until Sobolev norm too large

Note that Theorem 4.3.1 shows that there will be an analytic solution in a neighborhood unless the Sobolev norm blows up. After a calculation, one can check that the choice of threshold for blow up does not affect much the final result. More accurate results can be obtained by fitting some formula for the blow up.

In is interesting to compare the above criteria with other methods. The best known method [95] is based on the computation of periodic orbits which approximate the periodic solution. On the other hand, when V contains several harmonics, tracking periodic orbits becomes hard close to breakdown since they appear in complicated orders [135]. The formulation of the criterion in [95] does not seem clear in cases such as (4.10) where one cannot make sense of the residue. Another algorithm based on periodic orbits and their stable manifolds appear in [182]. Other algorithms based on variational methods for twist mappings are [110, 207, 145], but this do not generalize to (4.9), (4.10).

4.5 Numerical results

We implemented the continuation method prescribed by Algorithm 5.2.1 using the methods introduced in [37]. In this section, we present some numerical results.

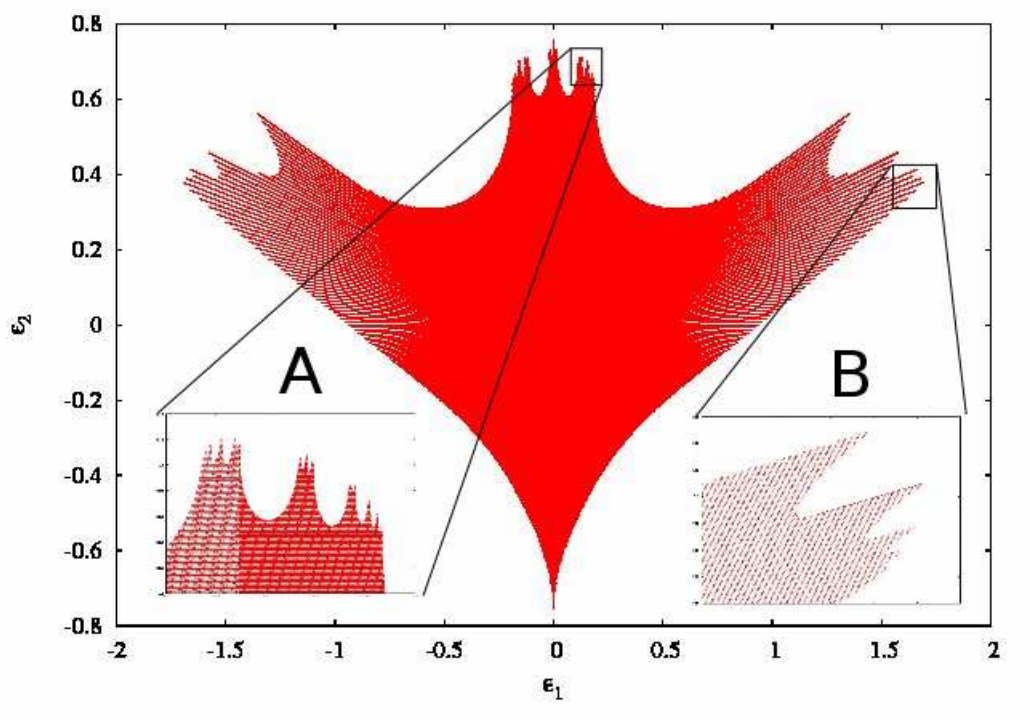


Figure 4.1: Domain of $\varepsilon_1, \varepsilon_2$, for which the model (4.1) with potential $V(x) = -\frac{\varepsilon_1}{(2\pi)^2}\cos(2\pi x) - \frac{\varepsilon_2}{(4\pi)^2}\cos(4\pi x)$ has an invariant circle of rotation golden mean.

In figure 4.1, we present the parameters $\varepsilon_1, \varepsilon_2$ neighborhood of existence of analytic hull functions, $h_{(\varepsilon_1,\varepsilon_2)}$ for $\omega = \frac{\sqrt{5}-1}{2}$, for the model (4.1) with potential $V(x) = -\frac{\varepsilon_1}{(2\pi)^2}\cos(2\pi x) - \frac{\varepsilon_2}{(4\pi)^2}\cos(4\pi x)$.

In the neighborhood of analyticity in figure 4.1 (a) we can find regions

with a smooth boundary and regions where the boundary has folds. We have found that as the parameter approaches a smooth boundary $\|h_\varepsilon - id\|_r \approx \alpha(\varepsilon - \varepsilon_{crit})^{\beta(r-1/2)}$, see figure 4.2 (a). However, as a parameter approaches a region that has folds the Sobolev norm has oscillations, see figure 4.2 (b). In figure 4.2 (a), we also present the Sobolev norm for the XY model (4.2).

In figure 4.3, we present the neighborhood of existence of invariant tori for the model (4.3) with $A_l = 1/l^k$ and potential $V(x) = -\frac{\varepsilon_1}{2\pi}\cos(2\pi x) - \frac{\varepsilon_2}{4\pi}\cos(4\pi x) - \frac{0.3}{6\pi}\cos(6\pi x)$ and $\omega = \frac{\sqrt{5}-1}{2}$.

4.6 Conclusions

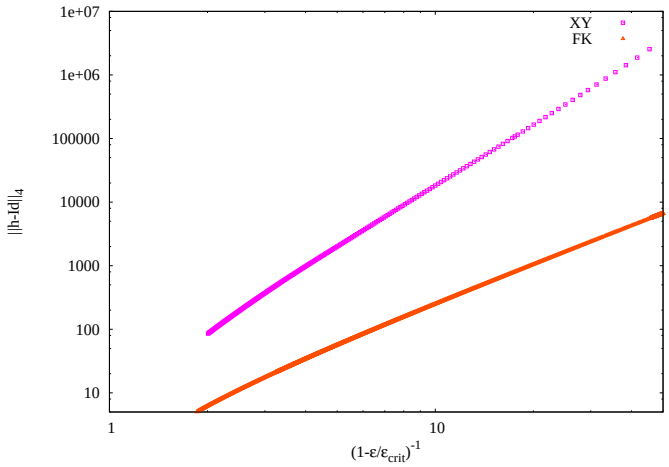
We have presented a method to detect the breakdown of analyticity of quasi-periodic solutions of statistical mechanics models by implementing an algorithm based on an efficient Newton Method.

Each step of the Newton Method requires $O(N\log(N))$ operations and $O(N)$ storage. The method converges by some theoretical analysis and is robust in practice.

We implemented the algorithm described above in FK, EFK, and XY models. We observed that for some parameter regimes the transition happens on a smooth boundary and there are scaling relations. These scaling relations are consistent with the Renormalization Group (RG) description of the transitions in the FK model. Our computations also indicate that there should exist a RG theory for the EFK and XY models.

In the parameter regimes where the boundary has folds our numerical experiments show a complicated behavior of the RG of the FK or EFK models.

a)



b)

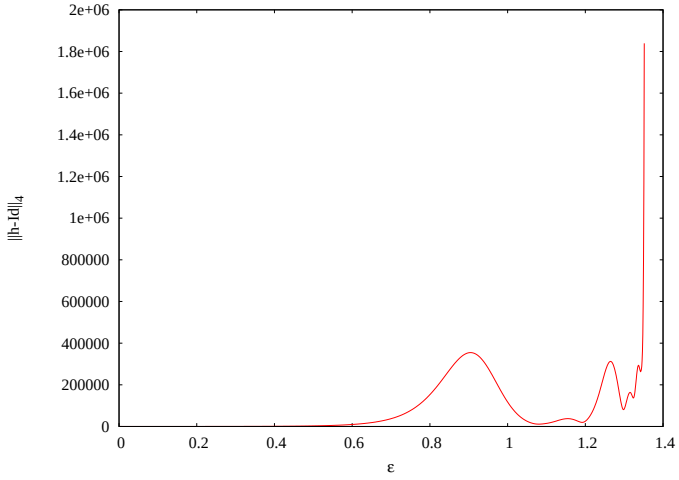


Figure 4.2: a) Double logarithmic scale plot of $\|h_\varepsilon - Id\|_4$ with respect to $(1-\varepsilon/\varepsilon_{crit})^{-1}$ for models (4.1) with $V(x) = -\frac{\varepsilon}{(2\pi)^2}\cos(2\pi x)$. and (4.2) with $B = -\frac{\varepsilon}{(2\pi)^2}$. b) $\|h_\varepsilon - Id\|_4$ with respect to ε for model (4.1) with $V(x) = -\frac{\varepsilon}{(2\pi)^2}\left(\cos(2\pi x) + \frac{\sqrt{2}-1}{4}\cos(4\pi x)\right)$.

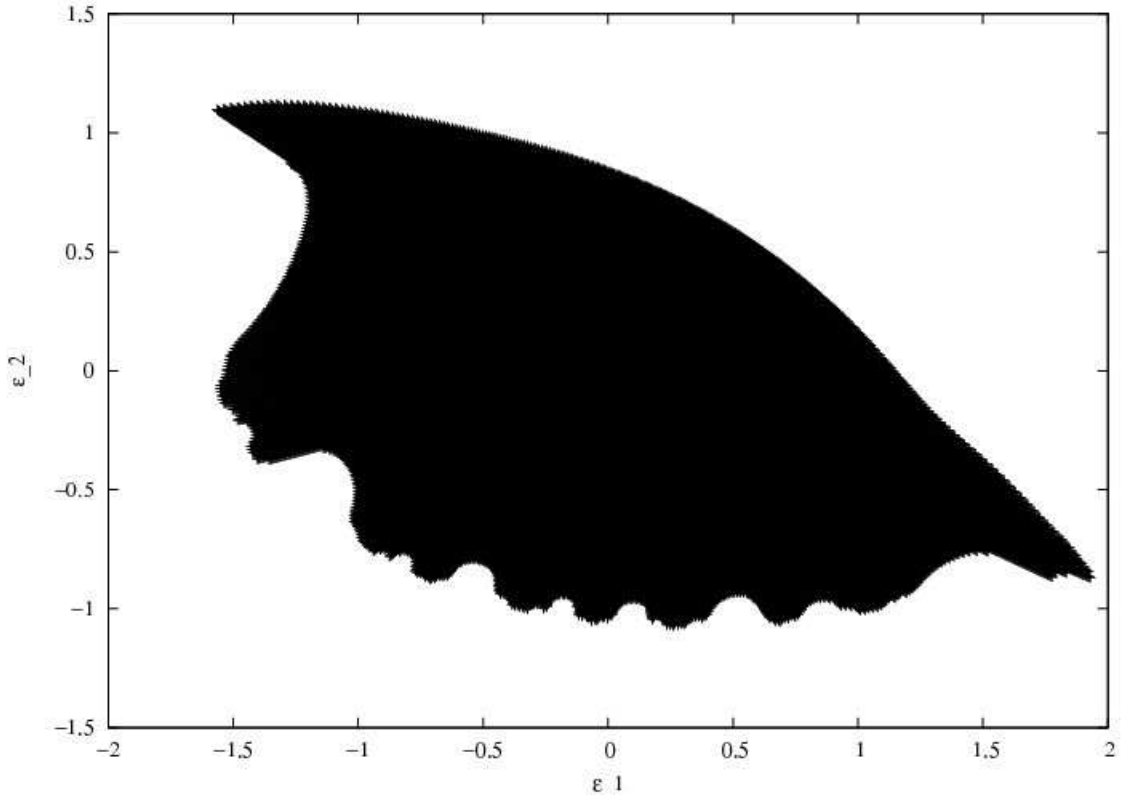


Figure 4.3: Neighborhoods of existence of invariant circles for the model (4.1) with $A_l = \frac{1}{l^2}$, $\omega = \frac{\sqrt{5}-1}{2}$, and potential $V(x) = -\frac{\varepsilon_1}{2\pi}\cos(2\pi x) - \frac{\varepsilon_2}{4\pi}\cos(4\pi x) - \frac{0.3}{6\pi}\cos(6\pi x)$ in the parameter space $(\varepsilon_1, \varepsilon_2)$.

Chapter 5

A criterion for the breakdown of quasi-periodic solutions and its rigorous justification

5.1 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 [187, 25, 171, 201] 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 [49] and established in [162]. 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, [174, 173, 132].

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 [14], 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. We also note that with the solid state motivation one is lead naturally to consider problems that do not reduce to twist mappings.

The analyticity breakdown transition for twist maps has been the subject of intensive numerical study starting with the pioneering [95] (see Appendix B for a comparison among different methods). The goal of this paper is to formulate a numerically efficient criterion for the computation of the analyticity breakdown of analytic tori in 1-D systems described by a variational principle (in particular in twist mappings) or in symplectic 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. They are uniquely defined and, as we will see, there are efficients algorithms for their computation.

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 5.2 for a precise formulation of the criterion. We have implemented this in [37], were we include algorithmic details. In the present paper, we concentrate on rigorous results that justify the numerical procedures.

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 [57] and this leads to rigorous proofs. Even if one does not want to get full rigor, one can get good indications of the reliability of the computation 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 [37, 104]. 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.2.1, 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 provides 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 [60] one can find statistical mechanics models that cannot be written as a dynamical system. On the other hand, non-twist mappings [70] can be treated as symplectic mappings but do not admit a variational formulation.

The very successful criteria of [95, 184] 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.

There are other *a posteriori* theorems in the literature such as the ones presented in [53, 42, 220]. 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.

5.2 Criterion for the breakdown

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

Algorithm 5.2.1.

Choose a path in the parameter space

starting in the integrable case.

Initialize the parameters and the solution at integrable

Repeat

Increase the parameters along the path

Run the iterative step

If (Iterations do not converge)

Decrease the increment in parameters

Else (Iteration success)

Record the values of the parameters

and the Sobolev norm of the solution.

Until Sobolev norm too large

In practice, one can find often that the 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, [51].

The previous algorithm is a continuation algorithm and shares all the shortcomings common to continuation algorithms. One can compute the connected component of

$$K_\omega = \{(\varepsilon, K_\varepsilon) | \varepsilon \in \mathbb{R}, \mathbb{C}\}$$

where K_ε is the parameterization of an invariant torus with frequency ω.

There remains the possibility that the set K_ω has several components. Of course. the local uniqueness results of [174, 220, 54, 60] show that the set K_ω is locally a manifold.

On the other hand, it remains the possibility that for certain values of ε, there are several invariant tori (recently, it has been shown [80] that this does not happen for twist maps, but it does happen for non twist maps). It can also happen that indeed the set of ε with at KAM tori is not connected.

Indeed, [34] presents numerical evidence that the twist maps

$$(p, q) \to (p + \varepsilon[\alpha \cos(2\pi x) + \beta \cos(4\pi x)], q + p + \varepsilon[\alpha \cos(2\pi x) + \beta \cos(4\pi x)])$$

the set of parameters with KAM tori has several components when $\alpha = 1, \beta > \approx \frac{\sqrt{2}-1}{4}$.

As is standard with continuation algorithms, the algorithm [33] can be extended to two dimensional parameter space. The easiest implementation is to sum the algorithm form a family of paths which covers the parameter space. For example, think of families of radii covering the plane.

This straightforward implementation does not compute the full connected component since there may be "overhangs" (points in the connected component which are not reachable by path in the family even if they are reachable by a path not in the family). There exist standard continuation algorithms to do higher dimensional continuation. Indeed, the examples of several components in one parameter family alluded in the previous paragraph were found [34] by doing a 2 dimensional configuration. In that respect, we point out that there are compelling (but still incomplete) arguments that indicate that the infinite dimensional sets of twist maps with a KAM torus of rotation ω is connected (in other words the different components found in finite dimensional family can be connected in a higher dimensional family).

5.3 A posteriori KAM estimates

The rigorous justification of the criterion is based on an *a posteriori* formulation of a KAM theorem and continuity properties of a functional equation.

The theorem with its proof can be interpreted as an implicit function theorem, [220, 221, 27]. It is possible to find a finite set of explicit conditions [125, 180] (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 [57] is

Theorem 5.3.1. *Let $\mathcal{X}_0 \subset \mathcal{X}_1$ be Banach spaces and $\mathcal{U} \subset \mathcal{X}_0$ and open set. For certain maps*

$$\mathcal{F} : \mathcal{U} \subset \mathcal{X}_0 \to \mathcal{X}_0,$$

there exists an explicit function $\varepsilon^* : \mathbb{R}^+ \times (\mathbb{R}^+)^n \to \mathbb{R}^+$ such that

$$\lim_{t \to \infty} \varepsilon^*(t, \cdot) = 0,$$

explicit functionals $f_1, ..., f_n : \mathcal{X}_0 \to \mathbb{R}^+$, and $M_0, M_1, ..., M_n \in \mathbb{R}^+$ satisfying the following property. Suppose $x_0 \in \mathcal{X}_0$ with $\|x_0\|_{\mathcal{X}_0} \leq M_0$, with the following property

$$f_1(x_0) \leq M_1, ..., f_n(x_0) \leq M_n,$$

and

$$\|\mathcal{F}(x_0)\|_{\mathcal{X}_0} < \varepsilon^*(M_0, ..., M_n).$$

Then there exists an $x^* \in \mathcal{X}_1$ such that $\mathcal{F}(x^*) = 0$ and

$$\|x_0 - x^*\|_{\mathcal{X}_1} \leq C_{M_0,...,M_n} \varepsilon^*(M_0, ..., M_n)$$

The theorem states that the existence of a true solution is implied if we can find an $x_0 \in \mathcal{X}_0$ that solves the functional equation very approximately as long as a finite number of conditions are satisfied. In practice, we work in subsets of $\mathcal{X}_0$ where the functionals $f_1, ..., f_n$ are bounded. Therefore, the

true solution breaks down if and only if the norm of the approximate solution blows up.

Remark 5.3.2. For our applications it is important that the Newton method starts on an arbitrary approximate solution. Some versions of Nash–Moser implicit function theorems, notably those of [220, 197], have this feature, but they require a special structure in the equations or invertibility of the derivative of the functional in a neighborhood about the initial guess.

Remark 5.3.3. Other examples of *a posteriori* KAM theorems have appeared in the literature. For example [53] considers whiskered tori, [41] considers 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 effective.

In section 5.5, we present a KAM theorem for symplectic mappings based in *automatic reducibility*. A version for the analytic spaces was presented in [54], but now we present a result for Sobolev spaces, which is well suited for numerical implementations.

In section 5.6, 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 [60].

Both theorems will be proved by applying an abstract Nash-Moser implicit function theorem which we present in Appendix A so that it can be read independently. Theorem A.2.1 combines features of the abstract theorems in [220, 198]. Of course, there is a large literature of implicit function theorems, which are useful in many contexts. For example, [199, 97, 103] but for us the feature of starting the iteration on just approximate solutions was very important.

For simplicity, in this paper we will present results for maps only, but there are analogous results for flows. [73, 54] show how to deduce results for flows from results from maps.

5.4 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 5.3 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 rather than C^r norms, see below for more details.

5.4.1 Sobolev Spaces

We denote the Fourier expansion of a periodic mapping $u : \mathbb{T}^n \to \mathbb{R}^d$ 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 it by

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

Definition 5.4.1. For $m \in \mathbb{R}^+$, the Sobolev Space H^m is the Banach space of functions from $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$ taking values in $\mathbb{R}^d$ defined by

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

Here $|\cdot|$ represents the maximum norm on the spaces $\mathbb{R}^d$ and $\mathbb{C}^d$, i.e. if $x = (x_1, \ldots, x_d) \in \mathbb{C}^d$, then

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

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.

We note that for $m \in \mathbb{Z}^+$ we have

$$C_1(\|D^m u\|^2 + |\operatorname{avg} \{u\}_\theta \,|^2) \leq \|u\|_m^2 \leq C_2(\|D^m u\| 2 + |\operatorname{avg} \{u\}_\theta \,|^2)$$

so that the norms are equivalent.

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) [62].

- 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 [37] since it is known that for the *universality class* the analyticity breakdown satisfies some scaling relations [137]. The scaling relations of Sobolev norms allow us to identify more accurately the breakdown point for families in the same universality class.

- It has been shown in [54, 60] that solutions of the invariance equations for twist mappings and for models in Statistical Mechanics which are Sobolev of a sufficiently high order are analytic. See remarks.

5.4.1.1 Some properties of Sobolev spaces

In the rest of the section we collect some standard material to set the notation. This section is meant to be used as reference.

The Sobolev spaces we have introduced are a Banach Algebra for large enough m. The following result is proven in [6] as a straightforward application of the Sobolev Imbedding Theorem.

Theorem 5.4.2. *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*

$$\|u \cdot v\|_m \leq K_1 \|u\|_m \|v\|_m \tag{5.1}$$

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

$$\tilde{M}^{-1} = \left[\sum_{n=0}^{\infty} M^{-1} (M - \tilde{M})^n \right] M^{-1} \tag{5.2}$$

and the Banach algebra properties.

It is also useful to have the following estimates on compositions (see for example [212, Section 13.3]).

Theorem 5.4.3. *Let $\mathcal{F} \in \mathcal{C}^m$ and assume $\mathcal{F}(0) = 0$. Then, for $u \in H^m \cap L^\infty$*

$$\|\mathcal{F}(u)\|_m \leq K_2(\|u\|_{L^\infty})(1 + \|u\|_m) \tag{5.3}$$

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

$$\begin{aligned} &||f \circ (u+v) - f \circ (u) - Df \circ (u)v||_m \\ &\qquad \leq C_{n,m}(\|u\|_{L^\infty})(1 + \|u\|_m)||f||_{C^{m+2}}||v||_m^2 \end{aligned} \tag{5.4}$$

Notice that by the Sobolev Imbedding Theorem we also have that

$$H^m \subset \mathcal{C} \cap L^\infty, \quad \text{for } m > \frac{n}{2} \tag{5.5}$$

so if $\mathcal{F} \in \mathcal{C}^m$ and $u \in H^m$ with $m > \frac{n}{2}$ then the hypotheses of Theorem 5.4.3 are immediately satisfied.

5.4.2 Number Theory

A standard definition in KAM theory is the Diophantine condition.

Definition 5.4.4. We say that $\omega \in \mathbb{R}^n$ is Diophantine if for some $\nu > 0$ and $\tau > n$ we have that

$$|p \cdot \omega - q| \geq \nu |q|_1^{-\tau} \qquad q \in \mathbb{Z}^n - \{0\}, \quad \forall p \in \mathbb{Z} \tag{5.6}$$

where $|l|_1 = |l_1| + |l_n| + ... + |l_n|$. We define $D(\nu, \tau)$ as the set of all frequency vectors satisfying (5.6).

5.4.3 Cohomology equations

It is also standard in KAM theory to solve for φ given ξ in the equation

$$\varphi(\theta \pm \omega) - \varphi(\theta) = \xi(\theta) \tag{5.7}$$

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

Estimates for (5.7) in Sobolev spaces are given by the following lemma, which is straight forward compared to the version in other spaces.

Lemma 5.4.5. *Let $\omega \in D(\nu, \tau)$. Given any function $\xi \in H^{m+\tau}$ satisfying $avg\{\xi\}_\theta = 0$ there is one and only one function $\varphi \in H^m$ satisfying*

$$\varphi(\theta \pm \omega) - \varphi(\theta) = \xi, \quad avg\{\varphi\}_\theta = 0 \tag{5.8}$$

Moreover,

$$\|\varphi\|_m \leq C\nu^{-1}\|\xi\|_{m+\tau} \tag{5.9}$$

Proof 5.4.6. From (5.8) 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

$$\begin{aligned} \|\varphi\|_m^2 &= \sum_{k\in\mathbb{Z}} (1+|k|^2)^m |\hat{\varphi}_k|^2 = \sum_{k\in\mathbb{Z}} (1+|k|^2)^m \frac{|\hat{\xi}_k|^2}{|e^{\pm 2\pi i k\cdot\omega} - 1|^2} \\ &\leq C\sum_{k\in\mathbb{Z}} (1+|k|^2)^m \frac{|\hat{\xi}_k|^2}{(2\pi k\cdot\omega)^2} \leq C\nu^{-2}\sum_{k\in\mathbb{Z}} (1+|k|^2)^{m+\tau}|\hat{\xi}_k|^2 \\ &= C\nu^{-2}\|\xi\|_{m+\tau}^2 \end{aligned} \tag{5.10}$$

5.5 The criterion for Symplectic Maps

In this section we introduce a justification of the criterion of breakdown of analyticity for Symplectic maps with a Diophantine rotation vector. Similar result hold for vector fields, see [54] for an argument that shows 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 criterion we present works also in the context of Variational Problems in Statistical Mechanics discussed in Section 5.6 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 [54]. 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.

5.5.1 Formulation of the invariance equation

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

$$(f \circ K)(\theta) = K(\theta + \omega) \tag{5.11}$$

where $K : \mathbb{T}^n = (\mathbb{R}/\mathbb{Z})^n \to \mathbf{U}$ 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 $a : U \to \mathbb{R}^{2n}$ be defined by

$$\alpha_z = a(z)dz \quad \forall z \in U \tag{5.12}$$

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

$$\Omega_z(\xi, \eta) =< \xi, J(z)\eta > \tag{5.13}$$

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

Notice that (5.11) 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 $K : \mathbb{T}^n = (\mathbb{R}/\mathbb{Z})^n \to \mathbf{U}$ satisfying

$$K(\theta + k) = K(\theta) + (k, 0) \qquad k \in \mathbb{Z}^n. \tag{5.14}$$

Notice that it is equivalent to say that K satisfies (5.14) 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 5.5.1. 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

$$N(\theta)\ \left(DK(\theta)^\top\, DK(\theta)\right) = I_n, \tag{5.15}$$

where I_n is the n-dimensional identity matrix.

N2 The average of the matrix-valued function

$$S(\theta){:=}P(\theta+\omega)^\top\ \left[\, Df(K(\theta))J(K(\theta))^{-1}P(\theta)\ - J(K(\theta+\omega))^{-1}P(\theta+\omega)\,\right] \tag{5.16}$$

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

$$M(\theta){:=}\left(\ DK(\theta)\qquad J(K(\theta))^{-1}DK(\theta)N(\theta)\ \right), \tag{5.17}$$

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 5.5.2. 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 5.5.3. Note that **N1** depends only on K whereas **N2** depends on K and f.

Note also that by the observation on series (5.2), the Condition **N3** is an open condition in H^m. As we will see condition **N3** will be implied for functions K which satisfy the invariance equation with good accuracy.

5.5.2 Statement of an *a posteriori* theorem for symplectic maps

Theorem 5.5.1. Let $m > \frac{n}{2} + 2\tau + 1$ and $f \in C^{m+34\tau-17}$, $f : \mathbf{U} \to \mathbf{U}$ 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 5.5.1).

H2. The map $f \in C^{m+34\tau-17}$ 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 (5.12) and (5.13), respectively,

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

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 σ, n, r, ρ_0, $|f|_{C^2,\mathcal{B}_r}$, $\|a\|_{C^{r+3}}$, $\|J\|_{C^{r+3}}$, $\|J^{-1}\|_{C^{r+3}}$, $\|DK_0\|_{m-2\tau+1}$, $\|N_0\|_{m-2\tau+1}$, $\left|(\text{avg}\,\{S_0\}_\theta)^{-1}\right|$ (where N_0 and S_0 are as in 5.5.1, replacing K by K_0) such that, if $\|e_0\|_{m-2\tau}$ verifies the following inequalities

$$c\,\nu^{-4}\|e_0\|_{m-2\tau+1} < 1, \tag{5.18}$$

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 5.5.3. In [94], it is shown that if f is analytic, $K \in H^m$, for $m \geq m_0$ and satisfies the invariance equation and Definition 5.5.1 then K is analytic. Here, m_0 depends on τ and n.

5.5.3 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 [54]

Since equation (5.11) can be formulated as finding zeros of

$$F(K) := f \circ K - K \circ T_\omega\,, \tag{5.19}$$

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

$$DF(K)\Delta(\theta) = Df(K(\theta))\Delta(\theta) - \Delta(\theta+\omega) = -e(\theta) \tag{5.20}$$

with error function

$$e(\theta) = F(K)(\theta) \quad \forall\theta \in \mathbb{R}^n \tag{5.21}$$

In [54], 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 (5.22).

$$M(\theta) := \begin{pmatrix} DK(\theta) & J(K(\theta))^{-1}DK(\theta)N(\theta) \end{pmatrix}, \tag{5.22}$$

that transforms the derivative Df into

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

with

$$C(\theta) := \begin{pmatrix} I_n & S(\theta) \\ 0 & I_n \end{pmatrix}, \tag{5.23}$$

and

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

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

$$\begin{pmatrix} I_n & S(\theta) \\ 0 & I_n \end{pmatrix} M^{-1}(\theta)\Delta(\theta) - M^{-1}(\theta+\omega)\Delta(\theta+\omega) = -M^{-1}(\theta+\omega)e(\theta). \tag{5.24}$$

Notice that equation (5.24) differs from the Newton step equation by a term $BM^{-1}\Delta$ which is quadratic in e (we will show latter the Δ is also estimates by $\|e\|$) so the modified Newton Method (5.24) gives rise to a quadratically convergent scheme.

Moreover, equation (5.24) can be solved in two steps. We are therefore led to the following algorithm.

Procedure 1. The iterative step is constructed as follows:

1) Compute

$$e(\theta) = f \circ K - K \circ T_\omega,$$

$$N(\theta) = (DK(\theta)^T DK(\theta))^{-1},$$

$$M(\theta) = (DK(\theta) \quad J^{-1}(K(\theta))DK(\theta)N(\theta)),$$

$$M^{-1}(\theta),$$

and

$$E(\theta) = M^{-1}(\theta)e(\theta).$$

2) Find a normalized function W_2 (i.e. $\operatorname{avg}\{W_2\}_\theta = 0$) solving the equation

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

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

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

3) We solve for W_2 from

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

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

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

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

$\tilde{K}$ is the improved solution.

We call attention that all the steps are diagonal either in Fourier space of in Real space. The fact that the steps are diagonal and that one can switch from Real space to Fourier using efficient Fast Fourier Transforms allows to have fast numerical implementations. Notice also the small storage requirements.

5.5.4 Estimates for the Quasi-Newton Method

In this section we provide estimates for the iterative step described in Algorithm 1. The form of the estimates we will prove is typical of the Nash-Moser strategy. We will show that the new error will be bounded (in a less smooth norm) by the square of the original error.

Actually, we will follow the formulation of the abstract implicit function theroem, Theorem A.2.1, and we will describe the Algorithm 1 by a linear operator η that produces the correction Δ out of the true error e. That is

$$\Delta = \eta[K]e \tag{5.25}$$

According to the strategy of Theorem A.2.1 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 [54], an approximate solution K of (5.11) with error e defined in (5.21). Define S, M, and C by (5.16), (5.22), and (5.23), respectively, and let us define $\mathcal{E}$ as

$$\mathcal{E}(\theta) := Df(K(\theta))M(\theta) - M(\theta+\omega)\,C(\theta). \tag{5.26}$$

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

Then

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

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 5.5.5. Let $m > \frac{n}{2} + 2\tau + 1$, $F[K] \in H^m$, and $F[K]$, $\eta[K]$ defined in 5.25.

Then we have the estimates

$$\begin{aligned} &\|(DF[K]\eta[K] - \mathrm{Id})F[K]\|_{m-2\tau-1} \\ &\qquad \leq C\nu^{-2}\|M\|_{m-1}^2\|M^{-1}\|_{m-2\tau-1}\|F[K]\|_{m-1}\|F[K]\|_m \end{aligned} \tag{5.27}$$

Proof 5.5.6. We have

$$\begin{aligned} &\|(DF[K]\eta[K] - \mathrm{Id})F[K]\|_{m-2\tau-1} \\ &\qquad \leq \|DF\eta[k]F[K] + M \circ T_\omega BM^{-1}\eta[K]F[K] \\ &\qquad - M \circ T_\omega BM^{-1}\eta[K]F[K] - F[K]\|_{m-2\tau-1} \\ &\qquad \leq \|M \circ T_\omega[(C+B)M^{-1}\eta[k]F[K] - (M^{-1}\eta[K]F[K]) \circ T_\omega] \\ &\qquad - M \circ T_\omega BM^{-1}\eta[K]F[K] - F[K]\|_{m-2\tau-1} \\ &\qquad \leq \|M \circ T_\omega BM^{-1}(\eta[K]F[K]) \circ T_\omega\|_{m-2\tau-1} \\ &\qquad \leq C\nu^{-3}\|M\|_{m-1}^2\|M^{-1}\|_{m-2\tau-1}\|F[K]\|_{m-1}\|F[K]\|_m \end{aligned} \tag{5.28}$$

which completes the estimates for the approximate inverse.

The final result follows from an application of Theorem A.2.1. In the context of Theorem A.2.1 we consider the previous estimates with $\alpha = 2\tau - 1$ and the result from of Theorem 5.3.

5.6 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 1-D models coming from statistical

mechanics. This includes as particular cases the breakdown of KAM tori for twist mappings. In section 5.6.1, we introduce the models considered. In section 5.6.6, 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.2.1). The statement of Theorem 5.6.1 asserts that if the Sobolev norms of an approximate solution are small enough and it satisfies the functional equation very approximately 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 5.6.7. The estimates used for the step are in 5.6.8 and the convergence is established using Theorem A.2.1 from the Appendix A.

5.6.1 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 $x : \mathbb{Z} \to \mathbb{R}$). Following [192], 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 multi-body interactions).

In this paper, we will be concerned with the existence of equilibrium states (see Definition 5.6.3) 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:

$$\mathbb{S}(\{x_n\}) = \sum_{L\in\mathbb{N}} \sum_{k\in\mathbb{Z}} H_L(x_k, ..., x_{k+L}) \tag{5.29}$$

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.

$$H_L(x_k, ..., x_{k+L}) = H_L(x_k + 1, \ldots, x_{k+L} + 1) \tag{5.30}$$

The property (5.30) is a rather weak periodicity condition. It is implied by the stronger property

$$H_L(x_k, ..., x_{k+L}) = H_L(x_k + \ell_0, \ldots, x_{k+L} + \ell_L) \tag{5.31}$$

for all $\ell_i \in \mathbb{Z}$. The latter property (5.31) is natural when the variables x_i are angles. For example, spin variables. The weaker property (5.30) has appeared in many situations. It is natural when considering twist maps of the annulus [165] or monotone recurrences [11].

ii) We will also require a decay condition for the criterion to hold. In section 5.6.8, we present the detailed description of the decay condition and in 5.2 we state its relevance for the persistence of quasi-periodic solutions.

5.6.2 Some examples of models

Models of the form (5.29) 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

$$\partial_1 \partial_2 H_1(x, y) \leq -c < 0. \tag{5.32}$$

  Then models of the form (5.29) appear as variational principles for twist mappings. In this case, the physical meaning of $\mathcal{S}$ is an action while the assumption (5.32) 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 in 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 [14], models of dislocations [83]), and in dynamical systems as twist maps, [168, 165].

- If Frenkel-Kontorova models are considered as models of dislocations, some more realistic models include longer range interactions [39].

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 $k \geq 2$

$$H_k(x_0, \ldots, x_k) = \frac{A_k}{2}(x_0 - x_k)^2 \tag{5.33}$$

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 (5.33) (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. [26, p. 600] considers possible long range interactions that are relevant for the model. Computations of the coefficients of these interactions is are discussed in [189].

- In [11], 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[22] and references there.

5.6.3 Equilibrium equations

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

$$\partial_{x_i} \mathbb{S}(\{x_n\}) = 0 \tag{5.34}$$

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 $\mathbb{S}$ 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 5.6.4) are ground states. This is often called Wierstass criterion. 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 (5.29) the Euler-Lagrange equations are:

$$\sum_{L\in\mathbb{N}}\sum_{j=0}^{L}\partial_j H_L(x_{k-j},...,x_{k-j+L})=0\quad\forall k\in\mathbb{Z} \tag{5.35}$$

We call attention that, in contrast with the sums defining $\mathbb{S}$ which are merely formal, the sums involved in equilibrium equations (5.35) are meant to converge.

A practical case of equilibria that has attracted a great deal of attention is ground states [153, 21, 166] (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.

5.6.4 Plane-like configurations and hull functions

We are interested in equilibrium configurations $\{x_n\}$ that can be written as

$$x_n = h(n\omega) \tag{5.36}$$

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

$$h(x+e)=h(x)+e\quad\forall e\in\mathbb{Z} \tag{5.37}$$

and is analytic.

The function h is often called the *hull function*. The periodicity condition (5.37) means that h can be considered as a map of the circle to itself. We

will use the notation

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

Were u is a periodic function.

5.6.5 Equilibrium equations in terms of hull functions

For configurations of the form (5.36), the equilibrium equations become:

$$\begin{aligned} E[u](\theta) \equiv \sum_{L} \sum_{j=0}^{L} \partial_j H_L(\theta - j\omega + u(\theta - j\omega), \ldots, \\ \theta + u(\theta), \ldots, \theta + (L-j)\omega + u(\theta + (L-j)\omega)) \\ =0 \end{aligned} \tag{5.38}$$

5.6.6 Statement of an *a posteriori* theorem for statistical mechanics models

Theorem 5.6.1. *Let $m > \frac{1}{2} + 2\tau$ and $H_L \in C^{m+34\tau}$ be translation invariant interactions as in (5.29) satisfying the periodicity condition (5.30). Let $\omega \in \mathbb{R}$. Let $h = \mathrm{Id} + u$, with $u \in H^{m+32\tau}$, $avg\{u\}_\theta = 0$ be a diffeomorphism of $\mathbb{T}$. Assume:*

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

$$|q\omega - p| \geq \nu |q|^{-\tau} \ \forall p, q \in \mathbb{Z} \tag{5.39}$$

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

Denote

$$M_L = K_m \|H_L\|_{C^{m+3}} \|(\mathrm{Id} + u')\|_m^2$$

$$a = \sum_{L \geq 2} M_L L^4$$

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

$$\|(\partial_0 \partial_1 H_1)^{-1}(u(\theta), u(\theta + \omega))\|_m \leq T.$$

$$\left(avg\left\{(\partial_0 \partial_1 H_1)^{-1}(u(\theta), u(\theta + \omega))\right\}_\theta\right)^{-1} \leq U.$$

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

a1) $\|(\mathrm{Id} + u')\|_m \leq N^+$.

a2) $\|(\mathrm{Id} + u')^{-1}\|_m \leq N^-$.

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

$$E[u^*] = 0 \tag{5.40}$$

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 (5.40) and $avg\{u^*\}_\theta = 0$.

Remark 5.6.2. In [60], 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 (and that of $(\mathrm{Id}+u')^{-1}$), 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 5.6.1. 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, and that $\mathrm{Id} + u'$ is bounded away from zero.

5.6.7 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 is the basis of very practical algorithms and it is the key to the proof of Theorem 5.6.1 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

$$h'(\theta)(DE[u]v)(\theta) - v(\theta)(DE[u]h')(\theta) = -h'(\theta)E[u](\theta). \tag{5.41}$$

Note that equation (5.41) differs from the Newton step equation by the term $v(\theta)(DE[u]h')(\theta)$. Using the identity

$$\frac{d}{d\theta}E[u](\theta) = DE[u]h'(\theta). \tag{5.42}$$

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 form equation (5.41). The advantage of (5.41) 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 [60]. 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 (5.41) transforms into:

$$\mathcal{L}_1[(\mathcal{C}_{0,1,1} + \mathcal{G})\mathcal{L}_{-1}w] = -h'E[u]. \tag{5.43}$$

where

$$\mathcal{C}_{i,j,L} = \partial_i\partial_j H_L \circ \gamma_L(\theta - j\omega)h'(\theta)h'(\theta - (i-j)\omega) \tag{5.44}$$

with

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

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

$$\varphi(\theta \pm \omega) - \varphi(\theta) = \xi(\theta) \tag{5.45}$$

Thus, equation (5.43) can be solved following the next algorithm:

Procedure 2. a) Check that $\operatorname{avg}\{h'E[u]\}_\theta = 0$.

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

$$\mathcal{L}_1\varphi = -h'E[u] \tag{5.46}$$

Therefore, if φ is a solution for (5.46) 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

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

c) We solve for w from

$$\mathcal{L}_{-1}w = (\mathcal{C}_{0,1,1} + \mathcal{G})^{-1}(\varphi + \mathcal{T}) \tag{5.47}$$

d) Finally we obtain the improved solution

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

We call attention that all the steps are diagonal either in Fourier space of in Real space. The fact that the steps are diagonal allows to have fast numerical implementations.

5.6.8 Estimates for the Quasi-Newton Method

The goal of this section is to provide precise estimates for the iterative step described in Section 5.6.7. Throughout this section we will assume that $\omega \in \mathbb{R}$ satisfies the Diophantine condition given in Definition 5.4.4.

The following lemma is proven in [60]

Lemma 5.6.3. *For every $m > 0$ we have:*

$$\begin{array}{rcl} \|\mathcal{L}_\ell \mathcal{L}_{\pm 1}^{-1}\|_m & \leq & |\ell| \\ \|\mathcal{L}_{\pm 1}^{-1}\mathcal{L}_\ell\|_m & \leq & |\ell| \end{array} \tag{5.48}$$

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

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

and K_1 is the constant of (5.1) 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

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

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

Then we have the following estimates on η

$$\|\eta[u]E[u]\|_{m-2\tau} \leq C\nu^{-2}(N^+)^2\|E[u]\|_m. \tag{5.49}$$

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

Lemma 5.6.5. *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

$$\|(DE[u]\eta[u] - \mathrm{Id})E[u]\|_{m-2\tau} \leq C\nu^{-2}(N^+)^2N^-\|E[u]\|_{m-2\tau-1}\|E[u]\|_m \quad (5.50)$$

Proof 5.6.6. Let $\psi = DE[u]\eta[u]E[u] - E[u]$, then we have that

$$\begin{aligned} \psi &= DE[u]\eta[u]E[u] + (-h')^{-1}\cdot\eta[u]E[u]\cdot DE[u]h' \\ &\quad -(-h')^{-1}\cdot\eta[u]E[u]\cdot DE[u]h' - E[u] \\ &= (-h')^{-1}\cdot(h'DE[u]\eta[u]E[u] - \eta[u]E[u]\cdot DE[u]h') \\ &\quad +(h')^{-1}\cdot\eta[u]E[u]\cdot DE[u]h' - E[u] \\ &= (h')^{-1}\cdot\eta[u]E[u]\cdot DE[u]h' \end{aligned} \quad (5.51)$$

Se we have that

$$\begin{aligned} &\|(DE[u]\eta[u] - \mathrm{Id})E[u]\|_{m-2\tau} \\ &\quad \leq \|\,(h')^{-1}\cdot\eta[u]E[u]\cdot DE[u]h'\|_{m-2\tau} \\ &\quad \leq C\nu^{-2}(N^+)^2N^-\|E[u]\|_{m-2\tau-1}\|E[u]\|_m, \end{aligned} \quad (5.52)$$

which completes the estimates for the approximate inverse.

The final result follows from an application of Theorem A.2.1. In the context of Theorem A.2.1 we consider the previous estimates with $\alpha = 2\tau$ and the estimates of Theorem 5.3.

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Appendices

Appendix A

An abstract Nash-Moser implicit function theorem

In this appendix we prove Theorem A.2.1, an abstract Nash-Moser implicit function theorem that is very well suited for the proof of Theorem 5.6.1. 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 do not have a bounded inverse from one space to itself. In our applications this unboundedness of the inverse of the derivative 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 looses 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

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.

The theorem A.2.1 is very close to the main theorem in [197] (see also the exposition in [198]) but we allow an extra term in the reminder as in [220]. We also remark that it suffices to estimate the approximate inverse in the range of the operator. As pointed out in [220] this extra condition, 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.2.1 which is very important for our purposes is that Theorem A.2.1 does not assume that the initial system is close to integrable.

Compared with the scheme in [220], the present scheme has the advantage that uses 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 [222]. Hence we can obtain the results there without requiring that the initial approximation is analytic, nevertheless, the differentiability loss is more severe than in [222].

Remark A.0.7. The proof we present follows very closely [197]. In particular, we have followed the choices of [197] 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 itself does not loose any derivatives.

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.2.1 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.1.1. Given a scale of spaces, we say that $\{S_t\}_{t\in\mathbb{R}^+}$ is a family of smoothing operators when

i)
$$\lim_{t\to\infty} \|(S_t - \mathrm{Id})u\|_0 = 0$$

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

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

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

$$\widehat{(S_t u)}_k = e^{-|k|/t} \hat{u}_k \tag{A.1}$$

Note that $S_t u$ is analytic. In our concrete applications we will use (A.1).

Lemma A.1.2. The operators S_t defined in (A.1) are smoothing operators in the sense of Definition A.1.1.

Proof A.1.3. Notice that for $0 \leq m, n < \infty$

$$\begin{array}{rcl} \|S_t u\|_m^2 & = & \sum e^{-2|k|/t}(1+|k|^2)^m |u_k|^2 \\ & = & \sum e^{-2|k|/t}(1+|k|^2)^{m-n}(1+|k|^2)^n |u_k|^2 \\ & \leq & \sum e^{-2|k|/t} t^{2m-2n} (1+\frac{|k|^2}{t^2})^{m-n}(1+|k|^2)^n |u_k|^2 \\ & \leq & C t^{2(m-n)} \|u\|_n^2 \end{array} \tag{A.2}$$

We also have that

$$\begin{array}{rcl} \|(S_t - \mathrm{Id})u\|_m^2 & = & \sum (e^{-|k|/t}-1)^2 (1+|k|^2)^m |u_k|^2 \\ & \leq & \displaystyle\sum \frac{(e^{-|k|/t}-1)^2}{\left(1+\frac{|k|^2}{t^2}\right)^n} t^{-2n}(1+|k|^2)^{m+n}|u_k|^2 \\ & \leq & C_n t^{-2n} \|u\|_{m+n}^2 \end{array} \tag{A.3}$$

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 [220].

Lemma A.1.4. 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 that for any $u \in \mathcal{X}^m$:

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

Proof. For all $t > 0$, $u = S_t u + (\mathrm{Id} - S_t)u$ and therefore, if $u \in \mathcal{X}^m$,

$$\|u\|_l \leq \|S_t\|_l + \|(\mathrm{Id} - S_t)u\|_l \leq t^{l-n}C_{n,l}\|u\|_n + t^{-(m-l)}C_{l,m}\|u\|_m.$$

Computation of the minimum of the function in t on the RHS of this inequality leads immediately to the result.

□

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

A.2 Formulation of Theorem A.2.1

In this section, we formulate and prove the abstract implicit function theorem TheoremA.2.1. 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.2.1. 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

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

and

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

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) $\mathcal{F}|_{\tilde{\mathcal{B}}_m \cap \mathcal{X}^r} : \tilde{\mathcal{B}}_r \cap \mathcal{X}^r \to \mathcal{X}^{r-\alpha}$ 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) $\|(D\mathcal{F}[u]\eta[u] - \mathrm{Id})z\|_{r-\alpha} \leq C\|\mathcal{F}[u]\|_r\|z\|_r$, $u \in \tilde{\mathcal{B}}_r, z \in \mathcal{X}^r$, 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.2.1. Note that in *iii)* we are only requiring estimates for two values of r. When *iii)* acts in the whole space, and the spaces $\mathcal{X}^r$ are interpolation spaces [209], this implies the bounds for the intermediate spaces.

Remark A.2.2. 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)′ $\|(D\mathcal{F}[u]\eta[u] - \mathrm{Id})\mathcal{F}[u]\|_{r-\alpha} \leq C\|\mathcal{F}[u]\|_r^2$, $u \in \tilde{\mathcal{B}}_r$, for $r = m$. Indeed in both of our applications the definition of the approximate inverse requires that some average of z is small which i true for functions in the range but not in general.

A.3 Proof of Theorem A.2.1

The proof is based on an iterative procedure combining the ideas of [197, 220]. 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 u^* such that $\mathcal{F}[u^*] = 0$.

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 will indicate them during the proof when they have been specified. We anticipate that there will be a finite number of inequalities of κ, μ, and δ for β large enough and other finite set of inequalities for the remaining quantities.

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

$$u_{n+1} = u_n - S_{t_n}\eta[u_n]\mathcal{F}[u_n] \tag{A.4}$$

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

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

Then if

$$\mu > 2, \tag{A.5}$$

$\{u_n\} \subset \mathcal{X}^m$ converges to some $u \in \mathcal{X}^m$.

Now, to prove $(p1; n)$, we notice that, using $\kappa^j \leq j(\kappa - 1)$ we have that

$$\begin{aligned}\|u_n - u_0\|_m &\leq C\nu \sum_{j=1}^{\infty} e^{\alpha\beta\kappa^j(2-\mu)} \\ &\leq C\nu \sum_{j=1}^{\infty} e^{\alpha\beta j(\kappa-1)(2-\mu)} \\ &\leq C\nu \frac{e^{\alpha\beta(\kappa-1)(2-\mu)}}{1-e^{\alpha\beta(\kappa-1)(2-\mu)}}\end{aligned} \tag{A.6}$$

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.

$$\begin{aligned}\|\mathcal{F}[u_n]\|_{m-\alpha} \quad \leq \quad & \|\mathcal{F}[u_n] - \mathcal{F}[u_{n-1}] + D\mathcal{F}[u_{n-1}]S_{t_{n-1}}\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-\alpha} \\ & + \|(\mathrm{Id} - D\mathcal{F}[u_{n-1}]\eta[u_{n-1}])\mathcal{F}[u_{n-1}]\|_{m-\alpha} \\ & + \|D\mathcal{F}[u_{n-1}](\mathrm{Id} - S_{t_{n-1}})\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-\alpha}.\end{aligned} \tag{A.7}$$

The right hand side of the inequality is obtained by adding and subtracting terms and using (A.4).

We estimate the first term of (A.7) using assumption *iii*) and the quadratic remainder of Taylor's theorem.

$$\begin{aligned}&\|\mathcal{F}[u_n] - \mathcal{F}[u_{n-1}] + D\mathcal{F}[u_{n-1}]S_{t_{n-1}}\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-\alpha} \\ &\qquad \leq C\|S_{t_{n-1}}\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_m^2 \\ &\qquad \leq Ce^{2\alpha\beta\kappa^{n-1}}\|\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-2\alpha}^2 \\ &\qquad \leq C\nu^2 e^{2\alpha\beta\kappa^{n-1}(2-\mu)}\end{aligned} \tag{A.8}$$

For the second term of (A.7) by assumption *iv*) we get

$$\|(D\mathcal{F}[u_{n-1}]\eta[u_{n-1}] - \mathrm{Id})\mathcal{F}[u_{n-1}]\|_{m-\alpha} \leq C\|\mathcal{F}[u_{n-1}\|_m^2. \tag{A.9}$$

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

$$\begin{aligned} \|\mathcal{F}[u_{n-1}]\|_m^2 &\leq C\|\mathcal{F}[u_{n-1}]\|_{m-\alpha}^{36/17}\|\mathcal{F}[u_{m-1}]\|_{m+16\alpha}^{2/17} \\ &\leq C\|\mathcal{F}[u_{n-1}]\|_{m-\alpha}^{36/17}(1+\|u_{n-1}\|_{m+17\alpha})^{2/17} \\ &\leq C\nu^2 e^{\alpha\beta\kappa^{n-1}(-\frac{36\mu}{17}+\frac{2\delta}{17})} \end{aligned} \tag{A.10}$$

For the third term of (A.7), we use the properties of the smoothing operators and the fact that the Fréchet derivative, $D\mathcal{F}[u_{n-1}]$, is bounded.

$$\begin{aligned} &\|D\mathcal{F}[u_{n-1}](\mathrm{Id} - S_{t_{n-1}})\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m-\alpha} \\ &\quad\leq C\|(\mathrm{Id} - S_{t_{n-1}})\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_m \\ &\quad\leq Ct^{-15\alpha}\|\eta[u_{n-1}]\mathcal{F}[u_{n-1}]\|_{m+15\alpha} \\ &\quad\leq Ct^{-15\alpha}\|\mathcal{F}[u_{n-1}]\|_{m+16\alpha} \\ &\quad\leq C\nu e^{-15\alpha\beta\kappa^{n-1}}(1+\|u_{n-1}\|_{m+17\alpha}) \\ &\quad\leq C\nu e^{\alpha\beta\kappa^{n-1}(\delta-15)} \end{aligned} \tag{A.11}$$

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

$$C(\nu e^{-\alpha\beta\kappa^{n-1}(2(\mu-2)-\mu\kappa)} + \nu e^{-\alpha\beta\kappa^{n-1}(-\frac{2\delta}{17}+\frac{36\mu}{17}-\mu\kappa)} + e^{-\alpha\beta\kappa^{n-1}(15-\delta-\mu\kappa)}) \leq 1. \tag{A.12}$$

Condition (A.12) is true whenever ν is small enough and

$$\begin{aligned} \mu(2-\kappa) &> 4, \\ \mu(36-17\kappa) &> 2\delta, \\ 15-\mu\kappa &> \delta, \end{aligned} \tag{A.13}$$

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

Finally we note that

$$\begin{aligned} 1+\|u_n\|_{m+17\alpha} &\leq 1+\sum_{j=0}^{n-1}\|S_{t_j}\eta[u_j]\mathcal{F}[u_j]\|_{m+17\alpha} \\ &\leq 1+C\sum_{j=0}^{n-1}e^{2\alpha\beta\kappa^j}\|\eta[u_j]\mathcal{F}[u_j]\|_{m+15\alpha} \\ &\leq 1+C\sum_{j=0}^{n-1}e^{2\alpha\beta\kappa^j}\|\mathcal{F}[u_j]\|_{m+16\alpha} \\ &\leq 1+C\sum_{j=0}^{n-1}e^{2\alpha\beta\kappa^j}(1+\|u_j\|_{m+17\alpha}) \\ &\leq 1+C\sum_{j=0}^{n-1}e^{\alpha\beta(2+\delta)\kappa^j}. \end{aligned} \tag{A.14}$$

Thus

$$(1+\|u_n\|_{m+13\alpha})e^{-\delta\alpha\beta\kappa^n} \leq e^{-\delta\alpha\beta\kappa^n}+C\sum_{j=0}^{n-1}e^{\alpha\beta\kappa^j(2+\delta-\kappa\delta)} \tag{A.15}$$

To have $(p3;n)$ it suffices that the RHS of (A.15) is less than 1. If $\delta > \frac{2}{\kappa-1}$ the right side of (A.15) will be less than 1 for sufficiently large β.

If we consider $\kappa = 4/3$, $\delta = 6$, and $\mu = 61/10$ then (A.13) and

$$\delta > \frac{2}{\kappa-1} \tag{A.16}$$

are satisfied at the same time. To complete the induction, we fix β large enough so that (A.15) and (A.12) are satisfied.

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

$$\nu = \|\mathcal{F}[u_0]\|_{m-\alpha} e^{\alpha\beta\mu}. \tag{A.17}$$

From this choice of ν, together with (A.6) 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. $\square$

Note that if we assume Lipschitz dependence of $\mathcal{F}$ with respect to a parameter f in a Banach space $\mathcal{Y}$, we obtain Lipschitz dependence of the solution with respect to the parameter f.

Let $\mathcal{Y}$ be a Banach space and now assume in Theorem A.2.1 that $\tilde{\mathcal{B}}_{\Lambda,r} = \{(f,u) \in \mathcal{Y} \times (u_o + \mathcal{B}_r) | \|f - f_0\|_{\mathcal{Y}} < \Lambda\}$, for some fixed $\Lambda > 0$.

Corollary A.3.1. *Then we can consider the hypotheses of Theorem A.2.1. We also assume Lipshitz dependence with respect to the parameter f.*

$$\|\mathcal{F}[f,u] - \mathcal{F}[f',u]\|_{m-\alpha} \leq L\|f - f'\|_{\mathcal{Y}}$$

for $(f,u), (f',u) \in \tilde{\mathcal{B}}_{\Lambda,m-\alpha}$.

Then there exists a Λ such that the solution $(f, u(f))$ of $\mathcal{F}[f,u(f)] = 0$ is uniformly Lipschitz with respect to the parameter f.

Proof A.3.2. Let $(f,u(f)) \in \tilde{\mathcal{B}}_{\Lambda,m-\alpha}$ be the solution of $\mathcal{F}[f,u(f)] = 0$. Notice that for $(f',u) \in \tilde{\mathcal{B}}_{\Lambda,m-\alpha}$ then

$$\|\mathcal{F}[f',u]\|_{m-\alpha} = \|\mathcal{F}[f,u(f)] - \mathcal{F}[f',u]\|_{m-\alpha} \leq L\|f - f'\|_{\mathcal{Y}}$$

We choose Λ small enough so that by Theorem A.2.1 we have that there exists $u(f') \in \mathcal{X}^m$ so that $\mathcal{F}[f', u(f')] = 0$ and we have the Lipshitz dependence with respect to the parameter $f \in \mathcal{Y}$, i.e., for $f, f' \in \tilde{\mathcal{B}}_{\Lambda,r}$

$$\|u(f) - u(f')\|_m < CL\|f - f'\|_{\mathcal{Y}}.$$

□

Appendix B

Some remarks on the literature

Since the problem of the breakdown of analyticity has importance both in Mathematics and in Physics, there is an extensive literature on its computation.

In the following, we will describe the main methods that we know of and sketch some difference with the present method. We emphasize that we cannot claim to be systematic and give details of all the methods. In particular, we do not mention the all important issue of how can one assess the range of applicability of the methods. We certainly hope that more qualified author will make a more systematic survey.

B.1 Scalings and renormalization group

We do not discuss the (very important) phenomena that occur at breakdown. Notably, we do not cover asymptotic scalings and their explanations by a renormalization group. We just refer to [149, 123], to the survey [45], and the references there.

When scalings and renormalization group are present at breakdown, all the algorithms discussed here can be improved in two ways. First, using

the scaling relations it is possible to compute better the objects near breakdown since the scaling provides good initial points for the iterative methods. Second, using the scalings, one can post-process the results and fit powers law to the data. Furthermore, there are conjectures on the behavior of the renormalization group that show that some of these criterion are sharp, [61].

These improvements based on renormalization are very important for some of the methods and, it is quite customomary to use them. the relation of Greene's method and renormalization. Of course, when methods rely on scaling relations, they are powerless to assess whether indeed there are scalings. Fortunately, the method presented in the paper can work quite comfortably in situations when there is no scaling. The fact that there is a rigorous justification allows us to make sure that the method is working. See [37, 34] for reports on the numerical findings.

B.2 Several methods used in the literature

In this section we describe succinctly the methods that have been proposed in the literature and provide some notes on the possibility of implementing this numerically. In Section B.10 we will present some comparisons among the different methods.

Of course, the descriptions here are rather terse and the interested reader is urged to consult the original references.

B.3 Greene Method (GM)

This method was introduced in [95] for twist mappings. Partial justifications appear in [79, 142]. extensions (with justification) to complex values in [79], to non-twist mappings in [71] and to higher dimensions in [214].

The method (GM) consists in searching for periodic orbits and computing the *residue* (i.e $\frac{1}{4}(TrDf^n(x_n) - 2)$ The breakdown happens when the residue grows as n approaches to infinity. In [214] it is shown that the correct analogue in higher dimension is to study the spectrum of $Df^n(x_n)$ and to check whether all the eigenvalues remain close to 1 (equivalently, that the coefficients of the characteristic polynominal remain closer to those of $(\lambda - 1)^{2d}$.

B.4 Obstruction method (OM)

This method was introduced in [184]. The method searches for homoclinic connections between periodic orbits of nearby period. It is shown in [184] that if there is such a connection, there are no invariant circles with a rotation in the interval bounded by the rotation numbers of the periodic orbits exhibiting homoclinic connections.

In [61] it is shown that, under some hypothesis on the renormalization group appropriate for the rotation number ρ^*, the criterion is sharp in the universality class. Maps in the universality class either have an invariant circle of the a homoclinic connection between periodic orbits whose rotation numbers straddle ρ^*. Unfortunately, the renormalization theory of numbers

with bad approximation properties is not well understood.

B.5 Well ordered orbits (WOO)

In [29] it was shown that, for twist mappings, there are invariant circles if and only if the periodic orbits of all the convergents are *well ordered*. An orbit $\{x_k\}_{k\in\mathbb{Z}}$ is *well ordered* if when we fix $l, m \in \mathbb{Z}$ then for all $k \in \mathbb{Z}$ either $x_{k+m} + l \geq x_k$ or $x_{k+m} + l \leq x_k$. Computing all periodic orbits is, of course impossible, but finding a badly ordered periodic orbit, excludes the existence of invariant circles of several rotation numbers.

A preliminary assessment of the numerical efficiency of (WOO) is done in [130].

B.6 Peierls-Nabarro barrier (PNB)

In [151] it is shown that for twist mappings an invariant circle exists if and only if, the so-called Peierls-Nabarro barrier vanishes. This barrier is the difference in action between minimizers and other critical orbits of the same rotation number.

A different proof which extends to PDE's and to models with long range interactions in [67, 68, 66].

Note that lower bounds of the PN barrier can be computed just by considering the minimizing periodic orbit and another one. Of course, for irrational rotations, one needs to consider the limit. For twist mappings there

are a-priori bounds on the modulus of continuity of the PN barrier [161], so that, for twist mappings, one can, in principle, use this method to show that there are no invariant circles with a finite computation. At the moment, there do not seem to be in the literature a priori bounds.

We are not aware of any numerical implementation of these ideas.

B.7 A priori bounds for minimizers (APB)

When the mapping is a twist mapping, it was shown in [158] that invariant circles have a-priori bounds on the slope. Geometrically, this means that the circles passing through a point are contained in a cone with a-priori bounds in the slopes. The key step in the argument in the papers above is to show that the invariant circles have to be graphs over the angle coordinate. Then, one can observe that if we compose with an shear close enough to the identity, the map is still a twist map, so that the invariant circle has to be a graph over a tilted coordinate. For further improvements of this line of argument see [100, 129, 102, 13].

It was observed in [147] that, by studying carefully the maps one can show that if the a-priori bounds are satisfied in a region, then its image violates them (because the map rotates). By repeating this argument enough times (using computer assisted calculation) one can show that the circle does not exist [147].

In [139], MacKay follows theory of the calculus of variations, [178],

to prove that continuous families of critical points (an invariant circle) have to be a minimizers. This implies that the second derivative of the action along an orbit has to be positive definite. This gives a different proof to the cone criterion. Nevertheless, it is rather simple to compute orbits and decide whether the orbits are minimizers of the action.

This criterion for non-existence was shown to be sharp in [146] in the sense that, for twist maps, if there is no invariant circle, the cone method will prove this result with a finite computation.

B.8 Variational Shadowing (VS)

A method based on the variational theory of shadowing was introduced in [111]. We believe that the theory could be profitably recast in terms of viscosity sub-solutions and super-solutions of the Hamilton-Jacobi theory developed later.

This method can incorporate discussions of round off error and lead to rigorous proofs of nonexistence of invariant circles. Computer assisted results of are obtained in [111]. They produce results which seem to be extremely accurate and extremely fast. We are not aware of applications to statistical mechanics models.

B.9 The Padé method (PM)

In the case that the system is analytic and depends analytically on parameters, often one can compute some Lindstedt series expansion of the invariant torus. These series can be computed traditionally term by term, but there are also algorithms that allow to compute them by a quadratically convergent fast algorithm. It suffices to apply the quadratically convergent algorithms presented in this paper to power series. A Newton step will double the number of exact terms. Hence, it is possible to obtain polynomial approximations with high degree of accuracy.

These Lindstedt series were shown in [175] to have positive radii of analyticity when the rotation is Diophantine. The proof in [175] uses KAM methods. A later proof of convergence by exhibiting explicitly cancellations in the series was obtained [77]. The method of exhibiting explicitly cancellations in the series has lead to a very large literature, even if it is limited only to analytic systems. Among the first papers of these literature, we point out [47, 91] which deal with perturbations that do not depend on the action.

Strictly speaking, the domain of convergence of a power series expansion is a disk. Nevertheless, for analytic functions, whose domain of definition is not a disk, the power series determines the function and one can wonder whether the domain of definition of the function can be assessed from the Taylor expansion at one point.

From the numerical point of view, given a numerically computed power

series (of course, one only computes a polynomial) $F(\epsilon)$, a well known method to estimate the domain of convergence of the polynomial is to obtain a rational function $P(\epsilon)/Q(\epsilon)$ with P, Q polynomials of coefficients of degree N, M such that

$$F(\epsilon) = P(\epsilon)/Q(\epsilon) + O(\epsilon^{N+M+1}) \tag{B.1}$$

It can be readily seen that, there are unique polynomials of the indicated degrees that satisfy (B.1) and the normalization condition $Q(0) = 1$. The roots of Q give an approximation of the singularities of F.

There is a very large literature on the convergence of Padé methods for analytic functions. See, [19]. The application for the analyticity domains of KAM theory was started in [24] and they found that the domain of analyticity of the standard map is very close to a disk. The Padé method was compared with Greene's method for complex values in [78], not only for the standard map, but also for other maps with other harmonics. Further comparisons of this method with other methods were undertaken in [64, 63, 65]. In [65] one can find extensions of the method such as the multi-point Padé method.

It should be remarked that the Padé method is numerically very unstable. One can easily see that if one considers functions $F(\epsilon) = \sum_j a_j/(b_j - \epsilon)$, for which the Padé approximation indeed converges, we have that $F_n = \sum_j a_j (b_j)^{-n-1}$ so that, the poles farther away contribute much less than the closest poles. Equivalently, to get information on the poles farther away, one needs a very accurate computation of the coefficients F_n. It is, therefore, rather

fortunate that the standard map family has a domain of analyticity which is a circle.

Another problem with the Padé method is that it assumes that the singularities are poles. An easy numerical experiment – performed in [64, 65] – is to study the Padé approximants of $F(\epsilon) = \sum_j a_j/(b_j - \epsilon) + d_j\sqrt{e_j - \epsilon}$ and check whether they find the singularities b_j, e_n. It was empirically found that the square roots generate lines of zeros and poles in the Padé approximant accumulating at the branch point. This seems to generate much more instability.

Furthermore, [64, 65] presented heuristic arguments showing that one should expect that the boundary of analyticity of KAM tori is better described by an accumulation of branch points than by an accumulation of poles.

For example, if one considers periodic orbits, they satisfy an analytic equation depending on parameters, the generic bifurcation – easy to verify in many cases – is a branch point. Similarly, if one adds a small imaginary component to the frequency, one obtains that the invariance operator is compact and again, the bifurcation one expects is branch points (and indeed this is what one finds numerically). Since the analyticity domain is known to be well approximated by that of periodic orbits, see Section B.3, it follows that it is better to approximate by sums of branch points.

B.10 Comparison among the methods

Of course, in practice, all these different methods have different ranges of applicability, differ in their possibilities of extending them to other situations etc.

In the following remarks, we try to summarize some of the differences. Of course, we cannot hope to be completely systematic and, in particular, we omit many issues related to the implementation and numerical efficiency.

We concentrate on just a few issues. From the practical point of view, one question that interested us is whether the method depends on computing periodic orbits, (a task that seems to lead to be numerically difficult for some maps). In [95], following [69], it was shown that the calculation of periodic orbits is much simpler in the case that the map is *reversible*. Nevertheless, even for standard mappings with two frequencies it was shown [135] that, for some parameter values, the periodic orbits appear in complicate orders and there are many periodic orbits so that continuation methods have difficulty following them. Similar calculations were done in [78] for complex values. At the moment, it is not known if the smooth solutions for the models in statistical mechanics or in PDE's are approximated by periodic orbits.

From a more theoretical point of view it is interesting whether the method leads to conclusions after a finite computation (provided, of course, that one controls the round-off and truncation errors). In other words, whether one can turn the method into a computer assisted proof. Some of the methods

discussed in this section exclude the existence of invariant tori under a finite computation. The methods presented here, allow to conclude existence after a finite computation.

As for the conditions of applicability, we discuss whether the method depends on the system to be positive definite (as is the usual case in variational methods) or whether it is enough that the derivative of the frequency with respect of the action is invertible. Similarly, some of the methods extend to higher dimensional symplectic maps while others do not. Some methods extend to long range interactions and PDE's and others do not.

From the point of view of theoretical Physics, it is interesting to know whether the methods behave well under renormalization. Of course, the fact that there is no renormalization theory so far does not mean that there could not be one in the future.

A comparison between the methods discussed above is included in following table. We refer tho the headings of the sections for the meaning.

	GM	OM	WOO	PNB	APB	VS	Present
Conclusions after finite computation	N	$\not\exists$	$\not\exists$	$\not\exists$	$\not\exists$	$\not\exists$	$\exists$
Rigorous justification	$\Rightarrow$	$\Rightarrow$	$\Leftrightarrow$	$\Leftrightarrow$	$\Leftrightarrow$	$\Rightarrow$	$\Leftrightarrow$
Requires periodic orbits	Y	Y	Y	Y	N	N	N
Interpretation of the Renor. Group	Y	Y	N	?	?	Y	?
Requires Positive Def.	N	N	Y	Y	Y	Y	N
Long Range Models/ PDE	N	?	Y	Y	?	Y	Y

Bibliography

[1] *Dynamics and thermodynamics of systems with long-range interactions*. Springer Verlag, 2002.

[2] Juan J. Abad and Hans Koch. Renormalization and periodic orbits for Hamiltonian flows. *Comm. Math. Phys.*, 212(2):371–394, 2000.

[3] Juan J. Abad, Hans Koch, and Peter Wittwer. A renormalization group for Hamiltonians: numerical results. *Nonlinearity*, 11(5):1185–1194, 1998.

[4] Juan J. Abad, Hans Koch, and Peter Wittwer. Renormalization group analysis of Hamiltonian flows. In *XIIIth International Congress on Mathematical Physics (London, 2000)*, pages 209–216. Int. Press, Boston, MA, 2001.

[5] Milton Abramowitz and Irene A. Stegun. *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, volume 55 of *National Bureau of Standards Applied Mathematics Series*. For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 1964.

[6] Robert A. Adams. *Sobolev spaces*. Academic Press [A subsidiary of Harcourt Brace Jovanovich, Publishers], New York-London, 1975. Pure

and Applied Mathematics, Vol. 65.

[7] Eugene L. Allgower and Kurt Georg. *Introduction to numerical continuation methods*, volume 45 of *Classics in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2003. Reprint of the 1990 edition Springer-Verlag, Berlin;.

[8] Olivier Alvarez, Philippe Hoch, Yann Le Bouar, and Régis Monneau. Dislocation dynamics: short-time existence and uniqueness of the solution. *Arch. Ration. Mech. Anal.*, 181(3):449–504, 2006.

[9] Daniel J. Amit. *Field theory, the renormalization group, and critical phenomena*. McGraw-Hill International Book Co., New York, 1978. International Series in Pure and Applied Physics.

[10] Chris Anderson and Marie Dillon Dahleh. Rapid computation of the discrete Fourier transform. *SIAM J. Sci. Comput.*, 17(4):913–919, 1996.

[11] Sigurd B. Angenent. Monotone recurrence relations, their Birkhoff orbits and topological entropy. *Ergodic Theory Dynam. Systems*, 10(1):15–41, 1990.

[12] A. Apte, Rafael de la Llave, and Nikola P. Petrov. Regularity of critical invariant circles of the standard nontwist map. *Nonlinearity*, 18(3):1173–1187, 2005.

[13] Marie-Claude Arnaud. Fibrés de Green et régularité des graphes C^0-lagrangiens invariants par un flot de Tonelli. *Ann. Henri Poincaré*, 9(5):881–926, 2008.

[14] S. Aubry and P. Y. Le Daeron. The discrete Frenkel-Kontorova model and its extensions. I. Exact results for the ground-states. *Phys. D*, 8(3):381–422, 1983.

[15] S. Aubry, R. S. MacKay, and C. Baesens. Equivalence of uniform hyperbolicity for symplectic twist maps and phonon gap for Frenkel-Kontorova models. *Phys. D*, 56(2-3):123–134, 1992.

[16] Serge Aubry. Some nonlinear physics in crystallographic structures. In *Stochastic behavior in classical and quantum Hamiltonian systems (Volta Memorial Conf., Como, 1977)*, volume 93 of *Lecture Notes in Phys.*, pages 201–212. Springer, Berlin, 1979.

[17] C. Baesens and R. S. MacKay. Cantori for multiharmonic maps. *Phys. D*, 69(1-2):59–76, 1993.

[18] C. Baesens and R. S. MacKay. Cantori for multiharmonic maps. *Phys. D*, 69(1-2):59–76, 1993.

[19] George A. Baker, Jr. and Peter Graves-Morris. *Padé approximants*, volume 59 of *Encyclopedia of Mathematics and its Applications*. Cambridge University Press, Cambridge, second edition, 1996.

[20] I. Baldomá and T.M. Seara. Breakdown of heteroclinic orbits for some analytic unfoldings of the hopf-zero singularity. *Preprint*, 2005.

[21] V. Bangert. On minimal laminations of the torus. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 6(2):95–138, 1989.

[22] Peter W. Bates. On some nonlocal evolution equations arising in materials science. In *Nonlinear dynamics and evolution equations*, volume 48 of *Fields Inst. Commun.*, pages 13–52. Amer. Math. Soc., Providence, RI, 2006.

[23] A. Berretti, A. Celletti, L. Chierchia, and C. Falcolini. Natural boundaries for area-preserving twist maps. *J. Statist. Phys.*, 66(5-6):1613–1630, 1992.

[24] Alberto Berretti and Luigi Chierchia. On the complex analytic structure of the golden invariant curve for the standard map. *Nonlinearity*, 3(1):39–44, 1990.

[25] George D. Birkhoff. Dynamical systems with two degrees of freedom. *Trans. Amer. Math. Soc.*, 18(2):199–300, 1917.

[26] Stefan Blügel and Gustav Bihlmayer. Magnetism of low dimensional systems: theory. [128].

[27] Jean-Benoît Bost. Tores invariants des systèmes dynamiques hamiltoniens (d'après Kolmogorov, Arnol′d, Moser, Rüssmann, Zehnder, Her-

man, Pöschel, ...). *Astérisque*, (133-134):113–157, 1986. Seminar Bourbaki, Vol. 1984/85.

[28] Louis Boutet de Monvel, Adrien Douady, and Jean-Louis Verdier, editors. *Mathématique et physique*, volume 37 of *Progress in Mathematics*. Birkhäuser Boston, Mass., 1983. Lectures presented at the seminar held at the École Normale Supérieure, Paris, 1979/1982.

[29] Philip L. Boyland and Glen Richard Hall. Invariant circles and the order structure of periodic orbits in monotone twist maps. *Topology*, 26(1):21–35, 1987.

[30] O. M. Braun and Y. S. Kivshar. *The Frenkel-Kontorova model*. Texts and Monographs in Physics. Springer-Verlag, Berlin, 2004. Concepts, methods, and applications.

[31] Oleg M. Braun and Yuri S. Kivshar. Nonlinear dynamics of the Frenkel-Kontorova model. *Phys. Rep.*, 306(1-2):108, 1998.

[32] Xavier Cabré, Ernest Fontich, and Rafael de la Llave. The parameterization method for invariant manifolds. III. Overview and applications. *J. Differential Equations*, 218(2):444–515, 2005.

[33] R. Calleja and R. de la Llave. Fast numerical computation of quasi-periodic states in 1-D statistical mechanics, inluding twist maps. *To appear in Nonlinearity*, 2008.

[34] R. Calleja and R. de la Llave. Computation of the breakdown of analyticity in statistical mechanics models. *Preprint. Avaliable at mp_arc. http://www.ma.utexas.edu/mp_arc-bin/mpa?yn=09-56*, 2009.

[35] Renato Calleja and Rafael de la Llave. A criterion for the computation of the breakdown of analyticity in statistical mechanics models. in particular, for the breakdown of invariant circles in twist maps. *In preparation*, 2008.

[36] Renato Calleja and Rafael de la Llave. Fast numerical computation of quasi-periodic equilibrium states in 1-D statistical mechanics , including twist maps. *In preparation*, 2008.

[37] Renato Calleja and Rafael de la Llave. Fast numerical computation of quasi-peridoic equilibrium states in 1-d statistical mechanics, including twist maps. *To appear in Nonlinearity*, 2009.

[38] A. Candel and R. de la Llave. On the Aubry-Mather theory in statistical mechanics. *Comm. Math. Phys.*, 192(3):649–669, 1998.

[39] P. Cardaliaguet, F. Da Lio, N. Forcadel, and R. Monneau. Dislocation dynamics: a non-local moving boundary. In *Free boundary problems*, volume 154 of *Internat. Ser. Numer. Math.*, pages 125–135. Birkhäuser, Basel, 2007.

[40] A. Celletti and L. Chierchia. Construction of stable periodic orbits for the spin-orbit problem of celestial mechanics. *Regul. Chaotic Dyn.*,

3(3):107–121, 1998. J. Moser at 70 (Russian).

[41] A. Celletti and L. Chierchia. Quasi-periodic attractors and spin-orbit resonances. In *SPT 2007—Symmetry and perturbation theory*, pages 56–63. World Sci. Publ., Hackensack, NJ, 2008.

[42] Alessandra Celletti and Luigi Chierchia. A constructive theory of Lagrangian tori and computer-assisted applications. In *Dynamics reported*, volume 4 of *Dynam. Report. Expositions Dynam. Systems (N.S.)*, pages 60–129. Springer, Berlin, 1995.

[43] Alessandra Celletti and Luigi Chierchia. KAM stability and celestial mechanics. *Mem. Amer. Math. Soc.*, 187(878):viii+134, 2007.

[44] C. Chandre and H. R. Jauslin. Renormalization-group analysis for the transition to chaos in Hamiltonian systems. *Phys. Rep.*, 365(1):1–64, 2002.

[45] C. Chandre and H. R. Jauslin. Renormalization-group analysis for the transition to chaos in Hamiltonian systems. *Phys. Rep.*, 365(1):1–64, 2002.

[46] Xu-Yan Chen, Jack K. Hale, and Bin Tan. Invariant foliations for C^1 semigroups in Banach spaces. *J. Differential Equations*, 139(2):283–318, 1997.

[47] L. Chierchia and C. Falcolini. A direct proof of a theorem by Kolmogorov in Hamiltonian systems. *Ann. Scuola Norm. Sup. Pisa Cl. Sci. (4)*, 21(4):541–593, 1994.

[48] B. V. Chirikov. A universal instability of many-dimensional oscillator systems. *Phys. Rep.*, 52(5):264–379, 1979.

[49] Boris V. Chirikov. A universal instability of many-dimensional oscillator systems. *Phys. Rep.*, 52(5):264–379, 1979.

[50] P. Collet, J.-P. Eckmann, and H. Koch. Period doubling bifurcations for families of maps on $\mathbf{R}^n$. *J. Statist. Phys.*, 25(1):1–14, 1981.

[51] R. de la Llave. A renormalization group explanation of numerical observations of anal yticity domains. *J. Statist. Phys.*, 66(5-6):1631–1634, 1992.

[52] R. de la Llave. KAM theory for equilibrium states in 1-d statistical mechanics. *Ann. Henri Poincaré*, 9(5):835–880, 2008.

[53] R. de la Llave, E. Fontich, and Y. Sire. Construction of invariant whiskered tori by a parameterization method. part I: maps and flows in finite dimensions. *Preprint*, 2008.

[54] R. de la Llave, A. González, À. Jorba, and J. Villanueva. KAM theory without action-angle variables. *Nonlinearity*, 18(2):855–895, 2005.

[55] R. de la Llave and N. P. Petrov. Regularity of conjugacies between critical circle maps: an experimental study. *Experiment. Math.*, 11(2):219–241, 2002.

[56] R. de la Llave and N. P. Petrov. Boundaries of siegel disks – numerical studies of their dynamics and regularity. 2008. Preprint.

[57] R. de la Llave and D. Rana. Accurate strategies for K.A.M. bounds and their implementation. In *Computer aided proofs in analysis (Cincinnati, OH, 1989)*, volume 28 of *IMA Vol. Math. Appl.*, pages 127–146. Springer, New York, 1991.

[58] Rafael de la Llave. A tutorial on KAM theory. In *Smooth ergodic theory and its applications (Seattle, WA, 1999)*, pages 175–292. Amer. Math. Soc., Providence, RI, 2001.

[59] Rafael de la Llave. A tutorial on KAM theory. In *Smooth ergodic theory and its applications (Seattle, WA, 1999)*, volume 69 of *Proc. Sympos. Pure Math.*, pages 175–292. Amer. Math. Soc., Providence, RI, 2001.

[60] Rafael de la Llave. KAM theory for equilibrium states in 1-D statistical mechanics models. *Annales Henri Poincare*, 9(5):835–880, 2008.

[61] Rafael de la Llave and Arturo Olvera. The obstruction criterion for non-existence of invariant circles and renormalization. *Nonlinearity*, 19(8):1907–1937, 2006.

[62] Rafael de la Llave and Nikola P. Petrov. Regularity of conjugacies between critical circle maps: an experimental study. *Experiment. Math.*, 11(2):219–241, 2002.

[63] Rafael de la Llave and Stathis Tompaidis. Computation of domains of analyticity for some perturbative expansions of mechanics. *Phys. D*, 71(1-2):55–81, 1994.

[64] Rafael de la Llave and Stathis Tompaidis. Nature of singularities for analyticity domains of invariant curves. *Phys. Rev. Lett.*, 73(11):1459–1463, 1994.

[65] Rafael de la Llave and Stathis Tompaidis. On the singularity structure of invariant curves of symplectic mappings. *Chaos*, 5(1):227–237, 1995.

[66] Rafael de la Llave and Enrico Valdinoci. Critical points inside the gaps of ground state laminations for some models in statistical mechanics. *J. Stat. Phys.*, 129(1):81–119, 2007.

[67] Rafael de la Llave and Enrico Valdinoci. Ground states and critical points for generalized Frenkel-Kontorova models in $\mathbb{Z}^d$. *Nonlinearity*, 20(10):2409–2424, 2007.

[68] Rafael de la Llave and Enrico Valdinoci. Multiplicity results for interfaces of Ginzburg-Landau-Allen-Cahn equations in periodic media. *Adv. Math.*, 215(1):379–426, 2007.

[69] René De Vogelaere. On the structure of symmetric periodic solutions of conservative systems, with applications. In *Contributions to the theory of nonlinear oscillations, Vol. IV*, Annals of Mathematics Studies, no 41, pages 53–84. Princeton University Press, Princeton, N.J., 1958.

[70] D. del Castillo-Negrete, J. M. Greene, and P. J. Morrison. Area preserving nontwist maps: periodic orbits and transition to chaos. *Phys. D*, 91(1-2):1–23, 1996.

[71] Amadeu Delshams and Rafael de la Llave. KAM theory and a partial justification of Greene's criterion for nontwist maps. *SIAM J. Math. Anal.*, 31(6):1235–1269 (electronic), 2000.

[72] Amadeu Delshams and Rafael Ramírez-Ros. Melnikov potential for exact symplectic maps. *Comm. Math. Phys.*, 190(1):213–245, 1997.

[73] R. Douady. Une démonstration directe de l'équivalence des théorèmes de tores invariants pour difféomorphismes et champs de vecteurs. *C. R. Acad. Sci. Paris Sér. I Math.*, 295(2):201–204, 1982.

[74] A. Dutt and V. Rokhlin. Fast Fourier transforms for nonequispaced data. *SIAM J. Sci. Comput.*, 14(6):1368–1393, 1993.

[75] Freeman J. Dyson. An Ising ferromagnet with discontinuous long-range order. *Comm. Math. Phys.*, 21:269–283, 1971.

[76] J.-P. Eckmann, H. Koch, and P. Wittwer. A computer-assisted proof of universality for area-preserving maps. *Mem. Amer. Math. Soc.*, 47(289):vi+122, 1984.

[77] L. H. Eliasson. Absolutely convergent series expansions for quasi periodic motions. *Math. Phys. Electron. J.*, 2:Paper 4, 33 pp. (electronic), 1996.

[78] Corrado Falcolini and Rafael de la Llave. Numerical calculation of domains of analyticity for perturbation theories in the presence of small divisors. *J. Statist. Phys.*, 67(3-4):645–666, 1992.

[79] Corrado Falcolini and Rafael de la Llave. A rigorous partial justification of Greene's criterion. *J. Statist. Phys.*, 67(3-4):609–643, 1992.

[80] A. Fathi, A. Giuliani, and A. Sorrentino. Uniqueness of invariant lagrangian graphs in a homology or a cohomology class. *Preprint. Available at mp_arc. http://www.ma.utexas.edu/mp_arc-bin/mpa?yn=08-18*, 2008.

[81] Neil Fenichel. Persistence and smoothness of invariant manifolds for flows. *Indiana Univ. Math. J.*, 21:193–226, 1971/1972.

[82] E. Fermi, J. Pasta, and S. Ulam. Studies on nonlinear problems. *Document LA 1940*, 1955.

[83] J. Frenkel and T. Kontorova. On the theory of plastic deformation and twinning. *Acad. Sci. U.S.S.R. J. Phys.*, 1:137–149, 1939.

[84] G. Friesecke and R. L. Pego. Solitary waves on FPU lattices. I. Qualitative properties, renormalization and continuum limit. *Nonlinearity*, 12(6):1601–1627, 1999.

[85] G. Friesecke and R. L. Pego. Solitary waves on FPU lattices. II. Linear implies nonlinear stability. *Nonlinearity*, 15(4):1343–1359, 2002.

[86] G. Friesecke and R. L. Pego. Solitary waves on Fermi-Pasta-Ulam lattices. III. Howland-type Floquet theory. *Nonlinearity*, 17(1):207–227, 2004.

[87] G. Friesecke and R. L. Pego. Solitary waves on Fermi-Pasta-Ulam lattices. IV. Proof of stability at low energy. *Nonlinearity*, 17(1):229–251, 2004.

[88] Gero Friesecke and Jonathan A. D. Wattis. Existence theorem for solitary waves on lattices. *Comm. Math. Phys.*, 161(2):391–418, 1994.

[89] Matteo Frigo and Steven G. Johnson. The design and implementation of FFTW3. *Proceedings of the IEEE*, 93(2):216–231, 2005. special issue on "Program Generation, Optimization, and Platform Adaptation".

[90] Denis Gaidashev and Hans Koch. Renormalization and shearless invariant tori: numerical results. *Nonlinearity*, 17(5):1713–1722, 2004.

[91] Giovanni Gallavotti. Twistless KAM tori, quasi flat homoclinic intersections, and other cancellations in the perturbation series of certain

completely integrable Hamiltonian systems. A review. *Rev. Math. Phys.*, 6(3):343–411, 1994.

[92] Johannes Giannoulis and Alexander Mielke. The nonlinear Schrödinger equation as a macroscopic limit for an oscillator chain with cubic nonlinearities. *Nonlinearity*, 17(2):551–565, 2004.

[93] Gene H. Golub and Charles F. Van Loan. *Matrix computations*. Johns Hopkins Studies in the Mathematical Sciences. Johns Hopkins University Press, Baltimore, MD, third edition, 1996.

[94] A. González-Enríquez and R. de la Llave. Analytic smoothing of geometric maps with applications to KAM theory. *J. Differential Equations*, 245(5):1243–1298, 2008.

[95] John M. Greene. A method for determining a stochastic transition. *Journal of Mathematical Physics*, 20(6):1183–1201, 1979.

[96] O. H. Hald. On a Newton-Moser type method. *Numer. Math.*, 23:411–426, 1975.

[97] Richard S. Hamilton. The inverse function theorem of Nash and Moser. *Bull. Amer. Math. Soc. (N.S.)*, 7(1):65–222, 1982.

[98] A. Haro and R. de la Llave. A parametrization method for the computation of invariant tori and their whiskers in quasi-periodic maps: Rigorous results. *J. Diff. Eq.*, 228(2):530–579, 2006.

[99] A. Haro and R. de la Llave. A parameterization method for the computation of invariant tori and their whiskers in quasi-periodic maps: explorations and mechanisms for the breakdown of hyperbolicity. *SIAM J. Appl. Dyn. Syst.*, 6(1):142–207 (electronic), 2007.

[100] Michael-R. Herman. *Sur les courbes invariantes par les difféomorphismes de l'anneau. Vol. 1*, volume 103 of *Astérisque*. Société Mathématique de France, Paris, 1983. With an appendix by Albert Fathi, With an English summary.

[101] Michael-R. Herman. Sur les courbes invariantes par les difféomorphismes de l'anneau. Vol. 2. *Astérisque*, (144):248, 1986. With a correction to: *On the curves invariant under diffeomorphisms of the annulus, Vol. 1* (French) [Astérisque No. 103-104, Soc. Math. France, Paris, 1983; MR0728564 (85m:58062)].

[102] Michael-R. Herman. Inégalités "a priori" pour des tores lagrangiens invariants par des difféomorphismes symplectiques. *Inst. Hautes Études Sci. Publ. Math.*, (70):47–101 (1990), 1989.

[103] Lars Hörmander. On the Nash-Moser implicit function theorem. *Ann. Acad. Sci. Fenn. Ser. A I Math.*, 10:255–259, 1985.

[104] Gemma Huguet, Rafael de la Llave, and Yannick Sire. Fast numerical algorithms for the computation
of invariant tori in hamiltonian systems. *Preprint*, 2008.

[105] Gérard Iooss and Moritz Adelmeyer. *Topics in bifurcation theory and applications*, volume 3 of *Advanced Series in Nonlinear Dynamics*. World Scientific Publishing Co. Inc., River Edge, NJ, second edition, 1998.

[106] Gérard Iooss and Klaus Kirchgässner. Travelling waves in a chain of coupled nonlinear oscillators. *Comm. Math. Phys.*, 211(2):439–464, 2000.

[107] Gérard Iooss and Eric Lombardi. Polynomial normal forms with exponentially small remainder for analytic vector fields. *J. Differential Equations*, 212(1):1–61, 2005.

[108] Guillaume James and Yannick Sire. Travelling breathers with exponentially small tails in a chain of nonlinear oscillators. *Comm. Math. Phys.*, 257(1):51–85, 2005.

[109] Guillaume James and Yannick Sire. Travelling breathers with exponentially small tails in a chain of nonlinear oscillators. *Comm. Math. Phys.*, 257(1):51–85, 2005.

[110] I. Jungreis. A method for proving that monotone twist maps have no invariant circles. *Ergodic Theory Dynam. Systems*, 11(1):79–84, 1991.

[111] Irwin Jungreis. A method for proving that monotone twist maps have no invariant circles. *Ergodic Theory Dynam. Systems*, 11(1):79–84, 1991.

[112] Leo P. Kadanoff. *Statistical physics*. World Scientific Publishing Co. Inc., River Edge, NJ, 2000. Statics, dynamics and renormalization.

[113] L.P. Kadanoff. Renormalization equations: Conceptual basis and a simple example. In J.D. Gunton and M.S. Green, editors, *Renormalization Group in Critical Phenomena and Quantum Field Theory*, pages 21–38. Temple University Press, 1973.

[114] L.P. Kadanoff. Scaling, universality, and operator algebras. In C. Domb and M.S. Green, editors, *Phase Transitions and Critical Phenomena*, volume 5A. Academic Press, 1976.

[115] Tosio Kato. *Perturbation theory for linear operators*. Classics in Mathematics. Springer-Verlag, Berlin, 1995. Reprint of the 1980 edition.

[116] J. A. Ketoja and R. S. MacKay. Fractal boundary for the existence of invariant circles for area-preserving maps: observations and renormalisation explanation. *Phys. D*, 35(3):318–334, 1989.

[117] J. A. Ketoja and R. S. MacKay. Rotationally-ordered periodic orbits for multiharmonic area-preservin g twist maps. *Phys. D*, 73(4):388–398, 1994.

[118] J. A. Ketoja and R. S. MacKay. Rotationally-ordered periodic orbits for multiharmonic area-preserving twist maps. *Phys. D*, 73(4):388–398, 1994.

[119] Jukka A. Ketoja. Breakup of Kolmogorov-Arnol′d-Moser tori of arbitrary frequency in a two-parameter system. *Phys. Rev. A (3)*, 42(2):775–780, 1990.

[120] Donald E. Knuth. *The art of computer programming. Vol. 2.* Addison-Wesley Publishing Co., Reading, Mass., second edition, 1981. Seminumerical algorithms, Addison-Wesley Series in Computer Science and Information Processing.

[121] Hans Koch. A renormalization group for Hamiltonians, with applications to KAM tori. *Ergodic Theory Dynam. Systems*, 19(2):475–521, 1999.

[122] Hans Koch. A renormalization group fixed point associated with the breakup of golden invariant tori. *Discrete Contin. Dyn. Syst.*, 11(4):881–909, 2004.

[123] Hans Koch. A renormalization group fixed point associated with the breakup of golden invariant tori. *Discrete Contin. Dyn. Syst.*, 11(4):881–909, 2004.

[124] Hans Koch, Rafael de la Llave, and Charles Radin. Aubry-Mather theory for functions on lattices. *Discrete Contin. Dynam. Systems*, 3(1):135–151, 1997.

[125] A. N. Kolmogorov. On conservation of conditionally periodic motions for a small change in Hamilton's function. *Dokl. Akad. Nauk SSSR (N.S.)*, 98:527–530, 1954.

[126] Hyung-tae Kook and James D. Meiss. Periodic orbits for reversible, symplectic mappings. *Phys. D*, 35(1-2):65–86, 1989.

[127] S. M. Kozlov. Reducibility of quasiperiodic differential operators and averaging. *Trudy Moskov. Mat. Obshch.*, 46:99–123, 1983.

[128] Helmut Kronmüller and Stuart S. P. Parkin, editors. *Handbook of magnetism and advanced magnetic materials: Vol I Fundamentals and Theory*. John Willey, Chichester, 2007.

[129] Patrice Le Calvez. Propriétés dynamiques des difféomorphismes de l'anneau et du tore. *Astérisque*, (204):131, 1991.

[130] I. Leage and R. S. MacKay. Badly ordered periodic orbits of the standard map. *Phys. Lett. A*, 118(6):274–278, 1986.

[131] M. Levi and J. Moser. A Lagrangian proof of the invariant curve theorem for twist mappings. In *Smooth ergodic theory and its applications (Seattle, WA, 1999)*, volume 69 of *Proc. Sympos. Pure Math.*, pages 733–746. Amer. Math. Soc., Providence, RI, 2001.

[132] R. de la Llave. A tutorial on KAM theory. In *Smooth Ergodic Theory and Its Applications (Seattle, WA, 1999)*, pages 175–292. Amer. Math. Soc., Providence, RI, 2001.

[133] Eric Lombardi. Phenomena beyond all orders and bifurcations of reversible homoclinic connections near higher resonances. In *Peyresq lectures on nonlinear phenomena (Peyresq, 1998/1999)*, pages 161–200. World Sci. Publ., River Edge, NJ, 2000.

[134] H. E. Lomelí and J. D. Meiss. Heteroclinic intersections between invariant circles of volume-preserving maps. *Nonlinearity*, 16(5):1573–1595, 2003.

[135] Héctor E. Lomelí and Renato Calleja. Heteroclinic bifurcations and chaotic transport in the two-harmonic standard map. *Chaos*, 16(2):023117, 8, 2006.

[136] Héctor E. Lomelí and James D. Meiss. Heteroclinic primary intersections and codimension one Melnikov method for volume-preserving maps. *Chaos*, 10(1):109–121, 2000. Chaotic kinetics and transport (New York, 1998).

[137] R. S. MacKay. A renormalisation approach to invariant circles in area-preserving maps. *Phys. D*, 7(1-3):283–300, 1983. Order in chaos (Los Alamos, N.M., 1982).

[138] R. S. MacKay. Converse KAM theory. In *Singular behavior and nonlinear dynamics, Vol. 1 (Sámos, 1988)*, pages 109–113. World Sci. Publ., Teaneck, NJ, 1989.

[139] R. S. MacKay. A criterion for nonexistence of invariant tori for Hamiltonian systems. *Phys. D*, 36(1-2):64–82, 1989.

[140] R. S. MacKay. Scaling exponents at the transition by breaking of analyticity for in commensurate structures. *Phys. D*, 50(1):71–79, 1991.

[141] R. S. MacKay. Scaling exponents at the transition by breaking of analyticity for incommensurate structures. *Phys. D*, 50(1):71–79, 1991.

[142] R. S. MacKay. Greene's residue criterion. *Nonlinearity*, 5(1):161–187, 1992.

[143] R. S. MacKay. Greene's residue criterion. *Nonlinearity*, 5(1):161–187, 1992.

[144] R. S. MacKay and S. Aubry. Proof of existence of breathers for time-reversible or Hamiltonian networks of weakly coupled oscillators. *Nonlinearity*, 7(6):1623–1643, 1994.

[145] R. S. MacKay, J. D. Meiss, and J. Stark. Converse KAM theory for symplectic twist maps. *Nonlinearity*, 2(4):555–570, 1989.

[146] R. S. MacKay, J. D. Meiss, and J. Stark. Converse KAM theory for symplectic twist maps. *Nonlinearity*, 2(4):555–570, 1989.

[147] R. S. MacKay and I. C. Percival. Converse KAM: theory and practice. *Comm. Math. Phys.*, 98(4):469–512, 1985.

[148] R. S. MacKay and C. Tresser. Badly ordered orbits of circle maps. *Math. Proc. Cambridge Philos. Soc.*, 96(3):447–451, 1984.

[149] R.S. MacKay. *Renormalisation in area preserving maps.* PhD thesis, Princeton Univ., 1982.

[150] J. N. Mather. Destruction of invariant circles. *Ergodic Theory Dynam. Systems*, 8*(Charles Conley Memorial Issue):199–214, 1988.

[151] John Mather. A criterion for the nonexistence of invariant circles. *Inst. Hautes Études Sci. Publ. Math.*, (63):153–204, 1986.

[152] John N. Mather. Concavity of the Lagrangian for quasiperiodic orbits. *Comment. Math. Helv.*, 57(3):356–376, 1982.

[153] John N. Mather. Existence of quasiperiodic orbits for twist homeomorphisms of the annulus. *Topology*, 21(4):457–467, 1982.

[154] John N. Mather. Existence of quasiperiodic orbits for twist homeomorphisms of the annulus. *Topology*, 21(4):457–467, 1982.

[155] John N. Mather. Glancing billiards. *Ergodic Theory Dynam. Systems*, 2(3-4):397–403 (1983), 1982.

[156] John N. Mather. Nonuniqueness of solutions of Percival's Euler-Lagrange equation. *Comm. Math. Phys.*, 86(4):465–473, 1982.

[157] John N. Mather. Amount of rotation about a point and the Morse index. *Comm. Math. Phys.*, 94(2):141–153, 1984.

[158] John N. Mather. Nonexistence of invariant circles. *Ergodic Theory Dynam. Systems*, 4(2):301–309, 1984.

[159] John N. Mather. More Denjoy minimal sets for area preserving diffeomorphisms. *Comment. Math. Helv.*, 60(4):508–557, 1985.

[160] John N. Mather. Dynamics of area preserving maps. In *Proceedings of the International Congress of Mathematicians, Vol. 1, 2 (Berkeley, Calif., 1986)*, pages 1190–1194, Providence, RI, 1987. Amer. Math. Soc.

[161] John N. Mather. Modulus of continuity for Peierls's barrier. In *Periodic solutions of Hamiltonian systems and related topics (Il Ciocco, 1986)*, volume 209 of *NATO Adv. Sci. Inst. Ser. C Math. Phys. Sci.*, pages 177–202. Reidel, Dordrecht, 1987.

[162] John N. Mather. Destruction of invariant circles. *Ergodic Theory Dynam. Systems*, 8*(Charles Conley Memorial Issue):199–214, 1988.

[163] John N. Mather. Destruction of invariant circles. *Ergodic Theory Dynam. Systems*, 8*(Charles Conley Memorial Issue):199–214, 1988.

[164] John N. Mather. Minimal measures. *Comment. Math. Helv.*, 64(3):375–394, 1989.

[165] John N. Mather and Giovanni Forni. Action minimizing orbits in Hamiltonian systems. In *Transition to chaos in classical and quantum mechanics (Montecatini Terme, 1991)*, volume 1589 of *Lecture Notes in Math.*, pages 92–186. Springer, Berlin, 1994.

[166] John N. Mather and Giovanni Forni. Action minimizing orbits in Hamiltonian systems. In *Transition to chaos in classical and quantum me-*

chanics (Montecatini Terme, 1991), volume 1589 of *Lecture Notes in Math.*, pages 92–186. Springer, Berlin, 1994.

[167] Daniel C. Mattis. *The theory of Magnetism made simple.* World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2006.

[168] J. D. Meiss. Symplectic maps, variational principles, and transport. *Rev. Modern Phys.*, 64(3):795–848, 1992.

[169] B. Mestel. *A computer assisted proof of universality for Cubic critical mapsof t he circle with Golden mean rotation number.* PhD thesis, University of Warwick, 1984.

[170] Alexander Mielke. Über maximale L^p-Regularität für Differentialgleichungen in Banach- und Hilbert-Räumen. *Math. Ann.*, 277(1):121–133, 1987.

[171] Jürgen Moser. New results on the stability of periodic motions. In *Proc. Internat. Congr. Mathematicians (Stockholm, 1962)*, pages 584–586. Inst. Mittag-Leffler, Djursholm, 1963.

[172] Jürgen Moser. New results on the stability of periodic motions. In *Proc. Internat. Congr. Mathematicians (Stockholm, 1962)*, pages 584–586. Inst. Mittag-Leffler, Djursholm, 1963.

[173] Jürgen Moser. A rapidly convergent iteration method and non-linear differential equations. II. *Ann. Scuola Norm. Sup. Pisa (3)*, 20:499–535, 1966.

[174] Jürgen Moser. A rapidly convergent iteration method and non-linear partial differential equations. I. *Ann. Scuola Norm. Sup. Pisa (3)*, 20:265–315, 1966.

[175] Jürgen Moser. Convergent series expansions for quasi-periodic motions. *Math. Ann.*, 169:136–176, 1967.

[176] Jürgen Moser. On the construction of almost periodic solutions for ordinary differential equations. In *Proc. Internat. Conf. on Functional Analysis and Related Topics (Tokyo, 1969)*, pages 60–67. Univ. of Tokyo Press, Tokyo, 1970.

[177] Jürgen Moser. On the construction of almost periodic solutions for ordinary differential equations. In *Proc. Internat. Conf. on Functional Analysis and Related Topics (Tokyo, 1969)*, pages 60–67. Univ. of Tokyo Press, Tokyo, 1970.

[178] Jürgen Moser. Monotone twist mappings and the calculus of variations. *Ergodic Theory Dynam. Systems*, 6(3):401–413, 1986.

[179] Jürgen K. Moser. Lectures on Hamiltonian systems. In *Mem. Amer. Math. Soc. No. 81*, page 60. Amer. Math. Soc., Providence, R.I., 1968.

[180] John Nash. The imbedding problem for Riemannian manifolds. *Ann. of Math. (2)*, 63:20–63, 1956.

[181] A. Olvera and N.P. Petrov. Regularity properties of critical invariant circles of twist maps, and their universality. *SIAM J. Appl. Dyn. Syst.*, 2008.

[182] A. Olvera and C. Simó. An obstruction method for the destruction of invariant curves. *Phys. D*, 26(1-3):181–192, 1987.

[183] Arturo Olvera and Carles Simó. The obstruction method and some numerical experiments related to the standard map. In *Periodic solutions of Hamiltonian systems and related topics (Il Ciocco, 1986)*, pages 235–244. Reidel, Dordrecht, 1987.

[184] Arturo Olvera and Carles Simó. An obstruction method for the destruction of invariant curves. *Phys. D*, 26(1-3):181–192, 1987.

[185] I. C. Percival. Variational principles for the invariant toroids of classical dynamics. *J. Phys. A*, 7:794–802, 1974.

[186] I. C. Percival. A variational principle for invariant tori of fixed frequency. *J. Phys. A*, 12(3):L57–L60, 1979.

[187] Henri Poincaré. *New methods of celestial mechanics. Vol. 1-3*, volume 13 of *History of Modern Physics and Astronomy*. American Institute of Physics, New York, 1993. Translated from the French, Revised reprint of the 1967 English translation, With endnotes by V. M. Alekseev, Edited and with an introduction by Daniel L. Goroff.

[188] Jürgen Pöschel. On elliptic lower-dimensional tori in Hamiltonian systems. *Math. Z.*, 202(4):559–608, 1989.

[189] George Tibor Rado and Harry Shul, editors. *Magnetism, Vol IIB*. Academic Press, New York, 1963.

[190] D. Rana. *Proof of Accurate Upper and Lower Bounds to Stability Domains in Small Denominator Problems*. PhD thesis, Princeton Univ., 1987.

[191] Michel Remoissenet. Low-amplitude breather and envelope solitons in quasi-one-dimensional physicsl models. *Phys. Rev. B*, 33(4):2386–2392, 1986.

[192] David Ruelle. *Statistical mechanics*. World Scientific Publishing Co. Inc., River Edge, NJ, 1999. Rigorous results, Reprint of the 1989 edition.

[193] Helmut Rüssmann. On optimal estimates for the solutions of linear partial differential equations of first order with constant coefficients on the torus. In *Dynamical systems, theory and applications (Rencontres, Battelle Res. Inst., Seattle, Wash., 1974)*, pages 598–624.Lecture Notes in Phys., Vol. 38. Springer, Berlin, 1975.

[194] Helmut Rüssmann. Note on sums containing small divisors. *Comm. Pure Appl. Math.*, 29(6):755–758, 1976.

[195] Yousef Saad. *Iterative methods for sparse linear systems*. Society for Industrial and Applied Mathematics, Philadelphia, PA, second edition, 2003.

[196] D. Salamon and E. Zehnder. KAM theory in configuration space. *Comment. Math. Helv.*, 64(1):84–132, 1989.

[197] J. Schwartz. On Nash's implicit functional theorem. *Comm. Pure Appl. Math.*, 13:509–530, 1960.

[198] J. T. Schwartz. *Nonlinear functional analysis*. Gordon and Breach Science Publishers, New York, 1969. Notes by H. Fattorini, R. Nirenberg and H. Porta, with an additional chapter by Hermann Karcher, Notes on Mathematics and its Applications.

[199] Francis Sergeraert. Un théorème de fonctions implicites. Applications. *Ann. Inst. Fourier (Grenoble)*, 23(2):151–157, 1973. Colloque International sur l'Analyse et la Topologie Différentielle (Colloq. Internat. CNRS, No. 210, Strasbourg, 1972).

[200] B. I. Shraiman. Transition from quasiperiodicity to chaos: a perturbative renormalization-group approach. *Phys. Rev. A (3)*, 29(6):3464–3466, 1984.

[201] Carl Ludwig Siegel. Iteration of analytic functions. *Ann. of Math. (2)*, 43:607–612, 1942.

[202] Yannick Sire. Travelling breathers in Klein-Gordon lattices as homoclinic orbits to p-tori. *J. Dynam. Differential Equations*, 17(4):779–823, 2005.

[203] Yannick Sire. Travelling breathers in Klein-Gordon lattices as homoclinic orbits to p-tori. *J. Dynam. Differential Equations*, 17(4):779–823, 2005.

[204] Yannick Sire and Guillaume James. Travelling breathers in Klein-Gordon chains. *C. R. Math. Acad. Sci. Paris*, 338(8):661–666, 2004.

[205] Yannick Sire and Guillaume James. Travelling breathers in Klein-Gordon chains. *C. R. Math. Acad. Sci. Paris*, 338(8):661–666, 2004.

[206] Yannick Sire and Guillaume James. Numerical computation of travelling breathers in Klein-Gordon chains. *Phys. D*, 204(1-2):15–40, 2005.

[207] J. Stark. An exhaustive criterion for the nonexistence of invariant circles for area-preserving twist maps. *Comm. Math. Phys.*, 117(2):177–189, 1988.

[208] Jaroslav Stark. Determining the critical transition for circles of arbitrary rotation number. *Phys. Lett. A*, 163(4):258–265, 1992.

[209] Elias M. Stein. *Singular integrals and differentiability properties of functions*. Princeton Mathematical Series, No. 30. Princeton University Press, Princeton, N.J., 1970.

[210] Andreas Stirnemann. Towards an existence proof of MacKay's fixed point. *Comm. Math. Phys.*, 188(3):723–735, 1997.

[211] Eduardo Tabacman. Variational computation of homoclinic orbits for twist maps. *Phys. D*, 85(4):548–562, 1995.

[212] Michael E. Taylor. *Partial differential equations. III*, volume 117 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1997. Nonlinear equations, Corrected reprint of the 1996 original.

[213] Stathis Tompaidis. Approximation of invariant surfaces by periodic orbits in high-dimens ional maps: some rigorous results. *Experiment. Math.*, 5(3):197–209, 1996.

[214] Stathis Tompaidis. Approximation of invariant surfaces by periodic orbits in high-dimensional maps: some rigorous results. *Experiment. Math.*, 5(3):197–209, 1996.

[215] Stathis Tompaidis. Numerical study of invariant sets of a quasiperiodic perturbation of a symplectic map. *Experiment. Math.*, 5(3):211–230, 1996.

[216] A. Vanderbauwhede and G. Iooss. Center manifold theory in infinite dimensions. In *Dynamics reported: expositions in dynamical systems*, volume 1 of *Dynam. Report. Expositions Dynam. Systems (N.S.)*, pages 125–163. Springer, Berlin, 1992.

[217] A. P. Veselov. Integrable mappings. *Uspekhi Mat. Nauk*, 46(5(281)):3–45, 190, 1991.

[218] J. C. Ward. An identity in quantum eletrodynamics. *Physical Rev. (2)*, 78:182, 1950.

[219] J. Wilbrink. Erratic behaviour of invariant circles in standard-like mappings. *Physica*, 26D:358–368, 1987.

[220] E. Zehnder. Generalized implicit function theorems with applications to some small divisor problems. I. *Comm. Pure Appl. Math.*, 28:91–140, 1975.

[221] E. Zehnder. Generalized implicit function theorems with applications to some small divisor problems. II. *Comm. Pure Appl. Math.*, 29(1):49–111, 1976.

[222] Eduard Zehnder. Moser's implicit function theorem in the framework of analytic smoothing. *Math. Ann.*, 219(2):105–121, 1976.

[223] Albert B. Zisook and Scott J. Shenker. Renormalization group for intermittency in area-preserving mappings. *Phys. Rev. A (3)*, 25(5):2824–2826, 1982.

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Vita

Renato Calleja was born close to the town of Coyocan in Mexico City on 12 November 1978, the son of Juan Manuel Calleja Montes de Oca and Alma A. Castillo Gutierrez. He received the Bachelor in Science degree in Applied Mathematics from the Instituto Tecnológico Autónomo de México. The first day of classes at ITAM he met Claudia Masferrer in a Computing class.

While studying at ITAM, he spent a semester abroad in Barcelona, Spain, where he met many experts in dynamical systems theory including his Ph.D. advisor, Rafael de la Llave. Back in Mexico, Renato wrote an honors thesis about global heteroclinic bifurcations of the biharmonic standard map under the supervision of Hector Lomelí.

In the summer of 2004, Renato travelled to Austin, Texas to enter the Ph. D. program in Mathematics. In the summer of 2007, Claudia joined him to pursue a M.A. in Statistics with concentration in Sociological Sciences and Demography.

In the summer of 2009, Claudia and Renato will move to Montreal. Renato will be a postdoc at the Mathematics Department of McGill University. Claudia will pursue a Ph.D. in the Sociology Department.

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