A PARAMETERIZATION METHOD FOR THE COMPUTATION OF INVARIANT TORI AND THEIR WHISKERS IN QUASI-PERIODIC MAPS: NUMERICAL ALGORITHMS.

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Abstract. We develop numerical algorithms for the computation of invariant manifolds in quasi-periodically forced systems.

We show how to compute invariant tori and invariant manifolds associated to them. In particular, the stable and unstable manifolds of invariant tori, but also *non-resonant* invariant manifolds associated to spaces invariant under the linearization. These non-resonant manifolds include the slow manifolds which dominate the asymptotic behavior.

The algorithms are based on the parameterization method. Rigorous results about this method are proved in [HdlL01b]. In this paper, we concentrate on numerical issues of algorithm. Examples of implementations of the algorithms appear in the companion paper [HdlL01a].

1. Introduction: quasi-periodically forced systems and invariant manifolds.

In this paper we develop numerical algorithms for the computation of invariant manifolds in quasi-periodically forced systems.

The algorithms we present compute quasiperiodic *invariant tori* as well as *whiskers* around these tori. See respectively, Section 3 and Section 6.

In this paper, invariant tori will always mean a torus in which the motion is quasi-periodic. Whiskers of an invariant torus are invariant manifolds that contain the torus and characterized by the fact that they are tangent to a chosen invariant space of the linearization around the torus. It is obvious that the tangent spaces of invariant manifolds are invariant under the linearization. There is kind of converse to this observation. It has been show that provided that the rates of expansion of the linearization on an invariant space satisfy some non-resonance condition, then there is a smooth invariant manifold. We note that the usual (un)stable and strong (un)stable manifolds satisfy automatically these non-resonance conditions. Hence, in particular, we develop algorithms to compute stable and unstable manifolds. We can, however compute other invariant manifolds which include sometimes the *slow* invariant manifolds which are associated to the less contractive (or less expansive) space and, hence, control the approach to this stationary state.

In applications, one often has to consider a system subject to quasi-periodic perturbations. In this case, hyperbolic periodic orbits (in particular stable steady states) of the original system, persist as quasi-periodic orbits in the perturbed system. Moreover, the stable and unstable manifolds of the periodic orbits persist as stable and unstable manifolds of the quasi-periodic orbit. The persistence of these manifolds can be proved using the theory of normally hyperbolic manifolds. Classic works in this area are

[HP70, Fen72, Fen74, Fen77, HPS77]. We remark, however, that taking into account that the dynamics on the torus is a rotation, one can improve significantly the results of the general theory. In particular, one can improve the regularity and show that, when the map is analytic, the varieties remain analytic. Normally hyperbolic rotational tori are shown in [HdlL01b] to depend analytic dependence on parameters. As it is well known, these results are false for more general normally hyperbolic manifolds, for which the bundles are only finitely differentiable and there is only finite differentiability with respect to parameters.

Besides the usual stable and unstable manifolds, one is often interested in other invariant manifolds. For example, when we consider an stable steady state, the manifolds that govern the asymptotic behavior of the convergence to the stable steady state are the manifolds associated to the least stable eigenvalue. Even if these manifolds associated to an invariant space are not always smooth, provided that the eigenvalues satisfy certain non-resonance assumptions, it has been shown in [dlL97, ElB01, CFdlL03a, CFdlL03b, dlL03] that one can associate smooth invariant slow manifolds to this invariant spaces. When a system is perturbed quasi-periodically, the stable steady state persists and so do the non-resonant invariant manifolds. The persistence of these manifolds under quasi-periodic perturbations is studied rigorously in [HdlL01b].

The method we use is the parameterization method – we will describe it in more detail in Section 1.1 – which seeks to study functional equations of a parameterization of the invariant manifold. As we will see later, the parameterization method has important numerical advantages since it allows to work with functions of an small number of variables (we only need to deal with functions of d variables to compute objects of dimension d). As it is remarked in [HdlL01b], the functional equations to be solved have the advantage that they are differentiable in the unknowns. Hence, one can use methods based on the derivatives and use the differentiability in estimates etc. This allows to derive efficient numerical algorithms and to asses the reliability.

A theory of these invariant manifolds for quasi-periodic systems (in particular, quasi-periodic perturbation) is developed in [HdlL01b]. The theory of [HdlL01b], takes advantage of the fact that the system restricted to the torus is a rotation and obtains regularity results that are false for general normally hyperbolic manifolds. The theory in [HdlL01b] is developed very closely to the methods whose implementation we describe here. We will refer to [HdlL01b] for mathematical details. We will not repeat the mathematical details since the goal of this paper is numerical algorithms. On the other hand, we will briefly summarize in the following Section 1.1 the equations we will consider and summarize their geometric meaning.

One of the consequences of the theory in [HdlL01b] is that the algorithms satisfy *a posteriori bounds*. That is, if we compute an object that satisfy a functional equation up to an small accuracy and can show that it satisfy

some non-degeneracy assumptions, we can conclude that there exists an exact solution and that the distance from the exact solution to the computed one is bounded by the error in the solution of the functional equation.

This paper is organized as follows: In Section 1.1 we will present some generalities on the parameterization method. In particular, we present the functional equations we will be studying. In Section 2 we will present some generalities on the numerical algorithms and some general purpose numerical algorithms for nonlinear problems (e.g. the Newton method) applied to our case. We will also discuss the choices of discretizations consider. More sophisticated algorithms that take advantage of the structure of the problem, its geometry and special features such as reducibility are discussed in Section 3 and Section 6. These sections also include discussions of computation of other invariant objects such as invariant subbundles. The details of concrete implementations of these algorithms as well as representative results are discussed in more detail in [HdlL01a].

Remark 1.1. Even if the algorithms we present are justified here by the theory of normally hyperbolic manifolds, it is interesting to note that the methods we present, notably, the method of reducibility in Section 3.3 work empirically when the manifolds present some elliptic component.

The theory of persistence of manifolds with normally elliptic components is less developed than the theory of normally hyperbolic manifolds, since it is known since [Mn78] that the only manifolds which are topologically robust under all C^1 perturbations are normally hyperbolic. On the other hand, there are many theories of persistence of normally elliptic manifolds. For example, in the case that the systems have some Hamiltonian structure and that there are extra parameters, one can prove persistence for large sets of parameters, [Eli88, Pös89, JS96]. Particularly interesting for applications to numerical computation is the theorem in [JdlLZ99] which shows that if there is a family which solves approximately the invariance and reducibility equation and which is not degenerate, then, excluding a set of small measure, we can find invariant tori which are also reducible which are very close to the numerically computed ones. The estimates presented in [JdlLZ99] show that the measure of parameters that needs to be excluded is extremely small.

From the numerical point of view, this means that if we run the algorithms presented here in a system with normally elliptic components, provided that the non-degeneracy conditions in [JdlLZ99] are satisfied, then, there will be an true invariant torus if we choose the parameter in a set of a very large measure in a small ball.

In the paper [HdlL01a] we will present some examples of this calculations. In particular we will present examples of computations of bifurcations from a normally elliptic torus to a normally hyperbolic one. (The phenomenon of bifurcation of tori has been studied rigorously in [CI79a, CI79b, Sel79, BHTB90]).

1.1. **The parameterization method.** In this section, we formulate the functional equations that we will be considering in the rest of the paper.

For simplicity, we will start discussing maps. In Section 1.1.5, we will discuss the easy modifications needed to discuss flows. We note that the mathematical results for flows can be deduced from those for maps (by taking the time one maps). See [HdlL01b]. On the other hand, in practical applications, it may be advantageous to apply methods that are specifically designed for flows. A similar situation happens in the simpler case of periodic orbits [Cap04].

1.1.1. *Quasi-periodic maps.* A *rotating map* with frequency vector $\omega \in \mathbb{R}^d$ is a diffeomorphism $\bar{F} : \mathbb{R}^n \times \mathbb{T}^d \to \mathbb{R}^n \times \mathbb{T}^d$ given by the skew product

$$\begin{pmatrix} x \\ \theta \end{pmatrix} \longrightarrow \begin{pmatrix} F(x,\theta) \\ \theta + \omega \end{pmatrix}. \tag{1}$$

One should think of θ as an internal (d-dimensional) phase which keeps evolving at a linear speed. The internal phase affects the motion of the variables x but it is not affected by them.

Remark 1.2. We will almost always assume that $\omega \in \mathbb{R}^d$ is non resonant (that is, for all $k \in \mathbb{Z}^d \setminus \{0\}$ we have $k \cdot \omega \notin \mathbb{Z}$), which means that the dynamics on the base torus $\mathbb{T}^d$ is ergodic. If $\omega \cdot k \in \mathbb{Z}$ for some $k \in \mathbb{Z}^d - \{0\}$, the torus $\mathbb{T}^d$ is foliated by a one-parameter family of $(d-1)$-dimensional tori. The motion on each of these $(d-1)$-dimensional tori has the same frequency $\hat{\omega} \in \mathbb{R}^{d-1}$. By repeating the process, if necessary, we arrive to the study of r-parameter families of $d-r$-dimensional tori on which the motion is non-resonant.

Hence, the results for resonant ω reduce to results for families of non-resonant tori.

1.1.2. *Equations for invariant tori.* In this paper we will study invariant tori by looking for parameterizations in which the the motion is given by a a rotation with the frequency of the external perturbation.

That is, we seek maps $K : \mathbb{T}^d \to \mathbb{R}^n$ in such a way that

$$F(K(\theta), \theta) = K(\theta + \omega) \ . \tag{2}$$

If we consider the graph of K

$$\mathcal{K} = \{(K(\theta), \theta) \mid \theta \in \mathbb{T}^d\} \ .$$

We observe that (2) is equivalent to saying that $\mathcal{K}$ is invariant under the skew-product (1). Conversely, in [HdlL01b] it is shown that a wide class of tori can be written in this way. Moreover, it is also shown in [HdlL01b] that, assuming that ω is non-resonant, the set $\mathcal{K}$ – a graph over θ, determines the map K uniquely.

1.1.3. *Equations for invariant whiskers.* To study whiskers of a torus, we seek maps $W : \mathbb{R}^m \times \mathbb{T}^d \to \mathbb{R}^n$ and $\Lambda : \mathbb{R}^m \times \mathbb{T}^d \to \mathbb{R}^m$ in such a way that

$$F(W(\eta,\theta),\theta) = W(\Lambda(\eta,\theta),\theta+\omega), \tag{3}$$

$$\Lambda(0,\theta) = 0\ . \tag{4}$$

We note that the equation (3) again implies that the graph of W

$$\mathcal{W} = \{(W(\eta,\theta),\theta) \mid \eta \in \mathbb{R}^m\ , \theta \in \mathbb{T}^d\}$$

is invariant under the map (1). The equation (4) implies that

$$\mathcal{K} = \{(W(0,\theta),\theta) \mid \theta \in \mathbb{T}^d\}$$

is invariant. Indeed, using (4), we see that setting $K(\theta) = W(0,\theta)$ we obtain a K which satisfies the invariance equation (2). Therefore, the manifold $\mathcal{W}$ contains the torus $\mathcal{K}$.

Remark 1.3. In the following, even if the tori and its whisker are the range of K, W respectively, we will often abuse the language and refer to the language and refer to K and W as a torus and a whisker.

Remark 1.4. We note that, in contrast with (2), which have a unique solution, the equations (3), (4) have always several solutions.

If W, Λ are a solution, for any $\mu \in \mathbb{R} - \{0\}$, so are $\tilde{W}, \tilde{\Lambda}$ defined by

$$\begin{aligned} \tilde{W}(\eta,\theta) &= W(\mu\eta,\theta) \\ \tilde{\Lambda}(\eta,\theta) &= \mu^{-1}\Lambda(\mu\eta,\theta) \end{aligned} \tag{5}$$

The change of variables in (5) corresponds to changing the units in the variables along the directions transversal to the torus. This non-uniqueness, affects the algorithms we can use to solve the equations (e.g. a Newton method or a contraction method, which imply uniqueness cannot be applied without modifications). Also, once we decide on a numerical algorithm, a proper choice of the scale helps with the numerical properties.

For the purposes of the algorithmic implementation, we just note that the linearizations of the whisker $W_1(\theta) = \mathrm{D}_\eta W(0,\theta)$ and $\tilde{W}_1(\theta) = \mathrm{D}_\eta W(0,\theta)$ satisfy $\tilde{W}_1(\theta) = \mu W_1(\theta)$. Hence the choice of the different parameterizations is related to the choice of solutions for W_1. As we will see, W_1 will be required to satisfy an equation (8) which determines it up to a multiple.

In the case that m, the dimension of the whiskers, is 1, that ω, the frequency of the external perturbation, is Diophantine and that there are appropriate non-resonance conditions – satisfied e.g. in the case that the one-dimensional manifold is the strong stable manifold –, the equation (3) can be taken just

$$F(W(s,\theta),\theta) = W(\lambda s,\theta+\omega)\ , \tag{6}$$

where $s = \eta$ is a one-dimensional parameter. See Section 6 for details of the computation in this case.

In the case that the $|\lambda| < 1$ in (6), we see that, since

$$F^k(W(s,\theta),\theta) = W(\lambda^k s, \theta + k\omega) \ ,$$

the iterates of a point in $\mathcal{W}$ converge to a point in $\mathcal{K}$. That is, the manifold $\mathcal{W}$ is a submanifold of the stable manifold.

In general, to obtain submanifolds of the stable manifold, it suffices that

$$|\Lambda(\eta,\theta)| \leq \lambda|\eta|, \qquad \lambda < 1 \tag{7}$$

which does not assume that the contraction rate is uniform. Even if the theory allows more general conditions, for practical applications, (7) will be enough. Note that if we consider iterates of the original map, and (7) holds for them, then applying the algorithms to the iterates, the theory in [HdlL01b] shows that we obtain manifolds invariant for the original map.

We note that Λ – or λ in the one-dimensional case – is part of the unknowns that need to be computed. It corresponds to finding a representation of the dynamics on the stable manifold. For example, the λ is the Lyapunov multiplier on a small neighborhood of the invariant manifold.

In fact, by taking derivatives in (3) with respect to η, and evaluating them in $\eta = 0$, we obtain the equation for the linearization of the whisker:

$$\mathrm{D}_x F(W(0,\theta),\theta)\mathrm{D}_\eta W(\theta,0) = \mathrm{D}_\eta W(0,\theta+\omega)\mathrm{D}_\eta \Lambda(0,\theta) \ . \tag{8}$$

Similarly, if we take derivatives with respect to s on (6) and evaluate them at $s = 0$, we obtain:

$$\mathrm{D}_x F(W(0,\theta),\theta)\frac{\partial W}{\partial s}(0,\theta) = \frac{\partial W}{\partial s}(0,\theta+\omega)\lambda \ . \tag{9}$$

Hence, we obtain that the vector space based at $K(\theta) = W(\theta, 0)$ spanned by $W_1(\theta) = \mathrm{D}_\eta W(\theta, 0)$ is mapped into the corresponding vector space based at $K(\theta+\omega) = W(0, \theta+\omega)$ spanned by $W_1(\theta+\omega) = \mathrm{D}_\eta W(0, \theta+\omega)$ through the linear map $\Lambda_1(\theta) = \mathrm{D}_\eta \Lambda(0, \theta)$. In the one-dimensional case, we obtain also that the expansion rate is constant.

There may be, of course, several bundles invariant under the linearization. For each of these invariant bundles, we can try to find an invariant manifold.

Once we choose the invariant bundle, we determine $W_1(\theta)$ and $\Lambda_1(\theta)$. As we will see in Section 6 (See also Section 4 in [HdlL01b]) under non-resonance conditions in the spectrum, once we have made the choice of the invariant bundle, we can determine the Taylor expansion in η of W and of Λ. In Section 6, we will discuss the numerical issues arising in these computations. In particular, we will discuss algorithms to compute invariant subbundles in Section 2.4. We note that the invariant subbundles may be topologically non-trivial. Examples of invariant bundles which are not trivial happen naturally in the study of resonant tori and their bifurcations.

Remark 1.5. The parameterization method is very well adapted to numerical computations. Note that the functional equations that we study involve only functions of the minimum number of variables possible. That is, to study invariant objects of dimension d we only need to work with functions

of d variables, irrespective of what is the dimension of the ambient space or the dimension of the stable and unstable manifolds.

Also, the parametric representation is a very efficient way to describe objects such as stable and unstable manifolds, which turn around very much. Descriptions as graphs of functions run into trouble when the functions turn around.

Given the functional analysis theory developed in [HdlL01b], the method obtains directly estimates on the derivatives of the manifold.

We also note that the functional analysis framework discussed in [HdlL01b] shows that the operators considered are continuous or differentiable in the unknowns. This leads to a systematic application of the implicit function theorem to obtain regularity with respect to parameters. The good analytical properties of the operators considered are presumably related to the numerical stability properties of the algorithms discussed more in detail in [HdlL01a].

We also note that we can compute not just the usual stable and unstable manifolds of the invariant objects but also some non-resonant invariant manifolds, which in some cases correspond to slow invariant manifolds. The relevance of these manifolds is that, since they correspond to the stable eigenvalues closest to the unit circle, they are the leading asymptotic term of the approximation of orbits to the invariant torus.

1.1.4. *Periodic tori and subharmonic tori.* The previous theory adapts rather easily to the discussion of periodic tori, that is tori that get mapped to themselves after N applications of (1).

It suffices to find N functions $K_i : \mathbb{T}^d \to \mathbb{R}^n$, $i = 1, \dots, N$, in such a way that

$$F(K_i(\theta), \theta) = K_{i+1 (\mathrm{mod} N)}(\theta + \omega) \ . \tag{10}$$

Of course, the K_i satisfy the invariance equation for the N power of the map and conversely, the fixed points of the N power correspond to an N periodic orbit. However, we note that sometimes it is numerically more stable to introduce more variables and study (10) even if it requires more storage. The discussion of trade offs in implementations are discussed in [HdlL01a].

Similar considerations can be made for the study of whiskers around periodic tori.

In the numerical applications in [HdlL01a], we will present calculations of tori and their whiskers of period 2, and higher.

The equations (2) and (3) are easily adapted to find subharmonic tori and their whiskers. Subharmonic tori are invariant tori whose basic frequencies are submultiples of those of the perturbation. For the sake of simplicity, assume that the vector of frequencies of a subharmonic torus is $\tilde{\omega} = \omega/N$, where $N \in \mathbb{N}$ (if the submultiples are different, say $N_1, \dots, N_d$, we can take

N as their minimum common multiple). Let $\tilde{K} : \mathbb{T}^d \to \mathbb{R}^n$ the parameterization of the torus, in such a way that

$$\tilde{K} = \{(\tilde{K}(\varphi), N\varphi) \mid \varphi \in \mathbb{T}^d\}$$

is invariant under (1). Then, $\tilde{K}$ satisfies the invariance equation

$$F(\tilde{K}(\varphi), N\varphi) = \tilde{K}(\varphi + \omega/N) \ . \tag{11}$$

From the geometrical point of view, this procedure is equivalent to taking N-coverings of the torus. The map $N\cdot : \mathbb{T}^d \to \mathbb{T}^d$ given by $\varphi \to \theta = N\varphi$ defines obviously such an N-covering, and the lifting of (1) is

$$\begin{pmatrix} x \\ \varphi \end{pmatrix} \longrightarrow \begin{pmatrix} \tilde{F}(x, \varphi) \\ \varphi + \tilde{\omega} \end{pmatrix} \ , \tag{12}$$

where $\tilde{F}(x, \varphi) = F(x, N\varphi)$ and $\tilde{\omega} = \omega/N$. Notice that (11) is the equation (2) for the system (12). Similar considerations apply for the whiskers of these subharmonic tori.

Obviously, a torus (and a whisker) that is invariant for (1) can be lifted as an invariant torus (and a whisker) of the lifting. This observation plays an important role in numerical computations (see [HdlL01a]), because, taking double coverings (i.e., $N = 2$), we can make 1 dimensional bundles orientable and subharmonic whiskers appear naturally in resonances.

1.1.5. *The case of differential equations.* A quasi-periodic differential equation is an equation of the form

$$\dot{x} = X(x, \omega t) \tag{13}$$

where $X : \mathbb{R}^n \times \mathbb{T}^d \to \mathbb{R}^n$.

The parameterization of an invariant circle for a quasi-periodic vector field as in (13) is given by a map $K : \mathbb{T}^d \to \mathbb{R}^n$ which satisfies the equation

$$\mathrm{D}_\theta K(\theta)\omega = X(K(\theta), \theta) \ . \tag{14}$$

The equation (14) indicates that the direction of the flow is in the tangent to the image and that, moreover, in the parameterization of the torus considered, the flow consists in the motion of a rotation in the parameterization by a rotation of frequency ω.

Similarly, to find a whisker for an invariant torus we seek a map $W : \mathbb{R}^m \times \mathbb{T}^d \to \mathbb{R}^n$ and a quasi-periodic vector field given by $\Lambda : \mathbb{R}^m \times \mathbb{T}^d \to \mathbb{R}^m$ in such a way that:

$$\mathrm{D}_\eta W(\eta, \theta)\Lambda(\eta, \theta) + \mathrm{D}_\theta W(\eta, \theta)\omega = X(W(\eta, \theta), \theta) \ , \tag{15}$$

$$\Lambda(0, \theta) = 0 \ . \tag{16}$$

The map W is the parameterization of the torus and Λ is a representation of the dynamics along the stable direction. The equation (15) implies that the graph of W is invariant (The vector field is in the tangent space of the graph of W). The dynamics in the parameterization given by W is given by the rotation in the θ variables and by Λ in the normal directions.

To make sure that the whiskers we consider are submanifolds of the stable manifold (possibly, the whole stable manifold), we impose $\Lambda(\eta, \theta) \leq -\lambda\eta$ for some $\lambda > 0$.

The functional equations (13) and (15), (16), from the numerical point of view are very similar to the corresponding equations for quasi-periodic maps. The methods that we will develop for maps have analogues for the case of differential equations. One can study them either by an standard Newton method or by numerical algorithms that take advantage of the geometric features. We will develop the easy changes in remarks.

Superficially, the equations (13) (15), (16) look harder to study rigorously since they involve unbounded operators such as the derivative. This does not affect the numerical implementation of the algorithms we describe since the inverses of unbounded operators — that we consider in the Newton method — are very reasonable. The theory of the equations above is developed in [HdlL01b].

1.2. **Some information on the literature on numerical computation of invariant manifolds.** Let us review some papers about computation of invariant objects, and see where our methods fit in.

[BOV97] uses the graph transform operator [HPS77] to develop an algorithm to compute normally hyperbolic invariant manifolds, and its stable and unstable manifolds. The invariant manifold is approximated by means of a finite simplicial complex. The method produces linear approximations of the stable and unstable manifolds, and their intersection provide an approximation of the invariant manifold. So, the invariant manifold is not computed directly but as a byproduct of computing its stable and unstable manifolds, which are higher dimensional objects. Notice also that the globalization of the stable an unstable manifolds is computationally hard, since only linear approximations are provided. [KO98, OF00] apply the method to compute invariant tori in quasi-periodic systems, the ones considered in the present paper.

There are also algorithms based in set oriented numerical methods (see [DFJ01] and the references therein). These method have been applied to the numerical approximation of invariant sets (not only invariant manifolds, but also global attractors and chain recurrent sets)as well as other natural objects such as invariant measures and almost invariant sets. The basic concept behind these methods is a subdivision algorithm that covers the invariant object by boxes and then the dynamical behavior on the set is approximated by a Markov chain based on transition probabilities between elements of this covering.

Notice that the previous methods can be applied to rather general cases. We will used a method specially fitted to the objects we are computing: invariant tori and their whiskers in quasi-periodic systems. We parameterize those objects with a set of coordinates that not only fits the shape of the manifold but also its dynamics. There are two steps: computation of the

invariant torus and computation of their whiskers. The approach we present is based on studying (2) and (3) respectively.

The only discretization we are going to considered in the applications is to expand the functions considered in Fourier-Taylor series and to develop a toolkit to implement functionals such as those entering in (2) and (3) and in the algorithms for their solution. See [Sim89] for an overview of methods based on the manipulation of Fourier-Taylor series. Some of the considerations on the algorithms apply equally well to other possible discretizations, but our discussions on whether matrices are full or sparse, storage requirements, running times etc. depend on the discretization used.

The straightforward direct application of the Newton method to the functional equations (2) involves the solution of a linear equation whose dimension is the number of Fourier modes that we are considering [CJ00]. Since in applications this could be hundreds, thousands of millions, full matrices of this size are large matrices. We will see that, by taking advantage of the geometry of the problem, we can perform algorithms that do not require to invert such large matrix.

The parameterization method for computation of invariant tori in differential equations has precedents in [DLR91], where two approaches are proposed:

- solution of a system of functional equations, that for the systems considered here corresponds to solve (2) once one uses the Poincaré return map;
- solution of a systems of first-order partial differential equations, that correspond to solve (14).

The numerical solutions in [DLR91] are constructed using difference methods. Fourier methods for computation of invariant tori for differential equations based on both approaches have been introduced in [HKM97] (see also [Tru00]), where the study of spectral and pseudospectral methods is done in detail under dissipativity conditions. Numerical approximations of invariant KAM tori in periodically forced Hamiltonian systems based on Fourier methods appear in [War91].

The methods we develop for the computation of invariant tori are based in the abstract constructs of the theory of normally hyperbolic invariant tori, for the case of normally hyperbolic tori, and in the KAM theory, for reducible and almost reducible tori. By following the geometric constructions closely and taking advantage of the structure of the problem, we will be able to avoid having to deal with large matrices. Details of the implementation are in [HdlL01a].

2. Numerical algorithms: an overview

The bulk of this paper is devoted to numerical methods for solving the equations (2) for invariant tori, as well as (3), (4) for their whiskers. We will

also study their analogues for differential equations (14), (15) for differential equations.

We will describe algorithms that allow us to, given a F, produce a K or a W that satisfies (2) or (3) up to an small error measured in a C^r norm. More precisely, we will present algorithms that, given a moderately approximate solution, produce a more approximate one. By iterating these steps, one can obtain extremely accurate solutions. These refinements can be the basis of a continuation method [AG03]; in the problem of quasi-periodic perturbations, it is natural to start from the uncoupled system and use as a parameter the strength of the perturbation. Another practical application is to start the refinement from an approximate solution obtained from asymptotic expansions or other non-rigorous, but reasonable method.

Moreover, we will also describe algorithms that allow us to assert that the approximate solutions constructed satisfy hyperbolicity properties. In such a case, the theory developed in [HdlL01b] establishes that there is a true solution which is close to the computed one. The theory of [HdlL01b] shows, moreover that the distance between the computed solution and the true one, is bounded by the error in solving the appropriate equations (times a factor that depends on the hyperbolicity properties and the map). This error as well as the hyperbolicity properties, are accessible for the computation.

We also note that, even if rigorous results are not completely developed, it is empirically found that the methods we present here work also in the presence of some elliptic components. See [HdlL01a] and Remark 1.1. We hope that this is an stimulus for the development of rigorous results in this direction.

The numerical study of a functional equation, often involves two different steps. The first step is the choice of a discretization – a set of functions specified by a finite number of parameters. The second step is to choose algorithms to solve the resulting finite dimensional problem obtained when truncating the problem. Finally, if one wants to validate the results as indicated above, one has also to choose spaces of functions in which to apply the rigorous results of validation.

2.1. **Discretization in terms of Fourier-Taylor series.** In this paper and its companion [HdlL01a], all the methods will be based on discretizing the functions in terms of Fourier series for the invariant tori (2). We will use the notation

$$f(\theta) = \sum_{k \in \mathbb{Z}^d} f_k e^{2\pi \mathbf{i} k\theta} \ ,$$

where f is any function on the torus (including vector valued functions, matrix valued functions, etc.), keeping in mind that only a finite number of modes f_k can be stored in the computer. In the implementations in [HdlL01a], we have used real Fourier series (expansions in cos and sin).

This choice is very well adapted to the problem at hand, since the quasi-periodic dynamics makes the objects we consider very homogeneous. Hence,

there is little advantage in choosing methods such as finite elements or splines that can be refined to deal with local features.

Fourier series are also well adapted to deal with smooth functions and to obtain information on derivatives of high order, a property which is useful in studies of bifurcation problems.

Another important advantage of the basis of Fourier series is that translations by a rotation are diagonal in the space of Fourier series. As we will see, this allows to implement algorithms that take advantage of the special structure of the equations, notably reducibility. The resulting algorithms are not only faster, but also much more accurate and more reliable.

A final advantage is that Fourier series can be manipulated very systematically by implementing a toolkit that implements elementary operations among them. Such toolkits for the manipulation of Fourier series have been in use for a long time among astronomers [Rom61, RJB83, Sim96, Sim98a, Las89, Sch89] and in the *automatic differentiation* community [GC91]. See also the discussion of polynomial manipulation in [Knu97]. A survey particularly indeed, particularly close to our applications, is [Har04].

As we will see, the algorithms that appear in this paper do not require anything beyond the arithmetic operations from the toolkit. A delicate step in the algorithms is the solutions of cohomology equations, but this will require special methods. As we will see, it can be reduced to elementary operations and iterative algorithms in many cases taking advantage of the geometry of the problem. In the companion paper [HdlL01a] we will discuss in more detail some of the numerical issues involved in how to implement such a toolkit. Notably, what are efficient and stable algorithms to multiply these series or to perform non-linear operations.

We also note that Fourier series are natural series for spaces of different regularities. Hence, once we decide to work with Fourier series, there is no need to change the algorithms to work in spaces of more or less derivatives (as it would be the case, with splines, which would require more coefficients and different representations to deal with spaces of smoother functions).

As we will see in our numerical experiments [HdlL01a], using the specialized algorithms with the problem at hand, it has been possible to use 10^5 coefficients working in a slightly out of date desktop computer. This provides excellent accuracy both in the functions and in their derivatives.

In this paper, we will not consider any other choice for discretization of periodic functions. With the same spirit, for the discretization of the whiskers (3), (4) we have considered series involving polynomials whose coefficients are Fourier series. These are Fourier-Taylor series. Again, we note that the manipulation of these series has been standard in the numerical literature for a long time.

2.2. **Newton method for invariant tori.** It will be interesting to start discussing the Newton method. This is a general purpose algorithm for nonlinear equations and it is a natural starting point. The discussion of

the Newton method will bring forth important features such as the role of the differential of the functional equations considered. The numerical shortcomings of the Newton method will be the stimulus for a geometric analysis of some of the elements of the Newton method. Taking advantage of this geometric analysis will lead to more efficient algorithms.

The Newton method applied to (2) is based on a repeated application of the following iterative step:

From a guess K, whose error is

$$r(\theta) = F(K(\theta - \omega), \theta - \omega) - K(\theta) \ , \tag{17}$$

construct a new approximation $\tilde{K} = K + h$ by solving

$$\mathrm{D}F(K(\theta - \omega), \theta - \omega)h(\theta - \omega) - h(\theta) = -r(\theta) \ . \tag{18}$$

Where DF denotes the derivative of F with respect to the first argument.

The equation (18) is obtained by substituting $K + h$ in (2), expanding to first order in h and using the error (17). (For mathematically rigorous precisions of the meanings in which the formal first order expansions are indeed so, we refer to [HdlL01b]. In this paper, we will concentrate in numerical analysis issues.)

As we will see later, solubility of (18) is closely related to that of normal hyperbolicity.

In the Fourier representation, the linear equation (18) of each step of Newton method corresponds to an infinite linear system whose unknowns are the Fourier coefficients of h.

If implemented straightforwardly, the matrix that implements the linear equation is full and can be very large. We will refer to this as the "*large matrix problem*". More precisely, the size of the matrix is $O(N^2)$ where N is the number of coefficients considered. Of course, the number of coefficients $N = O(nD^d)$ where D is degree of the Fourier series considered and d is the dimension of the torus considered and n is the dimension of the ambient space. Note that the dependence of the number of coefficients on the ambient dimension is only linear, whereas the dependence on the dimension of the torus is exponential. When the tori are not very smooth, the degree needed to achieve a prescribed accuracy grows fast.

The large matrix problem causes several computational difficulties: it increases the computational time, and the storage requirements. Related to that, it decreases the accuracy of the calculations. One of the main goals of this paper is to produce algorithms to avoid both shortcomings of the large matrix problem. The basic tool to avoid the large matrix problem will be to take advantage of the geometric features of the linearized equation.

2.3. **Normal dynamics: linear cocycle and transfer operator.** It this section, we study geometric and analytic properties of the operators obtaining linearizing the functional equation (2). A much more mathematical study appears in [HdlL03a, HdlL03b] and in [HdlL01b]. Here, we will just

set up the notation and quote the results which will be useful for the implementation of numerical algorithms.

Given a torus K, the monodromy matrix $M(\theta) = \mathrm{D}F(K(\theta), \theta)$ defines a rotating linear map (or cocycle) by

$$\begin{pmatrix} v \\ \theta \end{pmatrix} \longrightarrow \begin{pmatrix} M(\theta)v \\ \theta + \omega \end{pmatrix}. \tag{19}$$

If the torus K is invariant, this linear skew product represents the linearization of the dynamics around the torus. If we think of v as an infinitesimal perturbation of the initial condition $K(\theta)$ (19) describes how the disturbance propagates.

The transfer operator acts on sections $v : \mathbb{T}^d \to \mathbb{R}^n$ of $E = \mathbb{R}^n \times \mathbb{T}^d$ by means of

$$(\mathcal{M}_\omega v)(\theta) = M(\theta - \omega)v(\theta - \omega) \ . \tag{20}$$

Remark 2.1. Since in this paper we are assuming that the bundle E is trivial, the space of continuous sections of E, $\Gamma_{C^0}(E)$, is identified with the space of continuous vector valued functions, $C^0(\mathbb{T}^d, \mathbb{R}^n)$.

Remark 2.2. Since we are interested in the analysis of the transfer operator using functional analysis and plan to use spectral theory, it is necessary to consider complex spaces. Hence, we use the complexification trick and consider the real valued sections which appear naturally in geometric considerations as particular cases of complex sections. See [HdlL03a, HdlL03b].

In the following, we summarize some of the properties of the spectrum and their relation with geometric features. We refer to [HdlL03a, HdlL03b] and [HdlL01b] for proofs and references to the literature.

- An annular gap in the spectrum in the space of continuous sections of the transfer (20) associated to the cocycle (19), that is assumed to be C^r smooth, produces an invariant C^r splitting

$$E_\theta = \mathbb{R}^n \times \{\theta\} = E_\theta^{<\lambda} \oplus E_\theta^{>\mu} \ . \tag{21}$$

  Here, $\lambda < \mu$ give the size of the gap in the spectrum, that is, the set $\mathcal{A}_{\lambda,\mu} = \{z \in \mathbb{C} | \lambda \leq |z| \leq \mu\}$ is contained in the resolvent of the transfer operator.

  That is, the spectral projections (constructed using functional analysis) correspond to projections over two subbundles invariant under the linear cocycle. This interplay between the functional analysis and the geometry is crucial for many results starting in [Mat68].

  The geometric bundles in (21) are characterized by

$$\begin{aligned} v \in E_\theta^{<\lambda} &\iff |M(\theta + (m-1)\omega) \cdots M(\theta)v| \leq C\lambda^m |v| \quad \forall m > 0 \\ v \in E_\theta^{>\mu} &\iff |M^{-1}(\theta + m\omega) \cdots M^{-1}(\theta - \omega)v| \leq C\mu^m |v| \quad \forall m < 0 \end{aligned} \tag{22}$$

- The transfer operators can be considered as operators on different spaces, depending on the regularity. A remarkable fact about the

transfer operators based on rotations is that the spectrum does not depend on such spaces [HdlL03b]. (This result is false if the motion on the base is not a rotation [HdlL03a].)

- If ω is irrational, the spectrum is rotationally invariant. That is

$$\mathrm{Spec}(\mathcal{M}_\omega) = \bigcup_{i=1}^{k} \mathcal{A}_{\lambda_i^-,\lambda_i^+} \ , \tag{23}$$

where $\lambda_1^- \leq \lambda_1^+ < \lambda_2^- \leq \lambda_2^+ < \cdots < \lambda_k^- \leq \lambda_k^+$.

Each *spectral annulus* $\mathcal{A}_i = \mathcal{A}_{\lambda_i^-,\lambda_i^+}$ has associated an invariant subbundle E_i, characterized by the rates of growth of its orbits: $E_i = E^{>\lambda_i^- - \varepsilon} \cap E^{<\lambda_i^+ + \varepsilon}$, and $E = \bigoplus_{i=1}^k E_i$. Notice that $k \leq n$.

As a consequence of the previous observations, an invariant torus with an irrational rotation is normally hyperbolic if and only if the whole unit circle is in the resolvent set of $\mathcal{M}_\omega$.

Also, checking that an invariant torus with an irrational rotation ω is normally hyperbolic is the same as checking that 1 is in the resolvent set of $\mathcal{M}_\omega$.

This is, of course, the same as to the solubility of (18) which appears in the Newton method.

When the torus is not invariant but only approximately invariant – the situation that happens in numerical analysis – the solubility of (18), which allows us to take a Newton step, amounts to the hyperbolicity of the cocycle associated to the linearization on the torus. In retrospect, one of the main motivations of the authors for developing a general theory of cocycles was precisely the study of numerical algorithms in which one has to linearize around approximately invariant tori.

2.4. **Computation of the stable and unstable subbundles.** Now, we describe the computation of the invariant subbundles. Besides their intrinsic interest, the invariant subbundles will be crucial in the design of efficient algorithms for the calculation of invariant tori and will also be the base of calculation of whiskers.

In this section, we will concentrate in the stable and unstable subbundles. In Section 4, we will describe algorithms for the computation of more general subbundles, which will be the basis of the computation of other manifolds.

For the computer representation of the invariant subbundles, we will assume that they are trivial. That is $E^s \simeq \hat{E}^s = \mathbb{R}^{n_s} \times \mathbb{T}^d$ and $E^u \simeq \hat{E}^u = \mathbb{R}^{n_u} \times \mathbb{T}^d$, where n_s and n_u are the dimensions of the stable and the unstable subbundles, respectively. Of course, these are the subbundles that are the easiest to deal with, since they can be constructed using global frames. An *adapted frame* is a set of sections $v_1^s, \dots v_{n_s}^s, v_1^u, \dots v_{n_u}^u : \mathbb{T}^d \to \mathbb{R}^n$ such that

$$E^s_\theta = \mathrm{span}\{v_1^s(\theta), \dots v_{n_s}^s(\theta)\} \ , \ E^u_\theta = \mathrm{span}\{v_1^u(\theta), \dots v_{n_u}^u(\theta)\} \ .$$

By defining the matrices

$$V^s(\theta) = \left(v_1^s(\theta), \dots v_{n_s}^s(\theta)\right) \ , \ V^u(\theta) = \left(v_1^u(\theta), \dots v_{n_u}^u(\theta)\right) \ .$$

we produce the matrices $\Lambda^s(\theta)$ and $\Lambda^u(\theta)$, of dimension $n_s \times n_s$ and $n_u \times n_u$, respectively. The condition that the bundle is invariant amounts to:

$$M(\theta)V^s(\theta) = V^s(\theta+\omega)\Lambda^s(\theta) \ , \ M(\theta)V^u(\theta) = V^u(\theta+\omega)\Lambda^u(\theta) \ . \tag{24}$$

The matrix $\Lambda^s(\theta)$ represents the dynamics on the bundle $E^s(\theta)$ expressed in the coordinates we have chosen. The matrix $\Lambda^u(\theta)$ expresses the dynamics on $E^u(\theta)$ in the coordinates chosen.

The transfer operators $\mathcal{L}^s_\omega$ and $\mathcal{L}^u_\omega$, associated to the vector bundle maps Λ^s and Λ^u over the rotation ω, respectively, satisfy

$$r_s(\mathcal{L}^s_\omega) < 1 \ , r_s((\mathcal{L}^u_\omega)^{-1}) < 1 \ ,$$

where r_s means the spectral radius of a linear operator.

The theory of transfer operators shows that it is possible to find an (adapted) Finsler metric on $\hat{E} = (\mathbb{R}^{n_s} \times \mathbb{R}^{n_u}) \times \mathbb{T}^d$. That is a θ-depending norm on each fiber of the form $|\hat{v}|_\theta = |\hat{v}^s|_\theta + |\hat{v}^u|_\theta$ for $\hat{v} = (\hat{v}^s, 0) + (0, \hat{v}^u) \in (\mathbb{R}^{n_s} \times \mathbb{R}^{n_u}) \times \{\theta\}$. The dependence on θ of the adapted Finsler metric may be assumed to be analytic.

As it is standard, a Finsler metric induces a norm on the space of continuous sections $\hat{v} : \mathbb{T}^d \to \mathbb{R}^{n_s} \times \mathbb{R}^{n_u}$:

$$\|\hat{v}\| = \max_{\theta \in \mathbb{T}^d} |\hat{v}(\theta)|_\theta. \tag{25}$$

The property of adapted Finsler metrics that is more delicate and more important for us is that, when we consider the norms of the operators measured in (25), we have:

$$\begin{aligned} &\|\mathcal{L}^s_\omega\| \leq \lambda \ , \\ &\|(\mathcal{L}^u_\omega)^{-1}\| \leq \lambda \ , \end{aligned} \tag{26}$$

where $\lambda < 1$. Notice we consider $\hat{v}_\theta$ as the representation of a vector v_θ in the adapted frame.

The use of the adapted metric allows to simplify significantly the expression of the a-posteriori bounds. For practical implementations, we note that it suffices to check that, in the usual coordinates (26) is satisfied. If they are not, it suffices in practice to study a power of the operator – which is very close to the theoretical construction of the adapted metric –. Therefore, the adapted metrics do not need to be computed explicitly in many cases. We also note that, when we can apply the reducibility method, described in Section 3.3, one of the byproducts is the calculation of an adapted norm. See, in particular the discussion in Remark 3.11.

In summary, the vector bundle map $P : (\mathbb{R}^{n_s} \times \mathbb{R}^{n_u}) \times \mathbb{T}^d \to \mathbb{R}^n \times \mathbb{T}^d$ (over the identity) defined by

$$P(\theta) = (V^s(\theta), V^u(\theta))$$

represent the change of variables giving the adapted frame, and the vector bundle map $\Lambda : (\mathbb{R}^{n_s} \times \mathbb{R}^{n_u}) \times \mathbb{T}^d \to (\mathbb{R}^{n_s} \times \mathbb{R}^{n_u}) \times \mathbb{T}^d$ (over the rotation ω), defined by

$$\Lambda(\theta) = \text{blockdiag}(\Lambda^s(\theta), \Lambda^u(\theta))$$

represent the dynamics on the bundles in the adapted coordinates. The invariance of the splitting reads

$$P(\theta + \omega)^{-1} \mathrm{D}F(K(\theta), \theta) P(\theta) - \Lambda(\theta) = 0 \ . \tag{27}$$

Note that the equation (27) allows us to parameterize non-trivial bundles in the manifold. One example that we will see in [HdlL01a] that appears in practice is when $d = 1$ and $n = 2$, The map P can be considered as a mapping from $\mathbb{T}^1$ – the base space of the invariant torus to $\mathbb{P}^1$, the space of one-dimensional directions. It is quite possible that the map P has an index, which makes the bundle non-trivial. Nevertheless, the fact that the bundle can be given by a representation of the form (27) is not as general as the theory in [HdlL01b] allows. On the other hand, in order to be able to use numerical methods based on Fourier series, it seems that some weak version of trivializability is needed.

Remark 2.3. The assumption of the fact that the bundles are given by an embedding as in (27) is a strong assumption in general.

However, we note that in the case that the bundles have rank one (i.e. they have one-dimensional fibers), the bundles can be made trivial by just taking covers. In [HdlL01a] we show some explicit examples in which this situation happens. Notice that taking double coverings on the torus is well suited for Fourier series (we have to double the angles).

When the bundles are higher dimensional there are other obstructions for trivializations, notably characteristic classes [MS74]. Since the characteristic classes agree with integrals of the curvature of a connection over the torus, they do not vanish by taking covers. Taking covers will only multiply the class by an integer.

We however note that in [HP70] one can find a construction that shows that that all bundles can be considered as subbundles of a trivial bundle. The dynamics in the complementary variables introduced in the construction can be made very contractive.

There are other possibilities such as using local patches. In this paper, we have not studied the numerical representation of non-trivial bundles using local patches. This problem deserves further investigation since non-trivial bundles given by (27) appear naturally in applications.

Remark 2.4. Notice that, in the present formulation, (24) is not an equation, but just an identity which follows from the choice of an adapted frame.

In Section 3.2 we will discuss the computation of adapted frames.

As we will see later, it is possible to choose the adapted frames in such a way that the $\Lambda^{s,u}$ are particularly simple. In particular in Section 3.3 we will show that, under some additional conditions – which are, however verified

in practice several times – it is possible to make the matrices $\Lambda^{s,u}$ diagonal and independent of θ.

2.5. **Computation of Whiskers.** Once we have a K satisfying (2) – or at least satisfying it very approximately – and invariant bundles of the linearization around it, it is natural to wonder about the existence of invariant manifolds containing the torus and that are tangent to the invariant bundles. These manifolds, the whiskers, are non-linear analogues of the invariant bundles for the linearization.

Following the philosophy of the parameterization method, we will study the whiskers by finding parameterizations for them. To find a whisker $\mathcal{W}$, we will seek a function $W : \mathbb{R}^m \times \mathbb{T}^d \to \mathbb{R}^n$ and a function $\Lambda : \mathbb{R}^m \times \mathbb{T}^d \to \mathbb{R}^m$, such that they satisfy the invariance equation

$$F(W(\eta, \theta), \theta) = W(\Lambda(\eta, \theta), \theta + \omega), \tag{28}$$

as well as with $\Lambda(0, \theta) = 0$ and $W(0, \theta) = K(\theta)$.

Note that (28) implies that $\mathcal{W}$, the range of W is invariant under the skew-product. The interpretation of $\Lambda : \mathbb{R}^m \times \mathbb{T}^d \to \mathbb{R}^m$ is the dynamics on the manifold.

We emphasize that the unknowns in (28) are both W and Λ. That is, we look for a parameterization of an invariant manifold $\mathcal{W}$ through $\mathcal{K}$ such that the dynamics is a skew product.

Note that in the representation in (28) we are assuming that the invariant bundle we are considering is of the form considered in (27), This assumption does not belong and the theory of [HdlL01b] does not require that. On the other hand, this assumption allows us to work with globally defined functions parameterizing the bundles and to use numerical methods based on Fourier series.

3. Computation of invariant tori

3.1. **Validation of numerical results.** In this section we will establish some rigorous bounds for the convergence of Newton method. We reproduce below the standard Newton-Kantorovitch theorem [KA81].

Theorem 3.1 (Newton-Kantorovitch)**.** *Let B be a Banach space. Let $\|\cdot\|$ be the B-norm. Let $\mathcal{F} : \Omega \subset B \to B$ a C^2 operator, defined in an open set Ω.*

Let $r > 0$ such that $\bar{B}_r = \bar{B}(x_0, r) \subset \Omega$ such that:

- *$\mathrm{D}\mathcal{F}(x_0)$ has continuous inverse. Denote $\Gamma_0 = (\mathrm{D}\mathcal{F}(x_0))^{-1}$;*
- *$\|\Gamma_0(\mathcal{F}(x_0))\| \leq \varepsilon$, where $\varepsilon > 0$;*
- *$\|\Gamma_0 \mathrm{D}^2\mathcal{F}(x)\| \leq \beta$ for all $x \in \bar{B}_r$, where $\beta > 0$.*

Suppose that

$$h = \beta\varepsilon \leq \frac{1}{2} ,$$

and define the constants

$$r_0 = \frac{1 - \sqrt{1 - 2h}}{h} \cdot \varepsilon \ , \quad r_1 = \frac{1 + \sqrt{1 - 2h}}{h} \cdot \varepsilon \ . \tag{29}$$

Then, if

$$r_0 \leq r \ , \tag{30}$$

then, it is possible to define recursively a sequence

$$x_{n+1} = x_n - (\mathrm{D}\mathcal{F}(x_n))^{-1}\mathcal{F}(x_n) \ ,$$

from an initial approximation $x_0 \in B$.

The sequence x_n *converges to a point* $x^* \in B_r$, *which satisfies*

$$\mathcal{F}(x^*) = 0 \ . \tag{31}$$

Moreover,

$$\|x^* - x_0\| \leq r_0 \leq 2\varepsilon \ ,$$

and the convergence is quadratic:

$$\|x^* - x_n\| \leq \frac{1}{2^n}(2h)^{2^n}\beta \ , \tag{32}$$

for $n = 0, 1, \ldots$

Finally, if

$$h < \frac{1}{2} \ , \ r < r_1 \quad \textit{or} \quad h = \frac{1}{2} \ , \ r \leq r_1 \tag{33}$$

then x^* *is the only solution of* (31) *in* $\bar{B}_r$.

The following Theorem 3.2 makes explicit the conditions for the application Newton method to the problem of computation of normally hyperbolic invariant tori and the invariant bundles of its linearization.

It is important to remark that the conditions of Theorem 3.2 can be computed once we have some mild information about the system considered (upper bounds of derivatives in a ball) and bounds on the size of the right hand side of the invariance equations evaluated in the approximate objects. These bounds are easily available from a knowledge of the approximate solutions. As we will see later, in practice, we can often obtain solutions which satisfy the equation with an error – measured in an analytic norm or a C^r norm — which is a few thousand times the round off error. It is shown in [HdlL01b] that the normally hyperbolic tori are as smooth as the map. Hence, for smooth maps, it is easy to choose enough Fourier coefficients so that the truncation error is negligible and, indeed the main part of the numerical error is just the round–off. The conditions of differentiability on the map are not very restrictive and in [HdlL01a] we present the results of numerical implementations for maps which are just Lipschitz. We will also see in [HdlL01a] that, for large perturbations, it could happen that there may be tori with very weak hyperbolicity properties in such a way that, even if they become smooth, their derivatives are large. These tori also require a large number of Fourier coefficients.

Hence, once we have a computed solution, we just need to verify some conditions and, if they are verified, Theorem 3.2 implies the existence of a

true solution which is close – in an analytic or a C^r norm – to the computed solution.

Note that, in particular, Theorem 3.2 is independent of the method that was used to compute the approximate solution. The numerical method used may include uncontrolled approximations which are justified a posteriori by the fact that the error obtained is small. Of course, the approximate solutions may be produced by other methods than numerical calculation, for example, asymptotic expansions. To validate asymptotic expansions, it is enough to verify that the asymptotic expansion verifies the equation with a very small remainder. (In [HdlL01b], this technique is used to show that a formal Taylor expansion of K is a bona-fide Taylor expansion and that, therefore, K is differentiable.)

If one was interested in *"computer assisted proof"* it would be enough to establish – by computer, using, e.g. interval arithmetic and rigorous functional analysis [Lan87, Ran87, dlLR91, KSW96] – the hypothesis of Theorem 3.2. Of course, in normal practice, one can obtain reliable assessments of the error by the standard methods of changing the level of truncation or the precision of the calculations.

The important point is that Theorem 3.2 reduces the estimates of the error in the result to the error in the evaluation the functional.

Theorem 3.2. *Let $F : \mathbb{R}^n \times \mathbb{T}^d \to \mathbb{R}^n$ be a continuous map, C^2 with respect to the x variables, defining a skew-product*

$$\begin{pmatrix} x \\ \theta \end{pmatrix} \longrightarrow \begin{pmatrix} F(x,\theta) \\ \theta + \omega \end{pmatrix}, \tag{34}$$

where $\omega \in \mathbb{R}^n$. Suppose that for a continuous torus $K_0 : \mathbb{T}^d \to \mathbb{R}^n$ there exists

1) *Two continuous matrix-valued maps $P_1, P_2 : \mathbb{T}^d \to M_n(\mathbb{R})$, where P_1 represents a vector bundle map (over the identity) giving the change of variables to an adapted frame, and P_2 is its approximate inverse;*
2) *A continuous block diagonal matrix-valued map*

$$\Lambda_0(\theta) = \text{blockdiag}(\Lambda_0^s(\theta), \Lambda_0^u(\theta)) \ ,$$

where $\Lambda_0^s : \mathbb{T}^d \to M_{n_s}(\mathbb{R})$ and $\Lambda_0^u : \mathbb{T}^d \to M_{n_u}(\mathbb{R})$ ($n = n_s + n_u$).

We recall that, as we will see later, the $\Lambda_0^{s,u}$ are approximations of the linear contraction on the bundles.
3) *An (adapted) Finsler metric $|\cdot|_\theta$, of the form $|\hat{v}|_\theta = |\hat{v}^s|_\theta + |\hat{v}^u|_\theta$ for $\hat{v} = (\hat{v}^s, 0) + (0, \hat{v}^u) \in \mathbb{R}^n = \mathbb{R}^{n_s} \times \mathbb{R}^{n_u}$, and the induced norm on continuous sections and vector bundle maps is denoted by $\|\cdot\|$;*
4) *Positive constants $\rho, \sigma, \tau, \lambda, r, b$ with $\lambda + \sigma + \tau < 1$;*

such that

5.1) *$R(\theta) = P_2(\theta)(F(K_0(\theta-\omega), \theta-\omega) - K_0(\theta))$ satisfies $\|R\|_{C^0} \leq \rho$ (as a section);*

5.2) $S(\theta) = P_2(\theta+\omega)\mathrm{D}F(K_0(\theta),\theta)P_1(\theta) - \Lambda_0(\theta)$ *satisfies*

$$\|S\|_{C^0} \leq \sigma$$

(as a vector bundle map over the rotation ω);

5.3) $T(\theta) = P_2(\theta)P_1(\theta) - \mathrm{Id}$ *satisfies*

$$\|T\|_{C^0} \leq \tau$$

(as a vector bundle map over the identity);

5.4) *Let $\mathcal{L}^s_\omega$, $\mathcal{L}^u_\omega$ be the transfer operators over the rotation ω induced by the vector bundle maps Λ^s_0 and Λ^u_0 in $\mathbb{R}^s \times \mathbb{T}^d$ and $\mathbb{R}^u \times \mathbb{T}^d$. We assume we have*

$$\|\mathcal{L}^s_\omega\| \leq \lambda$$
$$\|(\mathcal{L}^u_\omega)^{-1}\| \leq \lambda$$

6) *For all points (x,θ) in the strip*

$$\bar{D}(K_0,\bar{r}) = \{(x,\theta) \in \mathbb{R}^n \times \mathbb{T}^d \mid |P_2(\theta)(x - K_0(\theta))|_\theta \leq \bar{r}\} \ ,$$

where $\bar{r} = r(1+\tau)$,

$$\|P_2(\theta+\omega)\mathrm{D}^2F(x,\theta)[P_1(\theta)\cdot, P_1(\theta)\cdot]\| \leq b$$

(as a bilinear vector bundle map over the rotation ω).

Define the constants

$$\varepsilon = \frac{\rho}{1-(\lambda+\sigma+\tau)} \ , \ \beta = \frac{b}{1-(\lambda+\sigma+\tau)} \ , \ h = \beta\varepsilon \ .$$

Assume that

7) $h < \frac{1}{2}$

and define

$$r_0 = \frac{1-\sqrt{1-2h}}{h} \cdot \varepsilon \ .$$

Finally. Assume that

8) $r_0 \leq r$.

Under the hypothesis 1)-8):

a) *There exists an invariant torus $K_* : \mathbb{T}^d \to \mathbb{R}^n$ to which Newton method converges quadratically from the initial approximation K_0, and*

$$|P_1(\theta)^{-1}(K_*(\theta) - K_0(\theta))|_\theta \leq r_0 < 2\varepsilon \ .$$

b) *The torus K_* is normally hyperbolic.*

Let $\hat{\lambda} = \|\Lambda_0\|$. Define the constant

$$\mu = \frac{\lambda}{1-\lambda^2}\frac{1}{1-\tau}\left(br_0 + \sigma + \hat{\lambda}\tau\right) \ .$$

and suppose that, moreover;

9) $\mu < \frac{1}{4}$.

Then:

c) *The stable and unstable bundles differ from the initial approximate invariant bundles in a distance smaller than* $\frac{\mu}{\sqrt{1-4\mu}}$*, and can be computed using the contraction principle.*

We note that the proof of Theorem 3.2 we present is very constructive and leads naturally to algorithms. Basically, the idea of the proof is to describe an iterative algorithm for the objects considered and estimate its convergence properties. Later, we will develop other algorithms that are more efficient from the numerical point of view but harder to estimate.

Remark 3.3. Notice that to apply Newton-Kantorovich theorem presented in this paper we need $\mathcal{F}$ to be C^2 when acting on continuous tori. To conclude that, it suffices that F is C^2 with respect to the x variables and that it is continuous with respect to θ. Of course, there are less demanding Newton-Kantorovich theorems, but they seem to be less quantitative. It is notable that we need much less regularity in the θ variables.

Proof. a) By using P_1 as a change of coordinates on the bundle $\mathbb{R}^n \times \mathbb{T}^d$, we write $\hat{K} = P_1^{-1} K$ and the functional on $C^0(\mathbb{T}^d, \mathbb{R}^n)$ we will consider is

$$\hat{\mathcal{F}}(\hat{K})(\theta) = P_2(\theta)(F(P_1(\theta-\omega)\hat{K}(\theta-\omega), \theta-\omega) - P_1(\theta)\hat{K}(\theta)) \ .$$

The norm we consider in $C^0(\mathbb{T}^d, \mathbb{R}^n)$ is that induced by the Finsler:

$$\|\hat{\Delta}\| = \max_{\theta \in \mathbb{T}^d} |\hat{\Delta}(\theta)|_\theta \ .$$

From the regularity properties of the composition operator, discussed in [HdlL01b] and [dlLO99] we have $\hat{F}$ is C^2 when acting on C^0 functions. This will allow us to use the mean value theorem, etc.

First, we estimate the error in the approximate invariant torus, that in the new coordinates is $\hat{K}_0 = P_1^{-1} K_0$. Hence, from 5.1):

$$\|\hat{\mathcal{F}}(\hat{K}_0)\| = \|R\| \leq \rho \ . \tag{35}$$

Now, we compute $(\mathrm{D}\hat{\mathcal{F}}(K_0))^{-1}$ and estimate its norm. The differential of $\hat{F}$ is defined by

$$\begin{aligned} (\mathrm{D}\hat{\mathcal{F}}(\hat{K}_0)\hat{\Delta})(\theta) &= P_2(\theta)\mathrm{D}F(P_1(\theta-\omega)\hat{K}_0(\theta-\omega), \theta-\omega)P_1(\theta-\omega)\hat{\Delta}(\theta-\omega) - \\ &\quad P_2(\theta)P_1(\theta)\hat{\Delta}(\theta) \\ &= (\Lambda_0(\theta-\omega) + S(\theta-\omega))\hat{\Delta}(\theta-\omega) - \hat{\Delta}(\theta) - T(\theta)\hat{\Delta}(\theta) \ . \end{aligned}$$

Denoting $\mathcal{L}_\omega$,$\mathcal{S}_\omega$ the transfer operators associated to $\Lambda_0(\theta)$ and $S(\theta)$ (over the rotation by ω), and $\mathcal{T}$ the transfer operator associated to $T(\theta)$ (over the identity), i.e.

$$\mathcal{L}_\omega\hat{\Delta}(\theta) = \Lambda_0(\theta-\omega)\hat{\Delta}(\theta-\omega) \ , \ \mathcal{S}_\omega\hat{\Delta}(\theta) = S(\theta-\omega)\hat{\Delta}(\theta-\omega) \ ,$$
$$\mathcal{T}\hat{\Delta}(\theta) = T(\theta)\hat{\Delta}(\theta) \ ,$$

we write

$$\mathrm{D}\hat{\mathcal{F}}(\hat{K}_0) = (\mathcal{L}_\omega - \mathrm{Id}) + \mathcal{S}_\omega - \mathcal{T} \ .$$

Notice that, from 5.3), both $\mathcal{L}^s_\omega - \mathrm{Id}$ and $\mathcal{L}^u_\omega - \mathrm{Id}$ have continuous inverses, with

$$\|(\mathcal{L}^s_\omega - \mathrm{Id})^{-1}\| \leq \frac{1}{1-\lambda} \ , \ \|(\mathcal{L}^u_\omega - \mathrm{Id})^{-1}\| \leq \frac{\lambda}{1-\lambda} \ ,$$

and then $\mathcal{L}_\omega - \mathrm{Id}$ has continuous inverse with

$$\|(\mathcal{L}_\omega - \mathrm{Id})^{-1}\| \leq \frac{1}{1-\lambda} \ . \tag{36}$$

Hence, we write

$$\mathrm{D}\hat{\mathcal{F}}(\hat{K}_0)^{-1} = (\mathrm{Id} + (\mathcal{L}_\omega - \mathrm{Id})^{-1}(\mathcal{S}_\omega - \mathcal{T}))^{-1}(\mathcal{L}_\omega - \mathrm{Id})^{-1}$$

and, from 5.2) and 5.3), we have the estimate

$$\|\mathrm{D}\hat{\mathcal{F}}(\hat{K}_0)^{-1}\| \leq \frac{1}{1-\frac{\sigma+\tau}{(1-\lambda)}} \frac{1}{1-\lambda} = \frac{1}{1-(\lambda+\sigma+\tau)} \ . \tag{37}$$

Notice that we use condition 4): $\lambda + \sigma + \tau < 1$.

We estimate now the norm of $\mathrm{D}^2\hat{\mathcal{F}}$ on functions in

$$\bar{B}(\hat{K}_0, r) \ = \ \{\hat{K} \in C^0(\mathbb{T}^d, \mathbb{R}^n) \mid \|\hat{K} - \hat{K}_0\| \leq r\} \ .$$

Notice that, if $\hat{K} \in \bar{B}(\hat{K}_0, r)$, then

$$|P_2(\theta)(P_1(\theta)\hat{K}(\theta) - P_1(\theta)\hat{K}_0(\theta))|_\theta \leq (1+\tau)r = \bar{r} \ ,$$

where $\bar{r}$ is defined in 6), and we can apply condition 6) to obtain

$$\begin{aligned} &\mathrm{D}^2\hat{\mathcal{F}}(\hat{K})[\hat{\Delta}_1, \hat{\Delta}_2](\theta+\omega) \\ &\qquad = P_2(\theta+\omega)\mathrm{D}^2F(P_1(\theta)\hat{K}(\theta), \theta)[P_1(\theta)\hat{\Delta}_1(\theta), P_1(\theta)\hat{\Delta}_2(\theta)]. \end{aligned}$$

That is,

$$\|\mathrm{D}^2\hat{\mathcal{F}}(\hat{K})\| \leq b \tag{38}$$

for any $\hat{K} \in \bar{B}(\hat{K}_0, r)$.

Once we have the estimates (35), (37) and (38), the only argument we need to prove a) is to verify the conditions of Newton-Kantorovitch theorem, that is, to compute the constants ε and β of Theorem 3.1. From (35) and (37) we obtain the estimate

$$\|\mathrm{D}\hat{\mathcal{F}}(\hat{K}_0)^{-1}\hat{\mathcal{F}}(\hat{K}_0)\| \ \leq \ \frac{1}{1-(\lambda+\sigma+\tau)} \cdot \rho = \varepsilon \ ,$$

and using (38) and (37) we obtain

$$\|\mathrm{D}\hat{\mathcal{F}}(\hat{K}_0)^{-1}\mathrm{D}^2\hat{\mathcal{F}}(\hat{K})\| \ \leq \ \frac{b}{1-(\lambda+\sigma+\tau)} = \beta \ ,$$

for any $\hat{K} \in \bar{B}(\hat{K}_0, r)$. The rest of the proof of a) is a straightforward application of Theorem 3.1. So, the Newton method converges quadratically to an invariant torus $K_*(\theta) = P_1(\theta)\hat{K}_*(\theta)$ from the initial approximation $K_0(\theta) = P_1(\theta)\hat{K}_0(\theta)$, and $\|\hat{K}_* - \hat{K}_0\| \leq r_0$, where r_0 is defined in 7).

b) We will prove that, for any $\hat{K}(\theta) \in \bar{B}(\hat{K}_0, r_0)$, the resolvent of the transfer operator associated to $M(\theta) = \mathrm{D}F(K(\theta), \theta)$, with $K(\theta) = P_1(\theta)\hat{K}(\theta)$,

contains the whole unit circle. (If ω is irrational, we just need to check that 1 is in the resolvent). In particular, this will prove that the invariant torus K_* is normally hyperbolic.

Hence, for any $z \in \mathbb{C}$ with $|z| = 1$, and given $\nabla \in C^0(\mathbb{T}^d, \mathbb{R}^n)$, we have to solve the equation

$$\nabla(\theta) = \mathrm{D}F(K(\theta-\omega), \theta-\omega)\Delta(\theta-\omega) - z\Delta(\theta) \ ,$$

which is equivalent to

$$\begin{aligned} P_2(\theta)P_1(\theta)\hat{\nabla}(\theta) =& P_2(\theta)\mathrm{D}F(K(\theta-\omega), \theta-\omega)P_1(\theta-\omega)\hat{\Delta}(\theta-\omega) - \\ & zP_2(\theta)P_1(\theta)\hat{\Delta}(\theta) \ , \end{aligned} \tag{39}$$

once we perform the change of variables giving rise $\Delta = P_1\hat{\Delta}$ and $\nabla = P_1\hat{\nabla}$.

A first step is to compare the transfer operators associated to $M(\theta) = \mathrm{D}F(K(\theta), \theta)$ and $M_0(\theta) = \mathrm{D}F(K_0(\theta), \theta)$. To do so, we consider the vector bundle map (over the rotation ω) defined by

$$\begin{aligned} B(\theta) =& P_2(\theta)(\mathrm{D}F(K(\theta), \theta) - \mathrm{D}F(K_0(\theta), \theta))P_1(\theta-\omega) \\ =& \int_0^1 P_2(\theta)\mathrm{D}^2F(K_t(\theta), \theta)[P_1(\theta)(\hat{K}(\theta) - \hat{K}_0(\theta)), P_1(\theta)\cdot] \ dt \ . \end{aligned} \tag{40}$$

where $K_t(\theta) = tK(\theta) + (1-t)K_0(\theta)$. Notice that $\|\mathcal{B}_\omega\| \leq br_0$.

Then, the equation to be solved (39) is:

$$\begin{aligned} (\mathrm{Id} + T(\theta))\hat{\nabla}(\theta) = & (\Lambda_0(\theta-\omega) + S(\theta-\omega) + B(\theta-\omega))\hat{\Delta}(\theta-\omega) \\ & - z(\mathrm{Id} + T(\theta))\hat{\Delta}(\theta). \end{aligned} \tag{41}$$

Using transfer operator notation, (41) becomes:

$$(\mathrm{Id} + \mathcal{T})\hat{\nabla} = ((\mathcal{L}_\omega - z\mathrm{Id}) + \mathcal{S}_\omega + \mathcal{B}_\omega - z\mathcal{T})\hat{\Delta} \ , \tag{42}$$

The solution of (42) is, using the contraction mapping principle:

$$\hat{\Delta} = \left(\mathrm{Id} + (\mathcal{L}_\omega - z\mathrm{Id})^{-1}(\mathcal{B}_\omega + \mathcal{S}_\omega - z\mathcal{T})\right)^{-1} (\mathcal{L}_\omega - z\mathrm{Id})^{-1}(\mathrm{Id} + \mathcal{T})\hat{\nabla} \ .$$

Notice that

$$\|\hat{\Delta}\| \leq \frac{1+\tau}{1 - (\lambda + \sigma + \tau + br_0)}\|\hat{\nabla}\| \ ,$$

If $\lambda + \sigma + \tau + br_0 < 1$, we can ensure that the operator is a contraction. To prove this bound, use hypothesis 7) of Theorem 3.2 and $r_0 < 2\varepsilon$ to obtain:

$$\frac{b}{1 - (\lambda + \sigma + \tau)} r_0 < 2\beta\varepsilon = 2h < 1 \ .$$

c) Once we have computed the invariant torus K_*, we are ready to compute its stable and unstable subbundles from the approximate invariant bundles.

The equation to be solved is

$$P(\theta + \omega)^{-1}\mathrm{D}F(K_*(\theta), \theta)P(\theta) - \Lambda(\theta) = 0 \ . \tag{43}$$

The unknowns in (43) are P and $\Lambda = \text{blockdiag}(\Lambda^s, \Lambda^u)$. Instead of using these unknowns, we will introduce new variables which take advantage of the fact that we have an approximate solution. We introduce the new variables Q, Δ^s, Δ^u by:

$$P(\theta) = P_1(\theta)(\mathrm{Id} + Q(\theta)) \ , \ \Lambda^s(\theta) = \Lambda^s_0(\theta) + \Delta^s(\theta) \ , \ \Lambda^u(\theta) = \Lambda^u_0(\theta) + \Delta^u(\theta) \ ,$$

with

$$Q(\theta) = \begin{pmatrix} 0 & Q^{su}(\theta) \\ Q^{us}(\theta) & 0 \end{pmatrix} \ . \tag{44}$$

From the geometrical point of view, this construction is just writing the stable bundle as a graph of a vector bundle map $Q^{us}(\theta) : \mathbb{R}^{n_s} \to \mathbb{R}^{n_u}$ and the unstable bundle as a graph of a vector bundle map $Q^{su}(\theta) : \mathbb{R}^{n_u} \to \mathbb{R}^{n_s}$. This is an standard procedure in the study of stability of invariant splittings. See, for example [HP70]. In Section 4 we will generalize the construction to more general splittings.

We will use the contraction principle to analyze (43). First, notice that the initial error (we take is $Q^{us} = 0$ and $Q^{su} = 0$), is

$$\begin{aligned} \tilde{S}(\theta) &= P_1(\theta+\omega)^{-1} \mathrm{D}F(K_*(\theta), \theta) P_1(\theta) - \Lambda_0(\theta) \\ &= (\mathrm{Id} + T(\theta+\omega))^{-1} (\Lambda_0(\theta) + S(\theta) + B(\theta)) - \Lambda_0(\theta) \\ &= ((\mathrm{Id} + T(\theta+\omega))^{-1} - \mathrm{Id}) \Lambda_0(\theta) + (\mathrm{Id} + T(\theta+\omega))^{-1} (S(\theta) + B(\theta)) \ , \end{aligned}$$

where B is defined in (40) with $K = K_*$. The norm is

$$\|\tilde{S}\| \leq \frac{\tau}{1-\tau} \hat{\lambda} + \frac{1}{1-\tau} (\sigma + b r_0) = \tilde{\sigma} \ . \tag{45}$$

The equation (43) reads

$$\begin{aligned} 0 &= P_1(\theta+\omega)^{-1} \mathrm{D}F(K_*(\theta), \theta) P_1(\theta)(\mathrm{Id} + Q(\theta)) - \\ &\quad (\mathrm{Id} + Q(\theta+\omega))(\Lambda_0(\theta) + \Delta(\theta)) \\ &= (\tilde{S}(\theta) + \Lambda_0(\theta))(\mathrm{Id} + Q(\theta)) - (\mathrm{Id} + Q(\theta+\omega))(\Lambda_0(\theta) + \Delta(\theta)) \\ &= \Lambda_0(\theta) Q(\theta) - Q(\theta+\omega) \Lambda_0(\theta) - \Delta(\theta) + \tilde{S}(\theta)(\mathrm{Id} + Q(\theta)) - Q(\theta+\omega)\Delta(\theta) \ . \end{aligned}$$

If we write

$$\tilde{S}(\theta) = \begin{pmatrix} \tilde{S}^{ss}(\theta) & \tilde{S}^{su}(\theta) \\ \tilde{S}^{us}(\theta) & \tilde{S}^{uu}(\theta) \end{pmatrix} \ ,$$

then we see that we can set Δ^s, Δ^u by

$$\Delta^s(\theta) = \tilde{S}^{su}(\theta) Q^{us}(\theta) + \tilde{S}^{ss}(\theta) \ , \tag{46}$$

$$\Delta^u(\theta) = \tilde{S}^{us}(\theta) Q^{su}(\theta) + \tilde{S}^{uu}(\theta) \ , \tag{47}$$

where Q^{us} and Q^{su} solve the equations

$$\begin{aligned} \Lambda^s_0(\theta) Q^{su}(\theta) - Q^{su}(\theta+\omega) \Lambda^u_0(\theta) &= -(\tilde{S}^{ss}(\theta) Q^{su}(\theta) - Q^{su}(\theta+\omega) \tilde{S}^{uu}(\theta)) + \\ &\quad Q^{su}(\theta+\omega) \tilde{S}^{us}(\theta) Q^{su}(\theta) - \tilde{S}^{su}(\theta) \end{aligned} \tag{48}$$

(49)
$$\Lambda_0^u(\theta)Q^{us}(\theta) - Q^{us}(\theta+\omega)\Lambda_0^s(\theta) = -(\tilde{S}^{uu}(\theta)Q^{us}(\theta) - Q^{us}(\theta+\omega)\tilde{S}^{ss}(\theta)) + Q^{us}(\theta+\omega)\tilde{S}^{su}(\theta)Q^{us}(\theta) - \tilde{S}^{us}(\theta) \ .$$

Hence, we have just to solve (48) and (49). We will just present the details (48), because the analysis of (49) follows along the same lines. (Indeed, the results for (49) can be obtained by applying the results for (48) to the inverse mapping.)

By defining the linear operator $\mathcal{L}_\omega^{su}$ acting on continuous vector bundle maps (over the identity) $Q^{su}(\theta) : \mathbb{R}^{n_u} \to \mathbb{R}^{n_s}$ by

$$\mathcal{L}_\omega^{su} Q^{su}(\theta) = \Lambda_0^s(\theta-\omega)Q^{su}(\theta-\omega)(\Lambda_0^u(\theta-\omega))^{-1}$$

the equation (48) reads

(50)
$$Q^{su} = (\mathcal{L}_\omega^{su} - \mathrm{Id})^{-1} \circ (-\tilde{\mathcal{S}}_\omega^{ss} Q^{su} + Q^{us}(\tilde{\mathcal{S}}_\omega^{su} Q^{us} + \tilde{\mathcal{S}}_\omega^{ss}) - \tilde{\mathcal{S}}_\omega^{us}) \circ (\mathcal{L}_\omega^u)^{-1} \ ,$$

where

$$\|(\mathcal{L}_\omega^{su} - \mathrm{Id})^{-1}\| \leq \frac{1}{1-\lambda^2} \ .$$

The right hand side is considered as an operator $Q^{su} \to \bar{Q}^{su}$.

An observation is that from the estimate (45) we obtain the estimates $\|\tilde{S}^{ss}\| \leq \tilde{\sigma}$, $\|\tilde{S}^{su}\| \leq \tilde{\sigma}$, $\|\tilde{S}^{us}\| \leq \tilde{\sigma}$, $\|\tilde{S}^{uu}\| \leq \tilde{\sigma}$, because the projections onto the approximate invariant subbundles have (adapted) norms bounded by 1.

We will find a closed ball of radius α in which (50) satisfies the contraction principle. First, if $\|Q^{su}\| \leq \alpha$ then

$$\|\bar{Q}^{su}\| \leq \frac{\lambda}{1-\lambda^2}\tilde{\sigma}(1+\alpha)^2 = \mu(1+\alpha)^2 \ ,$$

where μ is defined in 9) of Theorem 3.2. So, the ball of radius α is mapped into itself if

$$\mu(1+\alpha)^2 \leq \alpha \ . \tag{51}$$

A Lipschitz constant of $\bar{Q}^{su}$ is

$$L = 2\frac{\lambda}{1-\lambda^2}\tilde{\sigma}(1+\alpha) = 2\mu(1+\alpha) \ . \tag{52}$$

The invariance condition is satisfied, for instance, if

$$\alpha = \frac{1}{2\mu} - 1 - \frac{1}{2}\sqrt{\frac{1}{\mu}\left(\frac{1}{\mu} - 4\right)} \ ,$$

where we assume that $\mu < \frac{1}{4}$ by the hypothesis 9). In such a case, the Lipschitz constant is

$$L = 2\mu(1+\alpha) = 1 - \sqrt{1-4\mu} < 1 \ ,$$

and $\bar{Q}^{su}$ is a contraction in the ball of radius α.

Finally, notice that for the solution Q^{su} of (48):

$$\|Q^{su}\| \leq \frac{1}{1-L}\frac{\lambda}{1-\lambda^2}\tilde{\sigma} = \frac{\mu}{\sqrt{1-4\mu}} \ .$$

With this estimates we complete the proof of Theorem 3.2. □

3.2. **Projection method.** In this section, we describe an algorithm which is more efficient than the direct application of Newton method described before in Section 2.2 by using the geometry of the problem.

The basic idea of the method is that we observe that, by taking projections over the stable and unstable directions, the infinitesimal equations can be solved just by iterating (either in the future or in the past). This is the mechanism of the proof of Theorem 3.2 and has the flavor of the techniques of the general theory of normally hyperbolic invariant manifolds.

When we update the torus, the linearization changes, hence, immediately after we update the invariant torus, we update the invariant splitting using the perturbative arguments developed in the previous section.

This avoids storing and inverting the discretized matrix in (18). This gives a very important speed up with respect to the algorithm based in a straight implementation of the discretization if the number of coefficients is high and the gap in the spectrum around the unit circle is not too small.

We now give some more details about the algorithm.

Suppose that we have an approximate normally hyperbolic invariant torus given by K, and we have also produced an approximate adapted frame P, in such a way that

$$P(\theta)^{-1}(F(K(\theta-\omega),\theta-\omega) - K(\theta)) = R(\theta) \ , \tag{53}$$

and

$$P(\theta+\omega)^{-1}\mathrm{D}F(K(\theta),\theta)P(\theta) - \Lambda(\theta) = S(\theta) \ , \tag{54}$$

where R and S are small.

In order to improve the estimates K, P, Λ^s, Λ^u, we look for $\tilde{K} = K + PH$, $\tilde{P} = P + PQ$, $\tilde{\Lambda}^s = \Lambda^s + \Delta^s$, $\tilde{\Lambda}^u = \Lambda^u + \Delta^u$, respectively.

Equation (2) reads

$$\begin{aligned} 0 &= P(\theta+\omega)^{-1}(F(K(\theta)+P(\theta)H(\theta),\theta) - K(\theta+\omega)) - H(\theta+\omega) \\ &= R(\theta+\omega) + P(\theta+\omega)^{-1}\mathrm{D}F(K(\theta),\theta)P(\theta)H(\theta) + O(H^2) - H(\theta+\omega) \\ &= R(\theta+\omega) + (\Lambda(\theta)+S(\theta))H(\theta) - H(\theta+\omega) + O(H^2) \end{aligned}$$

and gives rise to

$$\Lambda(\theta)H(\theta) - H(\theta+\omega) = -R(\theta+\omega) \ , \tag{55}$$

where we are neglecting all the quadratically small terms.

If we split H and R in the stable and unstable components, (55) splits in the fixed point equations

$$H^s(\theta) = \Lambda^s(\theta-\omega)H^s(\theta-\omega) + R^s(\theta), \tag{56}$$

$$H^u(\theta) = (\Lambda^u(\theta))^{-1}(H^u(\theta+\omega) - R^u(\theta+\omega)) \ . \tag{57}$$

Since Λ^s is contracting and Λ^u is expanding, both equations are solvable by using simple iteration.

Once we have improved K, we improve P and Λ. Since S, H, Q and Δ are supposed to be small, we eliminate the quadratically small terms in the following computations:

$$\begin{aligned} 0 &= \tilde{P}(\theta+\omega)^{-1}\cdot \mathrm{D}F(\tilde{K}(\theta)),\theta)\cdot\tilde{P}(\theta)-\tilde{\Lambda}(\theta) \\ &= (\mathrm{Id}-Q(\theta+\omega))P(\theta+\omega)^{-1}\cdot \mathrm{D}F(\tilde{K}(\theta)),\theta)\cdot P(\theta)(\mathrm{Id}+Q(\theta))-\Lambda(\theta)-\Delta(\theta) \\ &= P(\theta+\omega)^{-1}\mathrm{D}F(\tilde{K}(\theta),\theta)P(\theta)-Q(\theta+\omega)\Lambda(\theta)+\Lambda(\theta)Q(\theta)-\Lambda(\theta)-\Delta(\theta) \end{aligned}$$

Hence, we reach to the equation

$$\Lambda(\theta)Q(\theta)-Q(\theta+\omega)\Lambda(\theta)-\Delta(\theta) = -\tilde{S}(\theta) \tag{58}$$

where

$$\tilde{S}(\theta) = P(\theta+\omega)^{-1}\mathrm{D}F(\tilde{K}(\theta),\theta)P(\theta)-\Lambda(\theta) \tag{59}$$

Using the block matrix notation

$$A=\begin{pmatrix} A^{ss} & A^{su} \\ A^{us} & A^{uu}\end{pmatrix},$$

equation (58) reads

$$\Lambda^s(\theta)Q^{ss}(\theta)-Q^{ss}(\theta+\omega)\Lambda^s(\theta) = -\tilde{S}^{ss}(\theta)+\Delta^s(\theta)\ , \tag{60}$$

$$\Lambda^s(\theta)Q^{su}(\theta)-Q^{su}(\theta+\omega)\Lambda^u(\theta) = -\tilde{S}^{su}(\theta)\ , \tag{61}$$

$$\Lambda^u(\theta)Q^{us}(\theta)-Q^{us}(\theta+\omega)\Lambda^s(\theta) = -\tilde{S}^{us}(\theta)\ , \tag{62}$$

$$\Lambda^u(\theta)Q^{uu}(\theta)-Q^{uu}(\theta+\omega)\Lambda^u(\theta) = -\tilde{S}^{uu}(\theta)+\Delta^u(\theta)\ . \tag{63}$$

In order to solve (60) and (63), we choose $Q^{ss}(\theta)=0$, $Q^{uu}(\theta)=0$ and $\Delta_s(\theta)=\tilde{S}_{ss}(\theta)$, $\Delta_u(\theta)=\tilde{S}_{uu}(\theta)$. The geometrical meaning of such an election of Q is that we modify the stable and unstable frames in the complementary directions. This is the trick we have used in the proof of Theorem 3.2, but other choices could be possible (see Section 3.3). We compute $Q^{us}(\theta)$ and $Q^{su}(\theta)$ using the contraction principle, by writing the equations as

$$Q^{su}(\theta) = (\Lambda^s(\theta-\omega)Q^{su}(\theta-\omega)+\tilde{S}^{su}(\theta-\omega))(\Lambda^u(\theta-\omega))^{-1}, \tag{64}$$

$$Q^{us}(\theta) = (\Lambda^u(\theta))^{-1}(Q^{us}(\theta+\omega)\Lambda^s(\theta)-\tilde{S}^{us}(\theta))\ . \tag{65}$$

We do minor modifications in the previous arguments to compute the inverse of the change of variables $P(\theta)$. We have just defined $P_2(\theta)=P(\theta)^{-1}$, and added the equation $P_2(\theta)P(\theta)-\mathrm{Id}=0$.

Hence, we arrive to:

Algorithm 3.4 (Projection Method)**.** *Let $K(\theta)$ be an approximate normally hyperbolic invariant torus, $P_1(\theta)$ the matrix of an approximate adapted frame and $P_2(\theta)$ an approximate inverse of $P_1(\theta)$, and $\Lambda(\theta)=\mathrm{blockdiag}(\Lambda^s(\theta),\Lambda^u(\theta))$*

representing the dynamics on the approximate stable and unstable invariant bundles. That is:

$$\begin{aligned} P_2(\theta)(F(K(\theta-\omega),\theta-\omega)-K(\theta)) &= R(\theta)\ , \\ P_2(\theta+\omega)\mathrm{D}F(K(\theta),\theta)P_1(\theta)-\Lambda(\theta) &= S(\theta)\ , \\ P_2(\theta)P_1(\theta)-\mathrm{Id} &= T(\theta)\ , \end{aligned}$$

where R, S, T are small.

Then, one step on the projection method is to compute $\tilde{K} = K + P_1 H$, $\tilde{P}_1 = P_1 + P_1 Q$, $\tilde{P}_2 = P_2 - (Q+T)P_2$, $\tilde{\Lambda}^s = \Lambda^s + \Delta^s$, $\tilde{\Lambda}^u = \Lambda^u + \Delta^u$, following the next recipe:

- *Compute the components of H from*

$$\begin{aligned} H^s(\theta) &= \Lambda^s(\theta-\omega)H^s(\theta-\omega)+R^s(\theta), \\ H^u(\theta) &= (\Lambda^u(\theta))^{-1}(H^u(\theta+\omega)-R^u(\theta+\omega))\ . \end{aligned}$$

  using simple iteration.
- *Compute*

$$\tilde{S}(\theta) = P_2(\theta+\omega)\mathrm{D}F(\tilde{K}(\theta),\theta)P_1(\theta)-\Lambda(\theta)-T(\theta+\omega)\Lambda(\theta)\ ,$$

- *Compute the components of the matrix*

$$Q(\theta) = \begin{pmatrix} 0 & Q^{su}(\theta) \\ Q^{us}(\theta) & 0 \end{pmatrix}$$

  from the equations

$$\begin{aligned} Q^{su}(\theta) &= (\Lambda^s(\theta-\omega)Q^{su}(\theta-\omega)+\tilde{S}^{su}(\theta-\omega))(\Lambda^u(\theta-\omega))^{-1}, \\ Q^{us}(\theta) &= (\Lambda^u(\theta))^{-1}(Q^{us}(\theta+\omega)\Lambda^s(\theta)-\tilde{S}^{us}(\theta))\ , \end{aligned}$$

  that are solved again by simple iteration.
- *Set $\Delta^s(\theta) = \tilde{S}^{ss}(\theta)$ and $\Delta^u(\theta) = \tilde{S}^{uu}(\theta)$.*

Remark 3.5. This method avoids the storage and inversion of a large matrix from the discretization in terms of Fourier series of the linear equation (18). The speed of the procedure depends strongly on the rate of contraction and expansion of Λ^s and Λ^u, respectively.

Remark 3.6. The computation of $P_1(\theta)^{-1}$ can be done at each step, using Newton method, and so eliminating $T(\theta)$. We can do this for the computation of $\Lambda^u(\theta)^{-1}$.

Remark 3.7. There are cases in which the inverse of the matrix $P_1 = P$ is easily computable. Such as the case when the system is conformal symplectic and so P is also symplectic. In Section 5 we develop an algorithm adapted to the conformal symplectic case. Another interesting case in when the system is reversible.

3.3. **Reducibility method.** The previous method assumed that there was a frame in the bundle and we just computed matrices. The idea of the reducibility method is that one can also optimize the choice of the frame in such a way that the linearization becomes diagonal and constant.

As we will see, this reduction to constant coefficients is not always possible in the quasi-periodic case – in the periodic case, this is possible because of Floquet theory –. However, under some extra non-resonance conditions, which we will detail, it is possible to make such reduction. The extra conditions are non-trivial. As we will see, they fail in several cases. On the other hand, they are verified in many cases and, when they do hold, the method is extremely fast and accurate.

Definition 3.8. *We say that the invariant K torus is reducible if the cocycle $M(\theta) = \mathrm{D}F(K(\theta), \theta)$ over the rotation ω is reducible, that is there exists a constant matrix Λ and a change of variables $P(\theta)$ such that*

$$P(\theta + \omega)^{-1} M(\theta) P(\theta) - \Lambda = 0 \ . \tag{66}$$

The vector bundle map over the identity given by $P(\theta)$ is known as Floquet transformation.

One important case when reducibility holds is when the invariant subbundles are one dimensional and ω is Diophantine [JS81]. In such a case we can obtain $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, where the entries are real. For more general cases, including complex entries and dependence on parameters see [Eli88, Pös89, JS92, JS96, JdlLZ99].

The key idea of the *reducibility method* is to consider both invariance equation (2) and reducibility equation (66), in such a way that at each step of Newton method, the linear equation to be solved is, in some sense, diagonalized. This is a technique widely used in KAM theory (see, for instance, [dlL01, JdlLZ99] and the references therein).

Suppose that we have an approximate solution of (66) that is, we have $K(\theta)$, Λ and $P(\theta)$ such that

$$P(\theta)^{-1}(F(K(\theta - \omega), \theta - \omega) - K(\theta)) = R(\theta) \ , \tag{67}$$

$$P(\theta + \omega)^{-1} \mathrm{D}F(K(\theta), \theta) P(\theta) - \Lambda = S(\theta) \ , \tag{68}$$

where $R(\theta), S(\theta)$ are supposed to be small. Let $\tilde{K}(\theta) = K(\theta) + P(\theta)H(\theta)$, $\tilde{P}(\theta) = P(\theta)(\mathrm{Id} + Q(\theta))$ and $\tilde{\Lambda} = \Lambda + \Delta$ be the corresponding improvements, where $\Delta = \mathrm{diag}(\delta_1, \ldots, \delta_n)$.

Repeating the arguments of Section 3.2 we obtain the equation

$$\Lambda H(\theta) - H(\theta + \omega) = -R(\theta + \omega) \ , \tag{69}$$

whose components are, for $i = 1, \ldots, n$:

$$\lambda_i H^i(\theta) - H^i(\theta + \omega) = -R^i(\theta + \omega) \ , \tag{70}$$

Writing the Fourier modes of (70) we obtain

$$H^i_k = \frac{1}{1-\lambda_i e^{2\pi \mathbf{i} k\omega}} R^i_k \ , \tag{71}$$

for each $k \in \mathbb{Z}^d$. Small divisors do not appear, provided the eigenvalues λ_i are not in the unit circle. If there are some eigenvalues in the unit circle, we need some Diophantine conditions involving those eigenvalues and ω.

The equation for Q and Λ is obtained again following the methods explained in Section 3.2, and it is

$$\Lambda Q(\theta) - Q(\theta+\omega)\Lambda - \Delta = -\tilde{S}(\theta) \tag{72}$$

where $\tilde{S}(\theta) = -P(\theta+\omega)^{-1} \mathrm{D}F(\tilde{K}(\theta),\theta)P(\theta) - \Lambda$.

Writing (72) componentwise we obtain, for any $i, j = 1, \dots, n$:

$$\lambda_i Q^{ij}(\theta) - Q^{ij}(\theta+\omega)\lambda_j = -\tilde{S}^{ij}(\theta) \ , \text{ if } i \neq j, \tag{73}$$

$$\lambda_i Q^{ii}(\theta) - Q^{ii}(\theta+\omega)\lambda_i - \delta_i = -\tilde{S}^{ii}(\theta) \ , \text{ if } i = j \ . \tag{74}$$

If the eigenvalues are all of them different and the non-resonance condition $\lambda_i/\lambda_j \neq e^{2\pi \mathbf{i} k\omega}$ for all $k \in \mathbb{Z}^d$, $i \neq j$ is satisfied, then (73) is formally solvable by

$$Q^{ij}_k = \frac{-1}{\lambda_i - \lambda_j e^{2\pi \mathbf{i} k\omega}} \tilde{S}^{ij}_k \ . \tag{75}$$

Notice that small divisors do not appear if the eigenvalues have different modulus. If this is not the case, suppose that $\lambda_i/\lambda_j = e^{2\pi \mathbf{i}\alpha}$, $\alpha \neq 0$ (for instance, if they are complex conjugated), then one needs some Diophantine conditions involving α and ω in order to avoid resonances.

About (74), we fix

$$\delta_i = \tilde{S}^{ii}_0 \ , \ Q^{ii}_0 = 0$$

and then for $k \neq 0$

$$Q^{ii}_k = \frac{-1}{\lambda_i(1 - e^{2\pi \mathbf{i} k\omega})} \tilde{S}^{ii}_k \ .$$

Small divisors appear again and we need Diophantine properties on ω.

Notice that we have some freedom to choose the averages of the solutions of $Q^{ii}(\theta)$. We could apply extra normalizing conditions to fix, for instance, the averages of the diagonal elements $P^{ii}(\theta)$.

Algorithm 3.9 (Reducibility Method)**.** *Let $K(\theta)$ be an approximate invariant torus. Let $P_1(\theta)$ be the matrix of an approximate adapted frame and $P_2(\theta)$ be an approximate inverse of $P_1(\theta)$, and $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_n)$ be the constant matrix representing the dynamics on the approximate complex 1-dimensional invariant bundles (generated by the columns of $P_1(\theta)$). That is:*

$$\begin{aligned} P_2(\theta)(F(K(\theta-\omega),\theta-\omega) - K(\theta)) &= R(\theta) \ , \\ P_2(\theta+\omega)\mathrm{D}F(K(\theta),\theta)P_1(\theta) - \Lambda &= S(\theta) \ , \\ P_2(\theta)P_1(\theta) - \mathrm{Id} &= T(\theta) \ , \end{aligned}$$

where R, S, T are small.

Then, one step on the reducibility method is to compute $\tilde{K} = K + P_1 H$, $\tilde{P}_1 = P_1 + P_1 Q$, $\tilde{P}_2 = P_2 - (T+Q)P_2$, $\tilde{\Lambda} = \Lambda + \Delta$, following the next recipe:

- *Compute the Fourier modes of $H = (H^1, \ldots, H^n)^\top$ by*

$$H_k^i = \frac{1}{1 - e^{-2\pi \mathbf{i} k\omega} \lambda_i} R_k^i \ . \tag{76}$$

- *Compute*

$$\tilde{S}(\theta) = P_2(\theta + \omega) \mathrm{D}F(\tilde{K}(\theta), \theta) P_1(\theta) - \Lambda - T(\theta + \omega)\Lambda \ . \tag{77}$$

- *For $i, j = 1, \ldots, n$, $i \neq j$, and for all $k \in \mathbb{Z}^d$ set*

$$Q_k^{ij} = \frac{-1}{(\lambda_i - e^{2\pi \mathbf{i} k\omega} \lambda_j)} \tilde{S}_k^{ij} \ . \tag{78}$$

- *For $i = 1, \ldots, n$, set*

$$\delta_i = \tilde{S}_0^{ii} \ , \ Q_0^{ii} = 0 \ ,$$

and for all $k \in \mathbb{Z}^d \setminus \{0\}$

$$Q_k^{ii} = \frac{-1}{\lambda_i (1 - e^{2\pi \mathbf{i} k\omega})} \tilde{S}_k^{ii} \ .$$

Remark 3.10. Note that the reducibility algorithm runs into problems if the denominators in (77) become zero. This can happen when the matrix Λ has two eigenvalues of the same modulus and whose phases differ by a rational angle. Of course, if the eigenvalues are not of modulus 1, the torus is normally hyperbolic and the other algorithms (Newton method, Projection method) described before work.

Hence, the reducibility method has more restrictions on the frequencies that the projection or the Newton method. Of course, the reducibility method yields more information since reducibility is a geometrically important property.

Remark 3.11. If the torus is normally hyperbolic and the spectrum of the associated transfer operator is decomposed in n circles, then there exists an splitting of $\mathbb{R}^n \times \mathbb{T}^d$ in n invariant subbundles of rank 1. We can trivialize them by a covering of a sufficiently high number of leaves of the torus $\mathbb{T}^d$.

Notice that Theorem 3.2 does not depend on the torus being reducible. It only depends on the approximate tori, and its hyperbolicity properties. Hence, in practice, we use the reducibility method to compute the approximate torus and the invariant subbundles of the linearization and, then, validate the computation using Theorem 3.2.

We note that the application of Theorem 3.2 to the results of a reducibility calculation are particularly easy. Issues such as the contractivity or the adapted metric are very easy. If Λ is diagonalized by $\Lambda = \mathrm{diag}(\lambda_1^s, \ldots, \lambda_{n_s}^s, \lambda_1^u, \ldots, \lambda_{n_u}^u)$, with

$$|\lambda_1^s| \leq \cdots \leq |\lambda_{n_s}^s| < 1 < |\lambda_{n_u}^u| \leq \cdots \leq |\lambda_1^u|$$

then we can take the Finsler norm as the sup-norm on the adapted coordinates (constant on the fibers). Notice that, if $\Lambda^s = \mathrm{diag}(\lambda^s_1, \ldots, \lambda^s_{n_s})$ and $\Lambda^u = \mathrm{diag}(\lambda^u_1, \ldots, \lambda^u_{n_u})$, then

$$\|\Lambda^s\| = |\lambda^s_{n_s}| \ , \ \|(\Lambda^u)^{-1}\| = \frac{1}{|\lambda^u_{n_u}|}$$

and $\lambda = \max(|\lambda^s_{n_s}|, \frac{1}{|\lambda^u_{n_u}|})$.

Remark 3.12. For a reducible torus, we have that the torus is normally hyperbolic if and only if the eigenvalues of Λ are outside of the unit circle.

Nevertheless, the numerical method does not distinguish on whether the eigenvalues are inside or outside of the unit circle. However, we note that in case that there are eigenvalues of Λ in the unit circle, there is the possibility of small divisors in the computation of H, described in (76), but, in practice, very often, the numerical calculation proceeds without interruption because the smallness of the divisors is compensated by the smallness of the numerators.

We note that the presence of elliptic eigenvalues is to be expected in the case of symplectic systems, but there is some justification for the use of the reducibility method based on KAM theory. The justification is not for a single torus, but rather for calculations in a family depending on a extra parameter μ. If the eigenvalues depend in such a way that the eigenvalues and their differences depend on μ, it is possible to exclude a set of parameters of small measure so that the small divisors in (76) and (78) are under control and hence, for these values of the parameter are invariant tori which are reducible. The stability theory of elliptic tori are covered in several references [Eli88, Pös89, JS96]. A formulation of the results for families which takes as a starting point the existence of an approximate solution of the invariance and reducibility equation and, which is, therefore, very close to the point of view of Theorem 3.2, we refer to [JdlLZ99].

We note that, in KAM theory, ensuring the reducibility requires to have control on the small divisors that appear in (78), besides the small divisors that appear in (76). The small divisors corresponding to (76) are called the *First Melnikov condition* and those corresponding to (78), the *Second Melnikov condition*.

One question that received attention in recent times – it is crucial in application of KAM theory in PDE's – was the proof of persistence of normally hyperbolic tori using only the first Melnikov condition. There are many solutions in the literature. Of particular interest for us is the solution based on quasi-reducibility introduced in [Eli01] and which we will study in Section 3.4.

Remark 3.13. In the presentation of the algorithm, we have only shown here how to improve reducibility using near identity transformations. In [MP84] it is shown how in the case of resonances one can improve reducibility using transformations which are not near the identity.

Notice that repeating indefinitely these transformations that are not near the identity is a non convergent procedure. On the other hand, it looks plausible that one could use them just a finite (and small) number of times in a continuation algorithm to avoid parameter values where reducibility stops due to resonances. See [Eli97, Eli01] for related results. In particular, [Eli01] shows that one can use this procedure to establish persistence of lower dimensional tori of Hamiltonian systems with only the first Melnikov condition.

We have implemented these transformations in [HdlL01a]. Our numerical experiments suggest that there are cases in which the resonances of elliptic eigenvalues are the place of birth of hyperbolic eigenvalues, and then reducibility is much better is those cases. Relatedly, the torus gains regularity when the strong perturbations make it become hyperbolic! (These sort of phenomena have been analyzed in [BHJ$^+$03] for quasiperiodically forced Hamiltonian systems with one degree of freedom.) In fact, the type of resonance has to do with the topology of the invariant bundles associated with those hyperbolic eigenvalues. As a result, the index of the embeddings giving the bundles is very related with the specific transformation not near the identity that one uses to gain reducibility. We can use this information to cross resonances [HdlL01a].

Remark 3.14. In [HdlL01a], one can find numerical results obtained studying a quasi-periodic perturbation of the standard map. We briefly summarize the observations of [HdlL01a] here since they are the motivation for some of the algorithms that we will describe now. In particular for the high precision calculation of invariant bundles and the multiplier on them.

In [HdlL01a], one can find a numerical continuation of an elliptic periodic orbit of period 3. It persists as an elliptic periodic torus for a (presumably) Cantor set of parameters. In the gaps, the periodic torus is normally hyperbolic (in one gap the stable and unstable invariant manifolds correspond to a bundle of index 2). At some value of the perturbation, the torus is normally hyperbolic, but it seems that eventually it is destroyed. The destruction of the invariant torus seems to be due to the fact that stable and unstable subbundles become closer, even if the hyperbolicity multipliers λ remain constant. From the point of view of functional analysis, the spectral projections associated to the two circles of the spectrum (one inside and the other outside of the unit circle) become unbounded and at the critical value, the spectrum is an annulus containing the unit circle. The periodic curve does not exist beyond this point.

Notice that the set of parameters for which the torus is normally hyperbolic (a saddle) is open. This is closely the well known phenomenon of semicontinuity of the spectrum [Kat76]. That is, if there is a gap in the spectrum, the torus is saddle-type, and the gap persists for a small enough perturbation.

On the other hand, it could well happen (and the experiments in [HdlL01a] suggest that this is the case) that the spectrum of the linearization contains a gap when the parameters lie in an open interval $(0, \varepsilon_0)$ but that nevertheless, at the boundaries of the interval, the gap is closed. The size of the gap can be uniform for $(0, \varepsilon_0)$ but the norm of the spectral projections grows.

Remark 3.15. Notice that in practice, we have just a rational approximation of ω, but Fourier expansions are truncated, and "zero" divisors do not appear if we are far from resonances. The numerical methods produce "almost" invariant objects. For results on effective reducibility, see [JRRV97].

Remark 3.16. When it is applicable, the reducibility method is the fastest of the methods we have discussed. It is specially appropriate for computation of high dimensional tori, because it not only avoids the large matrix problem, but also diagonalizes the linear equations at each step of Newton method.

Of course, when applying the reducibility method, we should be prepared to study the cases where reducibility fails but the torus persists.

Note that we expect problems when the eigenvalues have the same modulus. This – heuristically – means that, when continuing families, we should expect problems in sets of codimension one. When studying families (this appears naturally in homotopy methods, see Section 3.5), it is advantageous to use the reducibility method, but pay attention to the cases where it fails. In the cases that reducibility fails, but that normal hyperbolicity persists, we have to change to another of the methods. We will present a practical implementation in an example in [HdlL01a].

Remark 3.17. If we do not diagonalize the matrix Λ during the Newton process, then (69) reads in Fourier modes

$$(\Lambda - e^{2\pi \mathbf{i} k\omega}) H_k = -e^{2\pi \mathbf{i} k\omega} R_k \tag{79}$$

that is solved by

$$H_k = (\mathrm{Id} - e^{-2\pi \mathbf{i} k\omega} \Lambda)^{-1} R_k \ , \tag{80}$$

provided that the eigenvalues of Λ are different from $e^{-2\pi \mathbf{i} k\omega}$.

Moreover, (72) reads

$$\Lambda Q_0 - Q_0 \Lambda - \Delta = -\tilde{S}_0 \ , \tag{81}$$

$$\Lambda Q_k - e^{2\pi \mathbf{i} k\omega} Q_k \Lambda = -\tilde{S}_k \ \text{ for all } k \neq 0 \ . \tag{82}$$

A solution of (81) is

$$Q_0 = 0 \ , \ \Delta = \tilde{S}_0 \ .$$

The equations (82) are linear in the coefficients of the matrices Q_k.

A compact way of writing (82) is using Kronecker product. Recall that the Kronecker product of two matrices $A \in M_{m,n}$ and $B \in M_{p,q}$ is the

mp, np-matrix

$$A \otimes B \;=\; \begin{pmatrix} a_{1,1}B & a_{1,2}B & \dots & a_{1,n}B \\ a_{2,1}B & a_{2,2}B & \dots & a_{2,n}B \\ \vdots & \vdots & & \vdots \\ a_{m,1}B & a_{m,2}B & \dots & a_{m,n}B \end{pmatrix} .$$

We also use the notation

$$\mathrm{vec}(A) \;=\; (a_{1,1}, a_{2,1}, \dots, a_{m,1}, \dots, a_{1,n}, a_{2,n}, \dots, a_{m,n})^\top ,$$

that is, we stacking the columns of A.

Then, (82) is written as a linear system in $\mathrm{vec}(Q_k)$:

$$(\mathrm{Id}_n \otimes \Lambda - e^{2\pi \mathbf{i} k\omega} \Lambda^\top \otimes \mathrm{Id}_n)\mathrm{vec}(Q_k) = -\mathrm{vec}(\tilde{S}_k) \tag{83}$$

This equation has an unique solution if $\lambda_i \neq e^{2\pi \mathbf{i} k\omega}\lambda_j$ for all λ_i, λ_j eigenvalues of Λ.

This method is useful since we do not need to deal with complex eigenvalues and all the procedures can be set in the realm of real Fourier series.

Once we have computed the torus, we can diagonalize the matrix Λ to know the eigenvalues (real or complex).

3.4. **Almost reducibility.** Note that in the normally hyperbolic case, all the algorithms we have designed are contractions. Hence, there is room to maneuver and change the algorithms without altering their contraction properties.

In the reducibility case, the basic observation is that, if the only thing that we need is a computational step, we do not need that the torus is exactly reducible. If we detect that improving the reducibility becomes computationally hard, we just use the approximate solution of the reducibility equation to obtain an improved solution of the Newton step. Even if we do not achieve complete reducibility this is still more efficient than the projection method.

We give some more algorithm details.

Let $K_0(\theta)$ be the approximate invariant torus, whose monodromy matrix $M(\theta) = \mathrm{D}F(K_0(\theta), \theta)$ is close to be reducible. That is:

$$P(\theta)^{-1}(F(K_0(\theta - \omega), \theta - \omega) - K_0(\theta)) \;=\; R(\theta) , \tag{84}$$

$$P(\theta + \omega)^{-1} M(\theta) P(\theta) - \Lambda \;=\; S(\theta) , \tag{85}$$

where $P(\theta)$ and the constant matrix Λ are given, and $R(\theta), S(\theta)$ are assumed to be small.

We will look for the invariant torus as $K(\theta) = K_0(\theta) + P(\theta)H(\theta)$. We obtain that H has to satisfy the equation:

$$\begin{aligned} \Lambda H(\theta) - H(\theta + \omega) = & - S(\theta)H(\theta) \\ & - P(\theta + \omega)^{-1} \left[F(K_0(\theta) + P(\theta)H(\theta)) - K_0(\theta + \omega)\right. \\ & \left. - \mathrm{D}F(K_0(\theta), \theta)P(\theta)H(\theta)\right] . \end{aligned}$$

We can compute H using simple iteration: given H, we compute the right hand side $\hat{R}(\theta+\omega)$, and compute the new H solving $\Lambda H(\theta) - H(\theta+\omega) = \hat{R}(\theta+\omega)$.

3.5. **Continuation of invariant tori.** All the methods that we have discussed so far are methods that improve a sufficiently approximate solution. So far, we have not discussed how to obtain a solution approximate enough so that the improving algorithms start working.

A natural technique in this situation is to use a continuation method that follows a family connecting the problem we are interested in to another problem that can be solved explicitly. In many situations, the parameters connecting to a trivial problem have a physical interpretation (e.g. a coupling constant) but it is also quite common that the parameters are just introduced for numerical analysis purposes. These methods are often called homotopy methods. For a reference about general properties of homotopy methods, we refer to [AG03]. A general implementation of homotopy methods is `Hompack`. In our case, however, we can again take advantage to the geometric properties of the method and obtain homotopy methods that are more efficient than the general ones.

Let F_ε be a family of quasi-periodic maps, all of them with the same frequency vector ω. The continuation curve is the set of

$$(\varepsilon, K_\varepsilon) \ ,$$

where K_ε is an invariant torus for F_ε.

Suppose that we have computed an invariant torus $K_{\varepsilon_0} = K^0(\theta)$, and we want to estimate the invariant torus $K_\varepsilon(\theta)$ for F_ε, with $\varepsilon - \varepsilon_0$ small. We could just take K^0 as an initial guess for the Newton method for F_ε. One can, however, obtain better initial guesses. One general procedure, commonly used in homotopy methods is to extrapolate from previously computed points in the curve. In our case, however, we can compute rather efficiently the derivatives with respect to ε of K_ε. This can lead to more efficient methods.

Notice that in [HdlL01b] it is shown that when the tori are normally hyperbolic, the dependence on the parameters is as smooth as the family of maps. This serves a justification of the homotopy method when the tori remain normally hyperbolic.

Since

$$F_\varepsilon(K_\varepsilon(\theta), \theta) = K_\varepsilon(\theta+\omega),$$

by differentiating with respect to ε and evaluating at ε_0, we obtain that the first variation of the family K_ε in $\varepsilon = \varepsilon_0$,

$$K^1(\theta) = \frac{\partial K_\varepsilon}{\partial \varepsilon}_{|\varepsilon=\varepsilon_0}(\theta) \ ,$$

satisfies the linear equation

$$\mathrm{D}F_0(K^0(\theta),\theta)K^1(\theta) - K^1(\theta+\omega) = -F^1(K^0(\theta),\theta) \ , \tag{86}$$

where

$$F^1(x,\theta) = \frac{\partial F}{\partial \varepsilon}_{|\varepsilon=\varepsilon_0}(x,\theta) \ .$$

Hence, we can compute the derivative with respect to parameters by solving the linear equation (86), which is identical to the equations that we have studied in Section 3.2 or Section 3.3.

Notice also that an adapted frame for K_{ε_0} is an approximate adapted frame for K_ε. This allows us to use the computational effort invested in computing the guess into the refinement that we need to perform for the new value of ε.

It is also possible to compute other derivatives to obtain better guesses in the continuation method. The basic idea is to take more derivatives with respect to ε and match the terms. Each of the steps involves solving an equation of the same type that we have solved already for the first derivative. We will, however, not pursue this matter here.

4. Computation of invariant subbundles

In this section, we describe algorithms to compute invariant subbundles of the linearization once we have computed an invariant torus K. To do so, we study the spectral properties of the transfer operator associated to $M(\theta) = \mathrm{D}F(K(\theta),\theta)$, that are translated geometrically in the existence of invariant subbundles for the linear skew product

$$\begin{aligned} \bar v &= M(\theta) v \ , \\ \bar\theta &= \theta + \omega \ . \end{aligned} \tag{87}$$

We will develop algorithms for the study of the properties of the cocycle (87). The goal is to develop algorithms to compute invariant subbundles that correspond to different spectral annuli. For more information on properties of the spectrum of transfer operators and their relation to geometric properties of the cocycles, we refer to [HdlL03a, HdlL03b] and references there.

Notice that both Projection method and Reducibility method give information about the dynamics of the cocycle (87). We will isolate here the study of the cocycle from the computation of the invariant torus.

Remark 4.1. Note that, since we have results that tell us that the approximate solutions of the invariant circle are close to true solutions, we can easily estimate the difference between the true cocycle and the cocycle (87) evaluated on the approximate solution. The approximate solutions we will obtain for the invariance equations with the numerical approximation of the cocycle are also approximate solutions for the invariance equation of the true invariant torus.

Since we also have results that tell us that approximate solutions of the invariance equations are close to true solutions, we have that the approximates solutions of the invariance equations for an approximately invariant torus correspond to true solutions of the invariant torus.

4.1. **Computation of spectral subbundles.** Our first task is to construct frames for the different invariant subbundles. This is an extension of the algorithm that we used in Section 3.2. In that case, we used only two bundles, one stable and one unstable. In this case, we will try to study bundles separated by different expansion rates.

We will present an iterative algorithm that, given an approximate invariant frame produces a more approximate one. In practice, the following algorithm is used as part of a continuation method.

Algorithm 4.2. *Let $M(\theta) \in M_n(\mathbb{R})$ be a vector bundle map over the rotation ω. Let $P(\theta) \in M_n(\mathbb{R})$ be an approximate adapted frame, such that*

$$P(\theta+\omega)^{-1} M(\theta) P(\theta) - \Lambda(\theta) = S(\theta)$$

is small enough, where Λ is the block-diagonal matrix

$$\Lambda(\theta) = \text{blockdiag}(\Lambda_1(\theta), \dots \Lambda_k(\theta)) \ ,$$

with $\Lambda_i(\theta) \in M_{n_i}(\mathbb{R})$ ($n_1 + \cdots + n_k = n$). For a suitable Finsler metric $\|\cdot\|$, assume that

$$\|\Lambda_i\| \|\Lambda_j^{-1}\| < 1 \ , \tag{88}$$

for $i, j = 1, \dots, k$, $i < j$.

Then, we produce the invariant frame as $\tilde{P}(\theta) = P(\theta)(\text{Id} + Q(\theta))$, where

$$Q(\theta) \ = \ \begin{pmatrix} 0 & Q^{1,2}(\theta) & Q^{1,3}(\theta) & \dots & Q^{1,k}(\theta) \\ Q^{2,1}(\theta) & 0 & Q^{2,3}(\theta) & \dots & Q^{2,k}(\theta) \\ \vdots & & \ddots & \dots & \vdots \\ Q^{k,1}(\theta) & Q^{k,2}(\theta) & Q^{k,3}(\theta) & \dots & 0 \end{pmatrix}$$

and the $Q^{i,j}$ are $n_i \times n_j$ matrices that solve the equations

(89)

$$\begin{aligned} \Lambda_i(\theta) Q^{i,j}(\theta) - Q^{i,j}(\theta+\omega)\Lambda_j(\theta) = -S^{i,j}(\theta) - \sum_{l=1}^{k} S^{i,l}(\theta) Q^{l,j}(\theta) \\ + Q^{i,j}(\theta+\omega) \left(S^{j,j}(\theta) + \sum_{l=1}^{k} S^{j,l}(\theta) Q^{l,j}(\theta) \right) \ , \end{aligned}$$

for $i, j = 1, \dots, k$, $i \neq j$.

The dynamics on the subbundles are given by $\tilde{\Lambda}(\theta) = \Lambda(\theta) + \Delta(\theta)$, where block-diagonal matrix

$$\Delta(\theta) = \text{blockdiag}(\Delta_1(\theta), \dots, \Delta_k(\theta))$$

is given by

$$\Delta_i(\theta) = S^{i,i}(\theta) + \sum_{l=1}^{k} S^{i,l}(\theta) Q^{l,i}(\theta) \ .$$

When $i < j$, we rewrite the equations (89) as:

$$\begin{aligned} Q^{i,j}(\theta+\omega) = \Bigg[&\Lambda_i(\theta) Q^{i,j}(\theta) + \left(S^{i,j}(\theta) + \sum_{l=1}^{k} S^{i,l}(\theta) Q^{l,j}(\theta) \right) \\ &- Q^{i,j}(\theta+\omega) \left(S^{j,j}(\theta) + \sum_{l=1}^{k} S^{j,l}(\theta) Q^{l,j}(\theta) \right) \Bigg] \Lambda_j(\theta)^{-1} \ ; \end{aligned} \tag{90}$$

and when $i > j$ as

$$\begin{aligned} Q^{i,j}(\theta) = &\Lambda_i(\theta)^{-1} \Bigg[Q^{i,j}(\theta+\omega)\Lambda_j(\theta) - \left(S^{i,j}(\theta) + \sum_{l=1}^{k} S^{i,l}(\theta) Q^{l,j}(\theta) \right) \\ &+ Q^{i,j}(\theta+\omega) \left(S^{j,j}(\theta) + \sum_{l=1}^{k} S^{j,l}(\theta) Q^{l,j}(\theta) \right) \Bigg] \ . \end{aligned} \tag{91}$$

Because (88) we have that, for small S, Q the RHS of (91),(90) are contractions, when considered as functionals depending on Q. Hence, by iterating the RHS of (90),(91), we solve (89).

Remark 4.3. The theory of invariant manifolds in [HdlL01b] and the algorithms for invariant manifolds that we will discuss later in Section 6.1 do not require that the invariant subbundles out of which we construct the manifold are spectral subbundles. Indeed they do not require that they have invariant complements (an example of this situation is the eigenvector in a non-trivial Jordan block).

Invariant bundles without invariant complements appear in practice, for example in identical systems with master-slave coupling. Nevertheless, this situations are unstable under general perturbations. Hence, the algorithms to compute them cannot be general purpose algorithms such as the ones described here and have to rely on the specific properties of the system that we are considering.

4.2. **Computation of Floquet transformations.** The most precise information about normal behavior that one can obtain is when the cocycle is reducible that is, we can find a frame in which the cocycle (87) becomes a matrix independent of θ (see Definition 3.8). We will assume along this section that the frequency vector ω is Diophantine.

In this section, we discuss different algorithms to compute numerically the reducing change of variables, also known as Floquet transformation. Some of them are not perturbative.

A first observation is that the reducibility equation (66),

$$M(\theta)P(\theta) = P(\theta+\omega)\Lambda \ ,$$

is not uniquely solvable for $P(\theta)$ and Λ (besides linear and constant changes of variables). If the cocycle is reducible to a matrix

$$\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$$

through a change of variables $P(\theta)$, then it is also reducible to a matrix

$$\Lambda_k = \mathrm{diag}(e^{-2\pi \mathbf{i} k_1 \cdot \omega} \lambda_1, \ldots, e^{-2\pi \mathbf{i} k_n \cdot \omega} \lambda_k) \ ,$$

where $k = (k_1, \ldots, k_n) \in \mathbb{Z}^d$, through a change of variables $P_k(\theta) = P(\theta) E_k(\theta)$, where

$$E_k(\theta) = \mathrm{diag}(e^{2\pi \mathbf{i} k_1 \cdot \theta}, \ldots, e^{2\pi \mathbf{i} k_n \cdot \theta}) \ .$$

That is to say, $M(\theta) P_k(\theta) = P_k(\theta + \omega) \Lambda_k$. Notice that the transformations E_k for $k \neq 0$ are not near the identity [MP84]. This observation plays an important role in the theory of reducibility. We have used them in [HdlL01a] to cross resonances (see remarks 3.13,3.14).

Henceforth, in the following when we refer to the eigenvalues of the cocycle, we are referring to the eigenvalues of one of the reduced matrices. The election of one particular reduced matrix can follows from numerical computations, or from topological arguments, as we will see in the examples in [HdlL01a].

There are several algorithms to compute $P(\theta)$ and Λ which we have considered.

4.2.1. *Discretization method.* In [Jor01] the following heuristic method of solving (66) is proposed: discretize the infinite dimensional problem in a standard matrix eigenvalue problem, cutting off the tails of the Fourier series, and use a package of linear algebra to solve it. If one computes all the eigenvalues of the discretized problem, one has to choose the suitable ones. The method produces spurious eigenvalues, that have to be discarded (if fact, the discretized eigenvalue problem could even produce zero eigenvalues, that are not present in the spectral problem). Choosing the real eigenvalues is an easier task than choosing the pairs of complex conjugated eigenvalues. This method is slow, because we have to compute all the eigenvalues of a large matrix, and then we have to select the appropriate ones. See [Jor01] for details.

4.2.2. *Rational approximation of the frequencies.* In this method we start by choosing a sequence of rational vectors $p_i/n_i \in \mathbb{Q}^d$ ($p_i \in \mathbb{Z}^d$ and $n_i \in \mathbb{N}$) converging to the irrational vector ω. If $d = 1$ it is natural to use continuous fraction algorithm. If $d > 1$ there are several algorithms to generate rational approximations, one of the best known ones is the Jacobi-Perron algorithm. (See [LH86, HK02] for a survey of rational approximation algorithms in higher dimensional spaces.)

For each i we have,

$$P(\theta + n_i \omega)^{-1} M(\theta + (n_i - 1)\omega) \ldots M(\theta + \omega) M(\theta) P(\theta) = \Lambda^{n_i}$$

Since $\theta + n_i \omega$ is close to an integer vector and $P(\theta)$ is 1-periodic in all its variables, then $P(\theta + n_i \omega) \simeq P(\theta)$, and the eigenvalues of

$$M(\theta, n_i) = M(\theta + (n_i - 1)\omega) \ldots M(\theta + \omega) M(\theta) \tag{92}$$

will be close to the eigenvalues of Λ^{n_i}. Notice that the procedure is independent on θ (since ω is ergodic), and we can take $\theta = 0$. Once we have estimated the eigenvalues of Λ^{n_i}, we have to do the n_i-root of them to estimate the eigenvalues of Λ. Since there are n_i complex n_i-roots, we have also to decide what to choose.

This method improve the estimates of the eigenvalues at each step. Since the eigenvalues of Λ^{n_i} can grow or decrease very fast, we have to make scalings when iterating. Notice that this idea is very related with some methods of computation of Lyapunov multipliers.

Remark 4.4. From several estimates of an eigenvalue corresponding to several rational approximations, we can produce a new estimate by interpolation. A similar trick is proposed in [Sim98b] to compute invariant tori.

Remark 4.5. One of the most efficient methods to compute non-dominant Lyapunov multipliers is the reduction to upper triangular matrices. See [BGGS78, ER85, NY98, DVV02]. We recursively define

$$Q_{n+1}(\theta)R_{n+1}(\theta) = M(\theta + n\omega)Q_n(\theta)$$

where the Q are unitary and the R are upper triangular. Then, one can read off the Lyapunov exponents by just accumulating the diagonal elements of the R. The only steps of the method are multiplications by unitary transformations and the QR algorithm, which are rather robust to round off error.

The algorithm above is quite close to the proof in [Ose68] of the multiplicative ergodic theorem and it is useful in great generality, including non-uniformly hyperbolic systems with a singular invariant measure.

The cases considered here are notably simpler than the full generality of the theorem. We are assuming uniform hyperbolicity and the rotations are uniquely ergodic. In the case that the bundles are one-dimensional, the existence of negative (resp. positive) Lyapunov exponents is equivalent to uniform contractivity (resp expansivity). See Remark 4.8.

A bundle version of the above method has been developed in [DVV02].

Remark 4.6. Recall that Lyapunov multipliers are in the spectrum [SS78, HdlL03a], and in the reducible case the spectrum is a set of circles, so they can be computed easily. In fact, the degree of precision of the computation of the Lyapunov multipliers is an indicator of the reducibility of the cocycle. (See [HdlL01a] for numerical examples).

The computation of the eigenvalues of the matrices (92) is equivalent to the computation of the eigenvalues of the $\hat{M}$ matrices defined by:

$$\hat{M}_{n_i} = \begin{pmatrix} 0 & & \dots & & M_{n_i-1} \\ M_0 & 0 & \dots & & 0 \\ & M_1 & \dots & & 0 \\ & & \ddots & & \vdots \\ & & & M_{n_i-2} & 0 \end{pmatrix} \tag{93}$$

where $M_k = M(\theta + k\omega)$ [HdlL03b]. Although these matrices are very large, we can take advantage of the symmetry of their eigenvalues in order to perform the computations: if z is an eigenvalue of M_{n_i}, then $ze^{2\pi \mathbf{i} k/n_i}$ is also an eigenvalue, where $k = 0, \ldots, n_i - 1$.

4.2.3. *Power method applied to rank-one bundles.* One of the simplest methods to compute a dominant eigenvalue (and the corresponding eigenvalue) is just to iterate the application of the operator to a vector.

Applying the same idea, we can iterate the transfer on a section. Since there is a circle of dominant eigenvalues, applying the algorithm to real sections we will obtain the real dominant eigenvalue (if it exists). If the computation suggests that there are two dominant eigenvalues (for instance, they are complex conjugated), then we have to iterate a pair of sections, an so on. As is standard in the power method, we find it convenient to perform scalings at each step.

Assume we are in the simplest case that there is one dominating eigenvalue which is simple. Then, the power method produces a section v and a real function $m(\theta)$ such that

$$M(\theta)v(\theta) = m(\theta)v(\theta + \omega) \ .$$

The function $m(\theta)$ represent the dynamics on the invariant subbundle of rank 1 generated by $v(\theta)$.

Since the rotation ω is Diophantine, we can reduce the 1-dimensional cocycle associated to m and ω, that is, we look for a positive function $p(\theta)$ and a constant λ such that

$$m(\theta)p(\theta) = \lambda p(\theta + \omega) \ . \tag{94}$$

To do so, if $m(\theta) > 0$, we look for a positive λ. Then, by taking logarithms in both sides in (94), we obtain the equation

$$\log m(\theta) + \log p(\theta) = \log \lambda + \log p(\theta + \omega) \ , \tag{95}$$

that is a typical KAM equation for $l(\theta) = \log p(\theta)$. We fix, then,

$$\lambda = \exp \left(\int_{\theta \in \mathbb{T}^d} \log m(\theta) \ d\theta \right) \ , \tag{96}$$

and solve the equation for $l(\theta)$. Finally, $p(\theta) = \exp l(\theta)$.

If $m(\theta) < 0$, we look for a negative λ, and the equation to be solved is

$$\log \left(-m(\theta)\right) + \log p(\theta) = \log \left(-\lambda\right) + \log p(\theta + \omega) \ . \tag{97}$$

In this case,

$$\lambda = -\exp \left(\int_{\theta \in \mathbb{T}^d} \log \left(-m(\theta)\right) \ d\theta \right) \ . \tag{98}$$

Remark 4.7. It is very easy to see that (we refer to [HdlL03b] for details) for ω ergodic, the spectrum of the transfer operator associated to the cocycle m is a circle of radius

$$\rho = \exp\left(\int_{\theta\in\mathbb{T}^d} \log|m(\theta)|\ d\theta\right)\ .$$

Remark 4.8. It is worth remarking that in the one-dimensional case, uniform contractivity is equivalent to the – in principle much weaker – notion of negative Lyapunov exponent.

The following argument comes from [FdlL92]. We note that, for one dimensional bundles, negative Lyapunov exponents means that

$$\log\lambda = \lim_n \frac{1}{n}\sum_{i=0}^{n-1} \log|m(\theta+i\omega)| < 0\ .$$

In the one-dimensional case, however, the RHS of the equation above is a Birkhoff sum. If $\log m$ is continuous, using that an irrational rotation is uniquely ergodic we obtain that the Birkhoff sums converge uniformly in θ. Therefore, there is an N such that

$$\log|m(\theta+(N-1)\omega)\cdots m(\theta)| < N(\log\lambda+\delta) < 0.$$

This implies that the contraction rate of a power is uniform.

The power method is easily implementable as a numerical algorithm, but there is a a case that we should be aware of. In some cases, we have found that $m(\theta)$ vanishes in some points. This is perfectly consistent if $v(\theta)$ also vanishes at the zeros of m. Hence, v is not a good global frame for a bundle of rank one.

This is unavoidable if and we take as starting point of the iteration an embedding that has a different index than the index of the invariant bundle. (This complication happens in numerical implementations near resonances, when the invariant bundle changes index). If we apply the iterations of a bundle of the *"wrong"* topology, we find empirically that the iteration develops zeros. See the examples in [HdlL01a].

Remark 4.9. Related to the importance of the topology of the objects, notice that if a cocycle, considered as a map $M : \mathbb{T}^d \to GL(n,\mathbb{R})$ and a frequency ω, is non homotopic to the identity then it is non reducible. Moreover, in such a case, the corresponding transfer operator changes the homotopic invariants of continuous sections, as the index.

Remark 4.10. The power method to compute the dominant eigenvalue of a n-dimensional matrix A is equivalent to find the attracting fixed point of the dynamical system induced in the $(n-1)$-dimensional projective space by using iteration. Recall that the $(n-1)$-dimensional projective space $\mathbb{P}^{n-1}$ is the set of straight lines of $\mathbb{R}^n$ passing through the origin. Recall also that $\mathbb{P}^{n-1} = \mathbb{S}^{n-1}/a$, where $a : \mathbb{S}^{n-1} \to \mathbb{S}^{n-1}$ is the antipodal map $a(u) = -u$ (so we identify the points u and $-u$ of the unit sphere).

With this idea in mind, we can also projectivize the cocycle (87) and look for the attractors and repellors (or in general, invariant sets) in the projective bundle. First, we can work in the unit spheric bundle, so for $u \in \mathbb{R}^n$ with $\|u\| = 1$ and $\theta \in \mathbb{T}^d$, we define

$$\begin{aligned} \bar{u} &= M(\theta)u/\|M(\theta)u\| \ , \\ \bar{\theta} &= \theta + \omega \ . \end{aligned} \tag{99}$$

Then, we identify u with $-u$.

Some numerical experiments appear in [HdlL01b], where $n = 2$ and the 1-dimensional projective space is identified with $[0, \pi]/\{0 = \pi\}$ (it is parameterized by an angle α from 0 to π).

Remark 4.11. In its most straightforward implementation, the power method computes just the dominant bundle.

It is possible to use the very well known trick of *deflation* to compute the rest of the eigendirections. In our setting, deflation corresponds to the following general construction: if we know an invariant subbundle E_1, we construct a complementary subbundle E_2, and then the cocycle expressed using adapted frames to $E = E_1 \oplus E_2$ has triangular form:

$$M(\theta) = \begin{pmatrix} M^1(\theta) & N(\theta) \\ 0 & M^2(\theta) \end{pmatrix} \ .$$

The spectrum of the transfer $\mathcal{M}_\omega$ is the union of the spectra of $\mathcal{M}^1_\omega$ and $\mathcal{M}^2_\omega$. See [HdlL03a].

Remark 4.12. There are also other well known numerical methods to compute intermediate eigenvalues. General references are [Dem97, TB97].

We mention the algorithms of Wiedlandt. If λ is an approximate eigenvalue of $\mathcal{M}_\omega$, then $\mathcal{M}_\omega - \lambda \mathrm{Id}$ has an eigenvalue close to zero, whose inverse will be the dominant eigenvalue of $(\mathcal{M}_\omega - \lambda \mathrm{Id})^{-1}$. So, at each step we have to solve $(\mathcal{M}_\omega - \lambda \mathrm{Id})^{-1} v = w$, where v is the previous estimate of the eigensection, and w is the new one. This is equivalent to solving $(\mathcal{M}_\omega - \lambda \mathrm{Id}) w = v$, that can be done by discretization in Fourier series. Since the matrix is close to singular, it could be useful to employ singular value decomposition.

Another standard method – which, however we have not implemented – is Arnoldi's method.

In the numerical examples in [HdlL01a], all the cocycles are two dimensional, so we can use the power method to compute the two eigenvalues (if they are different). Even if this is the simplest case, our numerical experiments suggest new mathematical phenomena.

4.2.4. *Reducibility method.* In the core of the reducibility method to compute invariant tori, we use Newton method to reduce the linear skew product given by the monodromy matrix. We can use this "black box" to reduce the linear skew product, avoiding large matrices. This corresponds to apply

Algorithm 3.9 to the linear quasi-periodic map given by

$$F(x,\theta) = M(\theta)x$$

and ω. Obviously, the torus $K(\theta) = 0$ is invariant, but the algorithm looks for also the Floquet transformations.

Of course, Newton method needs good first approximations to converge. This can be obtained by continuation with respect to parameters. We can also apply first the other methods to obtain good starting guesses.

5. Geometric properties and computation

In case the system has geometrical properties (e.g. preserving a symplectic matrix), they are recovered by the invariant objects, and sometimes it is possible to adapt the algorithms so that they take advantage of these geometric properties.

For instance, when $n = 2m$ and F is symplectic, and the torus is normally hyperbolic, both stable and unstable subbundles are Lagrangian [HdlL03a] (for a normally hyperbolic torus in a general map, they are isotropic). Therefore, when one of them is known, it is straightforward to compute the other.

We give here some ideas of algorithms that take advantage of geometric structures.

For the purposes of this paper, a (trivial) symplectic bundle on the torus is a vector bundle $E = \mathbb{R}^{2m} \times \mathbb{T}^d$ equipped with a linear symplectic structure of each fiber $E_\theta = \mathbb{R}^{2m} \times \{\theta\}$. That is to say, we have a non-degenerate skew-symmetric matrix $J(\theta)$, depending smoothly on θ, defining a skew-symmetric product Ω_θ on each fiber:

$$\Omega_\theta(v_\theta, w_\theta) = v_\theta^\top J(\theta) w_\theta \ ,$$

for all $v_\theta, w_\theta \in E_\theta$. That is:

$$J(\theta)^\top = -J(\theta) \ . \tag{100}$$

Among the subbundles of E, the Lagrangian subbundles are particularly important. A Lagrangian subbundle L has rank m and satisfies

$$L(\theta)^\top J(\theta) L(\theta) = 0 \ , \tag{101}$$

where $L(\theta)$ is a (local) frame of L.

It is well known that there exist a complex vector bundle structure on the symplectic bundle [Wei77], that is to say, there exist a symplectic anti-involution on each fiber, $I(\theta)$, depending smoothly on θ:

$$I(\theta)^\top J(\theta) I(\theta) = J(\theta) \ , \ I(\theta)^2 = -\mathrm{Id} \ . \tag{102}$$

As a consequence, if the symplectic bundle E admits a Lagrangian subbundle L, there exist Lagrangian subbundles which are complementary to L: the subbundle IL is Lagrangian and satisfies $E = L \oplus IL$.

The vectors in IL are symplectic conjugated to those in L. A suitable frame for IL is

$$L(\theta)^* = I(\theta) L(\theta) b(\theta) \ ,$$

where

$$b(\theta) = (L(\theta)^\top J(\theta) I(\theta) L(\theta))^{-1} \tag{103}$$

is a $m \times m$ symmetric matrix. This election of the frame makes the matrix

$$P(\theta) = (L(\theta), L(\theta)^*)$$

to satisfy

$$P(\theta)^\top J(\theta) P(\theta) = J_0 \ , \tag{104}$$

where

$$J_0 = \begin{pmatrix} 0 & \mathrm{Id}_m \\ -\mathrm{Id}_m & 0 \end{pmatrix}$$

is the standard symplectic matrix in $\mathbb{R}^{2m}$. That is to say, $P(\theta)$ translates the symplectic form $J(\theta)$ to the standard J_0.

A conformal symplectic vector bundle map over a rotation ω is a linear skew-product

$$\begin{aligned} \bar{x} &= M(\theta) x \ , \\ \bar{\theta} &= \theta + \omega \ , \end{aligned} \tag{105}$$

such that

$$M(\theta)^\top J(\theta + \omega) M(\theta) = \sigma(\theta) J(\theta) \ ,$$

where $\sigma : \mathbb{T}^d \to \mathbb{R}$ is a non vanishing function.

Notice that for any $P(\theta)$ satisfying (104)

$$(P(\theta+\omega)^{-1} M(\theta) P(\theta))^\top J_0 (P(\theta+\omega)^{-1} M(\theta) P(\theta)) = \sigma(\theta) J_0 \ ,$$

that is, $P(\theta+\omega)^{-1} M(\theta) P(\theta)$ is conformal symplectic with respect to the standard form J_0.

Let L be a Lagrangian subbundle, invariant for (105). Let $\lambda(\theta)$ the vector bundle map on $\mathbb{R}^m \times \mathbb{T}^d$ over the rotation ω representing the dynamics on the subbundle:

$$M(\theta) L(\theta) = L(\theta + \omega) \lambda(\theta) \ . \tag{106}$$

We want to construct a complementary invariant Lagrangian subbundle.

First, notice that the frame

$$P(\theta) = (L(\theta), L(\theta)^*) \ ,$$

where $L(\theta)^* = L(\theta) a(\theta) + I(\theta) L(\theta) b(\theta)$, being $a(\theta)$ any $m \times m$ matrix, satisfies (104). So then, $P(\theta+\omega)^{-1} M(\theta) P(\theta)$ is conformal symplectic with respect to the standard form J_0. Since $M(\theta) L(\theta) = L(\theta+\omega)\lambda(\theta)$, then

$$P(\theta+\omega)^{-1} M(\theta) P(\theta) = \begin{pmatrix} \lambda(\theta) & c(\theta) \\ 0 & \sigma(\theta) \lambda(\theta)^{-\top} \end{pmatrix} \ ,$$

where

$$\begin{aligned} c(\theta) &= -L^*(\theta+\omega)^\top J(\theta+\omega)M(\theta)L^*(\theta) \\ &= \lambda(\theta)a(\theta) - \sigma(\theta)a(\theta+\omega)^\top \lambda(\theta)^{-\top} - d(\theta) \ , \end{aligned}$$

$$d(\theta) = b(\theta+\omega)^\top L(\theta+\omega)^\top I(\theta+\omega)^\top J_{\theta+\omega} M(\theta)I(\theta)L(\theta)b(\theta) \ .$$

Hence, we produce an invariant Lagrangian splitting $E = L \oplus L^*$ by solving the equation

$$\lambda(\theta)a(\theta) - \sigma(\theta)a(\theta+\omega)^\top \lambda(\theta)^{-\top} = d(\theta) \ . \tag{107}$$

In the projection method and the reducibility method, we can take advantage of the previous construction, because from an approximate stable invariant subbundle we can compute an approximate unstable invariant subbundle.

Similar constructions play also an important role in KAM theory [dlL01, GJdlLV00]. Other properties, such as reversibility, are useful to simplify the computations [HdlL03a].

6. Computation of the whiskers of an invariant torus

In this section we develop algorithms to compute invariant manifolds which are tangent to an invariant bundle around the linearization around an invariant torus. Algorithms for the computation of invariant tori and for invariant bundles of the linearization are described in Sections 3, 4.

The general theory works for manifolds associated to spectral subbundles that satisfy non-resonance conditions [HdlL01b]. In this paper, we will develop only algorithms in two special cases: stable/unstable manifolds and non-resonant manifolds associated to rank-1 bundles.

The algorithms for these two special cases present significant simplifications with respect to the general case and they seem to be important in practice. These are the algorithms we have implemented so far. We will present some possible modifications to cover the general case in remarks.

6.1. Computation of stable and unstable and other invariant manifolds.

We will assume that we have a very accurate numerical solution K of the invariance equation (2) and a frame $P(\theta)$ in which the linear normal dynamics given by the cocycle (87) is given by $\Lambda(\theta)$. That is:

$$P(\theta+\omega)^{-1} \mathrm{D}F(K(\theta),\theta) P(\theta) = \Lambda(\theta) \ .$$

We will denote $M(\theta) = \mathrm{D}F(K(\theta),\theta)$.

We will assume that $\Lambda(\theta)$ leaves invariant a subbundle, which we will call $P(\theta)E^s(\theta)$. We will denote by $P(\theta)E^u(\theta)$ a complementary subbundle. Hence, $\Lambda(\theta)$ expressed in these coordinates has the form

$$\Lambda(\theta) = \begin{pmatrix} \Lambda^s(\theta) & N(\theta) \\ 0 & \Lambda^u(\theta) \end{pmatrix} \ . \tag{108}$$

The notation E^s, E^u is meant to suggest that very important special cases is when the splitting is between stable and unstable bundles. Nevertheless, this is not necessary. The splitting need not correspond even to spectral subbundles. For example, if N is not zero, the bundle E^u is not invariant. The phenomenon of invariant bundles without invariant complements arises when we have identical oscillators in which one of them forces the other but there is no reverse effect. When the splitting indeed corresponds to spectral subbundles there are systematic ways of computing the P and the Λ described in Section 4.1. We recall that, by changing units in the stable direction, it is possible to adjust that $||N||$ is sufficiently small. (See [HdlL01b].)

The goal of this section is to compute invariant manifolds corresponding to invariant subspaces which satisfy appropriate non-resonance conditions. This includes as particular cases, the computation of (strong) stable and unstable manifolds, which we will treat in more detail.

Following the parameterization method, we will compute an invariant manifold of K by computing $W : \mathbb{R}^{n_s} \times \mathbb{T}^d \to \mathbb{R}^n$ and $\Lambda^s : \mathbb{R}^{n_s} \times \mathbb{T}^d \to \mathbb{R}^{n_s}$ in such a way that:

$$F(W(\eta, \theta), \theta) = W(\Lambda^s(\eta, \theta), \theta + \omega) \ . \tag{109}$$

We will discretize W as a Fourier-Taylor expansion

$$W(\eta, \theta) = \sum_{k=0}^{\infty} W_k(\eta, \theta) \ , \tag{110}$$

where $W_k(\eta, \theta)$ are homogeneous polynomials of order k in the η variables. So, we can write $W_k(\eta, \theta) = W_k(\theta)\eta^{\otimes k}$, where $W_k(\theta)$ is a k-multilinear symmetric form from $\mathbb{R}^{n_s}$ to $\mathbb{R}^n$.

$\Lambda^s(\eta, \theta)$ represents the dynamics on the invariant manifold, and it will be given by a polynomial of degree L in the η variables:

$$\Lambda^s(\eta, \theta) = \sum_{k=1}^{L} \Lambda^s_k(\eta, \theta) \ . \tag{111}$$

The degree L is a positive integer such that

$$\|\Lambda^s_1\|^{L+1}_{C^0} \|\Lambda^{-1}\|_{C^0} < 1 \, . \tag{112}$$

(One can choose L, but in practical computations, taking L as small as possible reduces the computations needed. On the other hand, near resonances, choosing L larger may give more numerical stability.)

The computation is based on substituting the expansions (110) and (111) in (109) to obtain a hierarchy of equations for the homogeneous terms of $W(\eta, \theta)$ and $\Lambda^s(\eta, \theta)$.

Notice that $W_0(\theta) = K(\theta)$, and so the 0-order equation

$$F(W_0(\theta), \theta) = W_0(\theta + \omega)$$

is verified.

Using the frame $P(\theta)$ we write

$$W(\eta,\theta) = K(\theta) + P(\theta)\sum_{k=1}^{\infty}\tilde{W}_k(\eta,\theta)\ . \tag{113}$$

Each term $\tilde{W}_k(\eta,\theta)$ is written as

$$\tilde{W}_k(\eta,\theta) = \begin{pmatrix} W_k^s(\eta,\theta) \\ W_k^u(\eta,\theta) \end{pmatrix}\ .$$

The 1-order equation is

$$\mathrm{D}F(W(0,\theta),\theta)W_1(\theta) = W_1(\theta+\omega)\Lambda_1^s(\theta)\ , \tag{114}$$

One possible solution of (114) is $W_1(\eta,\theta) = V^s(\theta)\eta$ and $\Lambda_1^s(\eta,\theta) = \Lambda_1^s(\theta)\eta$. That is to say,

$$\tilde{W}_1(\eta,\theta) = \begin{pmatrix} \eta \\ 0 \end{pmatrix}\ .$$

Remark 6.1. Note, however, that $W_1(\eta,\theta) = \mu V^s(\theta)\eta$ for each $\mu \in \mathbb{R}-\{0\}$ is also a solution of (114). This is closely related to the multiplicity of the solutions of (3) pointed out in Remark 1.4. Choosing W_1 amounts to choosing the scale in the coordinate η.

As we will see, once we make a choice for W_1, all the other terms in the expansion are determined. In the theory developed in [HdlL01b], it is shown that, provided that one chooses the domain of W_1 small enough, one can reduce the problem to a contraction mapping. However, we observe that if some of the computed coefficients are very small, this leads to numerical error since we lose information when adding the small coefficient to a larger one. In numerical implementations, it is advantageous to choose W_1 so that the coefficients for W decrease but as slowly as possible. In some cases, one can do a preliminary run, adjusting the choice of W_1 to obtain some information on the rate of decay of the coefficients. Then, one can restart the calculation with the appropriate choice of W_1.

Suppose we have computed all the terms of order less than k. In the following, a subscript $< k$ means that we only consider terms up to order $k-1$ and similarly for other symbols.

If we substitute the expansions (110) and (111) in (109), and equate terms of order k in η, we obtain the k-order equation

$$M(\theta)W_k(\eta,\theta) - W_k(\Lambda_1^s(\theta)\eta,\theta+\omega) - V^s(\theta+\omega)\Lambda_k^s(\eta,\theta) = R_k(\eta,\theta)\ , \tag{115}$$

where

$$R_k(\eta,\theta) = -\left(F(W_{<k}(\eta,\theta),\theta) - W_{<k}(\Lambda_{<k}(\eta,\theta),\theta+\omega)\right)_k$$

is known from the previous computations. Note that this k-homogeneous polynomial in η depends only on $\Lambda_1,\dots\Lambda_{k-1}, W_1,\dots W_{k-1}$.

Multiplying (115) on the right by $P(\theta+\omega)^{-1}$, using the notation (113), (108) and splitting the resulting equation into equations for the s-u components, we obtain:

(116)
$$\Lambda_1^u(\theta)\tilde{W}_k^u(\eta,\theta) - \tilde{W}_k^u(\Lambda_1^s(\theta)\eta,\theta+\omega) = \tilde{R}_k^u(\eta,\theta)$$

(117)
$$\Lambda_1^s(\theta)\tilde{W}_k^s(\eta,\theta) - \tilde{W}_k^s(\Lambda_1^s(\theta)\eta,\theta+\omega) = \tilde{R}_k^s(\eta,\theta) - N(\theta)\tilde{W}_k^u(\eta,\theta) + \Lambda_k^s(\eta,\theta)\ ,$$

where $\tilde{R}_k(\eta,\theta) = P(\theta+\omega)^{-1}R_k(\eta,\theta)$.

From the spectral properties of the transfer operators associated to Λ_1^s, Λ_1^u, (116) has an unique solution $\tilde{W}_k^u(\theta,\eta)$ provided that the spectrum of the linearized operator restricted to the bundle satisfies some non-resonance conditions, namely that the product of k points in the spectrum of the restriction is not a point in the spectrum. Once that we know $\tilde{W}_k^u$, we substitute it in (117). Again appropriate assumptions on the spectrum of Λ_1^s we can solve the equation (117). See [HdlL01b]. The theory of (117) is much richer than the theory for (116). Note that in (117) we want to find two unknowns $\tilde{W}_k^s$ and Λ_k^s. The choice that requires less computation is to set Λ_k^s to zero whenever possible. On the other hand, it can well be numerically advantageous to choose Λ so that we improve the condition of the resulting equation. Note that once we choose Λ_k^s, amounts to solving a linear equation for $\tilde{W}_k^s$. It is possible to choose Λ_k^s in such a way that the RHS of (117) does not include directions along which the operator in the LHS is hard to invert. This happens for example, if the product of k numbers in the spectrum of the transfer operator along E^s are close to points in the spectrum of the operator along E^u.

6.2. **The case of stable and unstable manifolds.** In the particular case that the splitting E^s, E^u is between stable and unstable components of the spectrum, the theory is much simpler. Note that in that case $N \equiv 0$.

A solution of (116), can be obtained by iterating the following equation, which is equivalent to it:

$$\tilde{W}_k^u(\eta,\theta) = (\Lambda_1^u(\theta))^{-1}\left[\tilde{W}_k^u(\Lambda_1^s(\theta)\eta,\theta+\omega) + \tilde{R}_k^u(\eta,\theta)\right]\ .$$

If $k \le L$, we take $\tilde{W}_k^s(\eta,\theta) = 0$ and $\Lambda_k^s(\eta,\theta) = -\tilde{R}_k^s(\eta,\theta)$. On the contrary, if $k > L$, then we take $\Lambda_k^s(\eta,\theta) = 0$ and $\tilde{W}_k^s(\eta,\theta)$ solves the equation

$$\Lambda_1^s(\theta)\tilde{W}_k^s(\eta,\theta) - \tilde{W}_k^s(\Lambda_1^s(\theta)\eta,\theta+\omega) = \tilde{R}_k^s(\eta,\theta)\ . \tag{118}$$

Notice that because $\tilde{W}_k^s$ is homogeneous of degree k we have

$$|\tilde{W}_k^s(\Lambda_1^s(\theta)\eta,\theta+\omega)| \le \|\tilde{W}_k^s\|_{C^0}\cdot\|\Lambda_1^s\|_{C^0}^k$$

Since (117) is equivalent to

$$\tilde{W}_k^s(\eta,\theta) = \Lambda^s(\theta)^{-1}\tilde{W}_k^s(\Lambda^s(\theta)\eta,\theta+\omega) - \Lambda_k^s(\eta,\theta) + \Lambda^s(\theta)^{-1}\tilde{R}_k^s(\eta,\theta)$$

we see that by (112), the RHS of the above equation is a contraction and we can solve (117) just iterating.

Remark 6.2. Note that the solution of (117), in general is not unique. We can make other choices for Λ_k^s than the ones we indicated. Notably, in the [HdlL01b] it is shown that one can choose $\Lambda_k^s = 0$ whenever the operator that to W_k^s associates the LHS of (117) is invertible. This is ensured by some non-resonance conditions on the spectrum of the transfer operator associated to Λ_1^s.

Remark 6.3. We can also represent the invariant manifold as a graph by taking $\tilde{W}_k^s(\eta, \theta) = 0$ and $\Lambda_k^s(\eta, \theta) = -\tilde{R}_k^s(\eta, \theta)$ for all $k \geq 2$.

Remark 6.4. At the moment, we have not implemented algorithms for non-resonant manifolds except in the rank-1 case, which will be discussed in the next Section. It looks possible that, in the case that the torus is reducible, there could be practical algorithms for these non-resonant manifolds even in the case that the rank is larger than 1.

6.3. **Invariant manifolds of rank 1 attached to an invariant torus.** In this section we will look for a manifold $W : \mathbb{R} \times \mathbb{T}^d \to \mathbb{R}^n$ and a real number λ with $|\lambda| \neq 1$ such that the invariance equation

$$F(W(s, \theta), \theta) = W(\lambda s, \theta + \omega), \tag{119}$$

is satisfied, with $W(0, \theta) = K(\theta)$. That is, we look for a parameterization of an invariant manifold W through K such that the normal dynamics is given by multiplication with λ. We will assume that ω is Diophantine.

By differentiating (119) with respect to s and taking $s = 0$, we have

$$\mathrm{D}F(K(\theta), \theta) \frac{\partial W}{\partial s}(0, \theta) = \lambda \frac{\partial W}{\partial s}(0, \theta + \omega). \tag{120}$$

Let $M(\theta) = \mathrm{D}F(K(\theta), \theta)$ be the differential of F along the invariant torus K (the monodromy matrix), that gives the normal behavior around the torus. Let W_1 be the first variation of W with respect to s in $s = 0$, that is,

$$W_1(\theta) = \frac{\partial W}{\partial s}(0, \theta).$$

Then, (120) just requires that $W_1(\theta)$ is an eigensection of the transfer operator $\mathcal{M}_\omega$, whose eigenvalue is λ.

As ω is Diophantine, the fact that there is a real eigenvalue of the transfer operator is equivalent to the fact that there is a rank one trivial invariant bundle. The invariant bundle is, clearly, the span of the eigenvalue. (See [JS81, HdlL03b].)

Notice that Algorithm 3.9, if it works, produces the invariant torus K, a constant cocycle Λ conjugated with the cocycle $M(\theta)$, and the corresponding conjugation $P(\theta)$ (Floquet transformation). See also Section 4.2. Notice that if λ is an eigenvalue of Λ, then $e^{2\pi \mathbf{i} k\omega}\lambda$ with $k \in \mathbb{Z}^d$ is an eigenvalue of $M(\theta)$, but we will refer to the eigenvalues of Λ as the eigenvalues of $M(\theta)$.

The eigensections are the columns of the matrix P, and are solutions of equation (120).

The equation (120), being an eigenvalue equation, determines λ – the eigenvalue – up to a choice and determines W_1 up to multiplication by a number. The fact that W_1 is determined up to a multiple is related to the indeterminacy pointed out in Remark 1.4. From the mathematical point of view, all choices are equivalent, but in numerical implementations, it is convenient to make a choice that minimizes the round-off error and increases the numerical stability. This choice is discussed in [HdlL01a]. See also the discussion in Remark 6.1.

Remark 6.5. In the following construction, the reducibility of the cocycle $M(\theta)$ is not strictly necessary, but just that it has a rank one trivial invariant subbundle whose dynamics, since ω is Diophantine, can be reduced to a constant λ. We also need non-resonance conditions similar to those in the previous section to reduce the dynamics on the whiskers to this constant λ.

Notice that the Floquet transformation decreases the degree of smoothness of the parameterizations, but it is very useful for computations.

We expand W as

$$W(s,\theta) = \sum_{k=0}^{\infty} W_k(\theta) s^k, \tag{121}$$

where the Taylor coefficients $W_k(\theta)$ are periodic functions. Notice that $W_0(\theta) = K(\theta)$ and $W_1(\theta)$ is, for the sake of simplicity, the first column in $P(\theta)$.

Substituting (121) in the invariance equation (119) and equating the terms containing s^k, we obtain

$$M(\theta) W_k(\theta) - \lambda^k W_k(\theta + \omega) = R_k(\theta). \tag{122}$$

where R_k is a polynomial expression which depends only on $W_1, \ldots, W_{k-1}$. Hence, it can be inductively assumed to be known. In practice, to compute R_k one just needs to feed the polynomial of degree $k-1$ to a program built using a package that manipulates Fourier-Taylor series. The coefficient of degree k is $R_k(\theta)$ and all the other coefficients of degree up to k should be 0. This provides a check of the accuracy of the calculation. An alternative that is significantly faster is to observe that if we keep all the intermediate terms in the evaluation of $F(W(s,\theta),\theta)$, one can keep the coefficients of the polynomial of degree up $k-1$ and only compute the coefficient of order k. The implementation of this procedure is very easy if F is obtained by repeated applications of of arithmetic operations and elementary transcendental functions. (See the references mentioned before for toolkits of Fourier-Taylor series or [Knu97].)

Notice that (122) has a solution if λ^k is not in the spectrum of the transfer operator $\mathcal{M}_\omega$. So, this gives a non-resonance condition to linearize the

dynamics on the whisker: $\lambda^k \notin \mathrm{Spec}(\mathcal{M}_\omega)$ for all $k > 1$. In fact, the non-resonance condition involves a finite number of conditions, since $|\lambda| \neq 1$.

We have several options to solve numerically equation (122):

- We can translate the system to a large linear system, whose unknowns are the coefficients of the Fourier series given W_k. This produces, of course a large matrix.
- Suppose we have computed the spectral annuli and their corresponding spectral subbundles of $\mathcal{M}_\omega$ (see Section 4.1). Since λ^k is in a gap of the spectrum, we can use the projection on the bundles $E^{<\lambda^k}$ and $E^{>\lambda^k}$ (both of them are direct sum of several spectral subbundles). On each projection, we solve the equations using iteration. This is similar to the constructions in Section 6.1.
- If the cocycle $M(\theta)$ is reducible to a constant cocycle Λ, and $P(\theta)$ is the reducing transformation, we write

  $$W_k(\theta) = P(\theta)\tilde{W}_k(\theta),$$

  where $\tilde{W}_k(\theta)$ solves the equation

  $$\Lambda\tilde{W}_k(\theta) - \lambda^k\tilde{W}_k(\theta+\omega) = P(\theta+\omega)^{-1}R_k(\theta),$$

  provided that the non resonance condition

  $$|\lambda|^k \neq |\lambda_i| \text{ for all } k > 1, i = 1, \ldots, n.$$

  Reducibility diagonalizes the linear system described in the first alternative.

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