

**ANALYSIS AND NUMERICAL METHODS IN SOLID STATE PHYSICS AND  
CHEMISTRY**

A Dissertation  
Presented to  
The Academic Faculty

By

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In Partial Fulfillment  
of the Requirements for the Degree  
Doctor of Philosophy in the  
School of Mathematics

Georgia Institute of Technology

August 2017

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**ANALYSIS AND NUMERICAL METHODS IN SOLID STATE PHYSICS AND  
CHEMISTRY**

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To my parents.

## ACKNOWLEDGEMENTS

I would like to thank all the people who helped me in this long and important journey in my life.

I would specifically thank my Ph.D. thesis advisor Prof. Rafael de la Llave, for his constant help and encouragement. Nothing will be achieved without his wholehearted help. I'd also like to thank Prof. Chongchun Zeng, Prof. Diego del-Castillo-Negrete, Prof. Luca Dieci, Prof. Molei Tao and Prof. Xifeng Su, for all the wise advise and beneficial discussions.

I am also deeply grateful for Dr. Federico Benetto, Dr. Michael Loss, Dr. Turgay Uzer, for serving as members of my committee and other help.

I will not forget the interesting and useful English class from Dr. Morag C. Burke and Ms. Cathy Jacobson.

I also want to thank my fellow graduate students and friends. Special thanks to Tongzhou Chen, Dawei He, Wuchen Li, Chenchen Mou, Hagop Toussounian, Mikel de Viana, Dong Xia, Xin Wang, Longmei Shu, Amir Salahshoor, for all the fun moments and interesting discussions.

Finally, I would like to thank my wife, Yan Shan, for her caring and support, and for making my life healthy and organized.

## TABLE OF CONTENTS

<b>Acknowledgments</b> . . . . .	v
<b>List of Figures</b> . . . . .	ix
<b>Chapter 1: Resonant quasi-periodic equilibria in quasi-periodic media: perturbative expansions</b> . . . . .	1
1.1 Introduction . . . . .	1
1.2 Models considered and formulation of the problem . . . . .	3
1.2.1 Equilibrium equations . . . . .	5
1.2.2 Quasi-periodic configurations, hull functions . . . . .	5
1.2.3 Resonances . . . . .	6
1.2.4 Quasi-periodic equilibria with resonant frequencies . . . . .	8
1.2.5 The symmetries of the invariance equation (1.13) . . . . .	10
1.2.6 A normalization of the solutions of the invariance equation (1.13) . . . . .	11
1.2.7 Diophantine condition . . . . .	11
1.3 Function spaces and linear estimates . . . . .	13
1.4 Lindstedt series for quasi-periodic solutions with resonant frequencies . . . . .	15
1.4.1 The auxiliary equation . . . . .	18
1.5 A dynamical interpretation of the equilibrium equations of Frenkel-Kontorova models . . . . .	20

1.5.1	On the global geometry of the constraints given by (1.39)	22
1.5.2	Lyapunov exponents and phonon localization	23
<b>Chapter 2: KAM Theory for resonant quasi-periodic equilibria in quasi-periodic media</b>		
		25
2.1	Introduction	25
2.1.1	The method of adding extra parameters to equations	27
2.2	Remarks on the role of parameters	28
2.2.1	Properties of the equilibrium equations (2.2) and its associated factorization equation (2.4)	33
2.3	Preliminaries	35
2.3.1	Spaces of functions we will use	35
2.3.2	Diophantine condition	37
2.3.3	Cohomology equations	37
2.3.4	Cohomology equations with non-constant coefficients	39
2.4	The KAM theorem	44
2.4.1	Statement of the main result	44
2.5	Proof of Theorem 3	47
2.5.1	Outline of the proof	47
2.5.2	Motivation for the iterative step	49
2.5.3	Solving the linearized equations	53
2.5.4	Formulation of the iterative step	55
2.5.5	Estimates on the corrections	57
2.5.6	Estimates on the improved error	59

2.5.7	Proof of convergence . . . . .	61
2.5.8	Proof of local uniqueness . . . . .	63
2.6	Consequences of Theorem 3 and its proof . . . . .	65
2.6.1	Perturbative series around any solution of invariance and factorization	65
2.6.2	Convergence of Lindstedt series for the equilibrium and the factor- ization equations . . . . .	69
<b>Chapter 3: Transition State Theory with Quasi-Periodic Forcing . . . . .</b>		<b>72</b>
3.1	The Model . . . . .	72
3.2	Numerical Calculations of Transition State . . . . .	72
3.2.1	The invariance and reducibility equations . . . . .	74
3.2.2	Newton's Method . . . . .	75
3.2.3	Some Remarks . . . . .	76
3.2.4	Numerical Results for the Invariant Manifolds . . . . .	77
3.3	Computation of Stable and Unstable Manifolds of Transition States . . . . .	79
3.3.1	Evolve the flow along curves . . . . .	79
3.3.2	The order by order method . . . . .	81
3.3.3	Reducibility Method . . . . .	82
<b>References . . . . .</b>		<b>90</b>
<b>Vita . . . . .</b>		<b>91</b>

## LIST OF FIGURES

3.1	Invariant Manifold Parameterized by $K$ with internal dynamics $f$ . . . . .	73
3.2	Invariant Torus in phase space Parameters: $A = 1, B = 2, \epsilon_1 = 1, \mu = 1, \omega = \frac{\sqrt{5}+1}{2}, \phi = \frac{\pi}{2}$ . . . . .	77
3.3	Invariant Torus, 3D Parameters: $A = 1, B = 2, \epsilon_1 = 1, \mu = 1, \omega = \frac{\sqrt{5}+1}{2}, \phi = \frac{\pi}{2}$	78
3.4	Angle between stable/unstable spaces Parameters: $A = 1, B = 2, \epsilon_1 = 1, \mu = 1, \omega = \frac{\sqrt{5}+1}{2}, \phi = \frac{\pi}{2}$ . . . . .	78

## SUMMARY

In the first part of the paper, we consider an atomic model of deposition over a quasi-periodic medium, that is, a quasi-periodic version of the well-known Frenkel-Kontorova model. We consider the problem of whether there are quasi-periodic equilibria with a frequency that resonates with the frequencies of the medium. We show that there are always perturbative expansions. We also prove a KAM theorem in a-posteriori form. We show that if there is an approximate solution of the equilibrium equation satisfying non-degeneracy conditions, we can adjust one parameter and obtain a true solution which is close to the approximate solution. The proof is based on an iterative method of the KAM type and a novel technique of supplementing the equilibrium equation with another equation that factors the linearization of equilibrium equation.

In the second part of the paper, we consider a model related to Transition State Theory in chemical reactions. We consider a particle with an initial position on the reactant side of a time-dependent energy barrier and study the invariant manifolds and associated bundles using the parameterization method.

This thesis is arranged as follows:

Chapter I and Chapter II are based on my papers [1] and [2] with Rafael de la Llave and Xifeng Su. Chapter I studies the quasi-periodic Frenkel-Kontorova model using formal perturbative expansions and Chapter II uses KAM method to get rigorous theorems.

Chapter III studies Transition State Theory using parameterization method.

**CHAPTER 1**  
**RESONANT QUASI-PERIODIC EQUILIBRIA IN QUASI-PERIODIC MEDIA:**  
**PERTURBATIVE EXPANSIONS**

**1.1 Introduction**

The goal of this paper is to formulate the theory of resonant equilibria in quasi-periodic Frenkel-Kontorova models. We argue that these equilibria play an important role in the phenomenon of pinning (the equilibria that survive after an extremal force is applied). In periodic Frenkel-Kontorova models, the role of resonances in pinning is well established.

We recall that in Frenkel-Kontorova models [3, 4], one considers configurations given by a sequence of real numbers (think of the position of a sequence of particles deposited on a 1-D material). The (formal) energy of the system is the sum of a term of interaction between nearest neighbors of the deposited material and a term modeling interaction with the media. In the quasi-periodic Frenkel-Kontorova models studied here, the interacting potential will be a quasi-periodic function of the position reflecting that the medium is quasi-periodic. We will be interested in equilibria, i.e., configurations such that the derivatives of the (formal) energy with respect to the position of each of the particles vanish. We note that even if the energy is a formal sum, the equilibrium equations are well defined. More details of the models will be discussed in Section 1.2.

In [5, 6], one can find a rigorous mathematical theory of quasi-periodic equilibria whose frequency is not resonant (indeed Diophantine) with the frequencies of the substratum. The rigorous theory of [5, 6] also leads to efficient algorithms that can compute these quasi-periodic solutions arbitrarily close to their breakdown. Implementations of these algorithms and investigation of the phenomena at breakdown appear in [7]. The paper [5], studies models with nearest neighbor interaction while [6] studies the case of long range

interactions.

Our motivation is to study the phenomena of “depinning”. When we add an external force (no matter how small) to the model, many quasi-periodic solutions disappear. Nevertheless, there are still other quasi-periodic solutions which survive and just get slightly deformed. This physically corresponds to the deposited material rearrange itself to withstand the force. It is well known in the periodic Frenkel-Kontorova models that the solutions which persist under forcing are resonant with the media. The papers [5, 6] also show that, in the quasi-periodic case, the smooth non-resonant solutions do not exist when there is an external force. Hence we are interested in resonant solutions present in the unperturbed system.

In this paper, we formulate the problem and develop in Section 1.4 a systematic perturbation theory and we show that there exist at least two formal power series in the amplitude of the coupling describing resonant solutions even in the presence of external forces. The delicate analytic question of convergence of these series is pursued in [2]. In Section 1.5 we also develop a dynamical interpretation of the equilibria as orbits of a dynamical system with very unusual properties. Using this dynamical interpretation, we show in this paper that the phonon gap of quasi-periodic equilibria is zero. We expect that this formulation can be used for a systematic numerical exploration.

We hope that this paper can lay the ground work for future explorations. In [2], we use rigorous mathematical tools to establish the convergence of the formal series developed here under some extra assumptions. We will also use numerical methods to explore in a non-rigorous but more quantitative way some of the phenomena discussed here.

Equilibria in quasi-periodic media with a resonant frequency have been investigated numerically in [8, 9, 10]. These papers also studied the phonon gap and found it to vanish when there are smooth solutions (in agreement with the results here).

The variational and topological methods that have been proved useful in the periodic case do not extend completely to the quasi-periodic case in its full strength. Homogeniza-

tion (existence of average energy for minimizers) is known to be true, but finer properties are not so clear. Several interesting counterexamples are in [11, 12]. Some results which carry from the periodic case into the quasi-periodic case (in somewhat weakened form) are in [13, 14, 15, 16]. It seems a very interesting question to clarify which parts of the periodic case carry to the quasi-periodic case.

We note that in the periodic case, there are other quasi-periodic solutions that play a role in depinning [17]. They can be understood geometrically as Secondary KAM tori. These solutions cannot be continued to the solutions in unperturbed case, hence, there are not accessible to the series considered in Section 1.4. On the other hand, they may be studied (numerically and theoretically) using the formalism in Section 1.5. In the periodic case, these problems were considered by [18]. The paper [19] presents a numerical exploration which leads to very precise quantitative conjectures. This is a question that deserves further study.

## 1.2 Models considered and formulation of the problem

We consider models of deposition in a quasi-periodic one-dimensional medium.

If  $x_n \in \mathbb{R}$  denotes the position of the  $n$ -th particle of the deposited material, the state of the system is specified by a configuration (i.e. a sequence  $\{x_n\}_{n \in \mathbb{Z}}$ ). We can associate the following formal energy to a configuration of the system

$$\mathcal{S}(x) = \frac{1}{2} \sum_{n \in \mathbb{Z}} (x_{n+1} - x_n - a)^2 - V(x_n \alpha) - \lambda x_n \quad (1.1)$$

where  $V : \mathbb{T}^d \rightarrow \mathbb{R}$  is an analytic function,  $\alpha \in \mathbb{R}^d$  is an irrational vector and  $a, \lambda$  are some real numbers.

A natural example often used is

$$\mathcal{S}(x) = \frac{1}{2} \sum_{n \in \mathbb{Z}} (x_{n+1} - x_n - a)^2 + A \cos x_n + B \cos(\sqrt{2}x_n + \phi) - \lambda x_n \quad (1.2)$$

which corresponds to  $\alpha = (1, \sqrt{2})$  and  $V(\theta_1, \theta_2) = -(A \cos \theta_1 + B \cos(\theta_2 + \phi))$ .

The term  $(x_{n+1} - x_n - a)^2$  represents the interaction among neighboring deposited atoms. The term  $V(x_n \alpha)$  represents the interaction with the substratum. The interaction at position  $x \in \mathbb{R}$  is the quasi-periodic function  $V(x_n \alpha)$ . This models that the substratum is quasi-periodic.

The term  $\lambda x_n$  has the interpretation of a constant field applied to the model. In the case of deposited materials, we can imagine that the sample is tilted and  $\lambda$  is the component of the gravity in the direction of the sample (or in other problems, the meaning could be a constant electric field). The physical meaning of the equilibria corresponding to  $\lambda \neq 0$  is that, when we apply a small external field, the configurations rearrange themselves so that they can respond to the force and do not slide. Of course, when the force is strong enough, no rearrangement is possible and all the configurations slide. This is the microscopic origin of static friction. The solutions that survive the application of a constant external field are called *pinned*. A heuristic principle (see later) is that orbits that are well equidistributed do not survive with a non-zero external field (the reason is that in equidistributed orbits, the force on a large sample is the average of the force, which is constant over all the phases; this argument can be made rigorous).

In the case of periodic media, the pinned solutions are known to correspond to resonant frequencies. Since the resonant tori do not survive, it is reasonable to consider resonant frequencies.

The consideration of non-zero external forces  $\lambda \neq 0$  in this paper is very important novelty with respect to the previous papers [5, 6]. It is shown in [5, 6] that if there is non-resonant quasi-periodic solution, then  $\lambda = 0$ . In our case, we will show how to construct quasi-periodic equilibria with nontrivial  $\lambda$  and will show how to compute perturbatively the range of such  $\lambda$  for which solutions with a prescribed frequency exist.

Without any loss of generality, we can assume that

$$k \cdot \alpha \notin \mathbb{N} \quad \forall k \in \mathbb{Z}^d - \{0\}. \quad (1.3)$$

If there exists a resonance  $k \cdot \alpha = 0$ , we could just use less frequencies to express the quasi-periodic function.

### 1.2.1 Equilibrium equations

A configuration is in equilibrium if the forces acting on all the particles vanish. Equivalently, the derivatives of the energy with respect to the position of the particles vanish. That is,

$$\frac{\partial \mathcal{S}}{\partial x_n}(x) = 0 \quad \forall n \in \mathbb{Z}.$$

In the model (1.1), the equilibrium equations are

$$x_{n+1} + x_{n-1} - 2x_n + \partial_\alpha V(x_n \alpha) + \lambda = 0 \quad \forall n \in \mathbb{Z} \quad (1.4)$$

where  $\partial_\alpha = \alpha \cdot \nabla$  and  $\nabla$  is the usual gradient.

Note that even if the energy (1.1) is just a formal sum, the equilibrium equations (1.4) are well defined equations.

It is very tempting to consider (1.4) as a dynamical system, so that we obtain  $x_{n+1}$  as a function of  $x_n$  and  $x_{n-1}$ . This system has very unusual properties. This will be pursued in Section 1.5.

### 1.2.2 Quasi-periodic configurations, hull functions

In this paper, we will be interested in quasi-periodic solutions of frequency  $\omega \in \mathbb{R}$ .

These are configurations of the form

$$x_n = n\omega + h(n\omega\alpha), \quad (1.5)$$

where  $h : \mathbb{T}^d \rightarrow \mathbb{R}$ .

A configuration given by a hull function (1.5) satisfies the equilibrium equation (1.4) if and only if the hull function  $h$  satisfies

$$h(n\omega\alpha + \omega\alpha) + h(n\omega\alpha - \omega\alpha) - 2h(n\omega\alpha) + \partial_\alpha V(n\omega\alpha + \alpha h(n\omega\alpha)) + \lambda = 0. \quad (1.6)$$

The equation (1.6) was considered in [5, 6] when  $\omega\alpha$  is Diophantine (in particular,  $n\omega\alpha$  is dense in the torus  $\mathbb{T}^d$ ).

In our case,  $n\omega\alpha$  will not be dense on the  $d$ -dimensional torus (see Section 1.2.3) and the equilibrium equations we will derive are different from those in [5, 6].

### 1.2.3 Resonances

The goal of this paper is to study situations when there are  $k \in \mathbb{Z}^d - \{0\}$  and  $m \in \mathbb{Z}$  such that

$$k \cdot \omega\alpha - m = 0. \quad (1.7)$$

When (1.7) holds we say that  $(k, m)$  is a discrete resonance for  $\omega\alpha$  and we refer to the pair  $(k, m)$  as a resonance.

**Remark 1.** *Note that these discrete resonances (1.7) are different from the resonances of the media we excluded before ( $k \cdot \alpha \neq 0, \forall k \in \mathbb{Z}^d - \{0\}$ ).*

**Remark 2.** *If*

$$k \cdot \alpha \neq 0 \quad \forall k \in \mathbb{Z}^d \setminus \{0\},$$

*given any  $k_0 \in \mathbb{Z}^d \setminus \{0\}$ ,  $m \in \mathbb{Z}$  we have that  $\omega = -m/(k_0 \cdot \alpha)$  is a resonant frequency. Since  $k_0 \cdot \alpha$  can be arbitrarily large, we see that the set of resonant frequencies is dense on the real line. Of course, once we fix  $\alpha$ , the set of resonant  $\omega$  is a countable set.*

### *Multiplicity of a resonance*

Clearly, if  $(k, m)$ ,  $(\tilde{k}, \tilde{m})$  are discrete resonances so is  $(k + \tilde{k}, m + \tilde{m})$ .

In mathematical language,

$$\mathcal{M}_{\omega\alpha} = \{(k, m) \in \mathbb{Z}^d \times \mathbb{Z} : k \cdot \omega\alpha - m = 0\}$$

is a  $\mathbb{Z}$ -module called the resonance module for  $\omega$ .

We denote by  $l(\omega) = \dim(\mathcal{M}_{\omega\alpha})$  the dimension of the resonance module and we call it the multiplicity of the resonance. The meaning of  $l(\omega)$  is the number of independent resonances. We can find  $(k_1, m_1), \dots, (k_l, m_l)$  in such a way that all resonances can be expressed as combinations of the basic resonances (and also no other set of basic resonances with smaller number of elements will allow to express all the resonances).

*Only resonances of multiplicity 1 appear in the models (1.1)*

In Hamiltonian mechanics for systems with  $d$  degrees of freedom, one can find resonances of all multiplicities up to  $d$ . As we will see later, in Section 1.5, one can give a dynamical interpretation of the equilibrium equations as a dynamical system in  $d + 1$  dimensions. Nevertheless, in our models only  $l = 1$  appears independently of the number of degrees of freedom. This highlights that the problem here is different from the Hamiltonian problem.

**Proposition 1.** *If  $\omega\alpha$  is resonant, i.e.  $\mathcal{M}_{\omega\alpha} \neq \{0\}$ , then  $l(\omega) = 1$*

*Proof.* Note that

$$k_1 \cdot \omega\alpha - m_1 = k_2 \cdot \omega\alpha - m_2 = 0$$

implies (because  $m_1 \neq 0$ ,  $m_2 \neq 0$  because of (1.3))

$$\omega = \frac{m_1}{k_1 \cdot \alpha} = \frac{m_2}{k_2 \cdot \alpha}$$

and therefore

$$\alpha \cdot (k_1 m_2 - k_2 m_1) = 0$$

and, because  $\alpha$  is non-resonant (1.3) we have

$$k_1 m_2 = k_2 m_1.$$

Therefore, the two resonant vectors are related. □

### *The intrinsic frequencies*

When  $\omega\alpha$  is resonant, we can find a matrix  $B \in SL(d, \mathbb{Z})$ ,  $\Omega \in \mathbb{R}^{d-1}$ ,  $L \in \mathbb{Z}^d$  in such a way that

$$B\omega\alpha = (\Omega, 0) + L \quad \text{with} \quad \Omega \cdot \hat{k} \notin \mathbb{Z} \text{ for } \hat{k} \in \mathbb{Z}^{d-1} - \{0\}. \quad (1.8)$$

We will refer to  $\Omega$ 's as the intrinsic frequencies. They are essentially unique, i.e., unique up to changes of basis in  $\mathbb{R}^{d-1}$  given by a matrix in  $SL(d-1, \mathbb{Z})$ .

In this case, the set  $\{n\omega\alpha\}_{n \in \mathbb{Z}}$  has a closure which is a  $d-1$  dimensional torus. This torus is invariant under the translation  $T_{\omega\alpha}$ . If we stay in this  $d-1$  dimensional torus,  $T_{\omega\alpha}$  can be described as  $T_\Omega$ . The torus  $\mathbb{T}^d$  is foliated by these  $\mathbb{T}^{d-1}$  indexed by another parameter  $\eta \in \mathbb{T}^1$ . We will write a point in  $\mathbb{T}^d$  as  $(\psi, \eta)$  where  $\psi$  is the coordinate corresponding to the position in  $\mathbb{T}^{d-1}$ . The coordinate  $\eta$  selects the  $d-1$  torus we are considering.

#### 1.2.4 Quasi-periodic equilibria with resonant frequencies

The natural notion of the hull functions in the resonant case would be to assume that the equilibrium solutions have the form

$$x_n = n\omega + v(n\Omega) \quad (1.9)$$

with  $v : \mathbb{T}^{d-1} \rightarrow \mathbb{R}$ .

Note that the physical meaning of  $\omega$  is still the mean spacing of the solutions (i.e., an inverse density). The term  $v(n\Omega)$  represents fluctuations that can be parameterized in terms of the intrinsic frequency  $\Omega$ . Of course, we could represent them in terms of the original frequencies, but it is more natural to change variables so that they become a part of the equation.

We will refer to the  $\eta$  variable as the *transversal phase*. The resonant solutions considered here, cover densely a torus of codimension one. The one-dimensional variable  $\eta$  measures the position of these codimension-one tori on the configuration space  $\mathbb{T}^d$  corresponding to the internal phases of  $V$ .

If we substitute the parameterization (1.9) into the equilibrium equation, we obtain that the equilibrium equation (1.4) is equivalent to:

$$v(n\Omega + \Omega) + v(n\Omega - \Omega) - 2v(n\Omega) + \partial_\alpha V(n\omega\alpha + \alpha v(n\Omega)) + \lambda = 0. \quad (1.10)$$

If we furthermore introduce the notation  $\partial_\alpha V(\theta) = W(B\theta)$  and  $B\alpha = \beta$ , and observe that the  $n\Omega$  is dense on  $\mathbb{T}^{d-1}$ , we see that for continuous functions  $v$ , (1.10) is equivalent to:

$$v(\psi + \Omega) + v(\psi - \Omega) - 2v(\psi) + W((\psi, 0) + \beta v(\psi)) + \lambda = 0. \quad (1.11)$$

Note that we can also consider solutions of the form

$$x_n = n\omega + v(n\Omega + \xi_1) + \xi_2 \quad (1.12)$$

for any fixed  $\xi_1$  and  $\xi_2$ . This will give us freedom to add the transversal phase  $\eta$  as an additional parameter in (1.11). So the equilibrium equation we will consider is

$$v(\psi + \Omega) + v(\psi - \Omega) - 2v(\psi) + W((\psi, \eta) + \beta v(\psi)) + \lambda = 0. \quad (1.13)$$

By simple calculations, it can be shown that (1.13) is equivalent to (1.4) when the hull

function is of the form (1.12) and  $B\alpha\xi_2 = (\xi_1, \eta)$ .

**Remark 3.** *Because  $\beta$  has components both in the  $\psi$  and the  $\eta$  directions, the equation (1.13) cannot be considered as a parameterized version of the equations considered in [5]. As we will see, the symmetries of the equation involve transformations that mix the dependence in  $\psi$  and in  $\eta$ .*

### 1.2.5 The symmetries of the invariance equation (1.13)

The equation (1.13) possesses remarkable symmetries that make the solutions not unique. The origin of these symmetries is the choice of the origin of the phases parameterizing the quasi-periodic solution. In the non-resonant case, since the orbits of a rotation are dense on  $\mathbb{T}^d$ , the origin of the parameterization is only a  $d$  dimensional parameter. In the resonant case, however, since the orbits are dense on  $\mathbb{T}^{d-1}$ , we can choose an origin for every value of the transversal phase. Therefore, in the resonant case considered here, the symmetries of the problem involve a function and the group of symmetries here is infinite dimensional. This causes several differences.

Note that to discuss smooth dependence on parameters, etc. we need to impose normalizations which select one solution among all the solutions related by the symmetries. See Section 1.2.6.

Even if we will not discuss it here, when we have variational models with symmetries, we can obtain identities (called Ward identities in field theory). In [20, 5, 6] these Ward identities are used to develop a KAM method in the periodic case. In the resonant case, the KAM method developed in [2] has to be very different because the Ward identities are very different.

More precisely, the main observation is that if  $(v, \lambda)$  is a solution of (1.13), then, for every  $\iota(\eta) : \mathbb{T}^1 \rightarrow \mathbb{R}$ , the pair  $(\tilde{v}, \tilde{\lambda})$  is also a solution of (1.13) where we denote  $\beta = (\beta_\psi, \beta_\eta)$

and  $\tilde{v}, \tilde{\lambda}$  are defined by:

$$\begin{aligned}\tilde{v}(\psi, \eta) &= v(\psi, \eta) + \iota(\eta)\beta + \iota(\eta), \\ \tilde{\lambda}(\eta) &= \lambda(\eta + \iota(\eta)\beta_\eta).\end{aligned}\tag{1.14}$$

Notice that the symmetry (2.5) involves changing not only the argument  $\psi$  but also the argument  $\eta$ . Note the space of symmetries of the equation is not just a finite dimensional space (as in the periodic case) but rather an infinite dimensional space of functions.

### 1.2.6 A normalization of the solutions of the invariance equation (1.13)

For later applications, it will be useful to have local uniqueness of the solutions (e.g. to discuss smooth dependence on parameters, perturbative expansions on parameters), here we impose the normalization

$$\int_{\mathbb{T}^{d-1}} v(\psi, \eta) d\psi = 0.\tag{1.15}$$

Since the symmetry (2.5) involves changes of arguments, given a  $v_\eta$ , finding the  $\iota(\eta)$  that accomplishes the normalization involves solving the implicit equation

$$I(\eta + \beta_\eta \iota(\eta)) + \iota(\eta) = 0\tag{1.16}$$

where  $I(\eta) \equiv \int_{\mathbb{T}^{d-1}} v(\psi, \eta) d\psi$ .

If  $I$  and its derivative are small, one can solve (2.6) using implicit function theorem.

### 1.2.7 Diophantine condition

In this paper, we will only consider the existence of formal asymptotic expansions and will not discuss their convergence. In contrast with KAM theory, which establishes convergence, we will not need very delicate estimates on the solutions and hence, we can deal with Diophantine conditions much more general than those in KAM theory.

We will assume that  $\Omega$  satisfies

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sup_{|\hat{k}| \leq N, m \in \mathbb{Z}} \left| \ln |\hat{k} \cdot \Omega - m| \right| = 0. \quad (1.17)$$

Note that the condition (2.83) is much weaker than the usual Diophantine conditions and even than the Bjruno-Rüssmann conditions. The condition(2.83) is the natural condition in the study of existence of series to all orders.

The following proposition shows that the sets of frequencies we are considering are abundant.

Fix a vector  $k \in \mathbb{Z}^d \setminus \{0\}$ ,  $m \in \mathbb{Z} \setminus \{0\}$  and assume without loss of generality that there is no common divisor in the components of  $k$ . For any  $\alpha \in \mathbb{R}^d$  satisfying  $\alpha \cdot k \neq 0$ , we can find a unique  $\omega$  such that  $\alpha \cdot k\omega - m = 0$ . Fix a  $B_k \in SL(d, \mathbb{Z})$  such that the last row of  $B$  equals  $k$  (It's possible to find such  $B$  since the components of  $k$  has no common divisor). Then, let  $B_k \alpha \omega = (\Omega, 0) + m$ . Hence, for any  $k, m$  and  $\alpha$  satisfying  $\alpha \cdot k \neq 0$ , we can define  $\Omega$  as a function of  $\alpha$ . Denote  $\Omega = F_{k,m}(\alpha)$ .

**Proposition 2.** *The set of  $\alpha$  for which  $F_{k,m}(\alpha)$  satisfies (2.83) for all  $k, m$  is of full measure in  $\mathbb{R}^d$ . In other words, for a full measure set of medium frequencies, we can find a countable many resonant frequencies that lead to intrinsic frequencies satisfying (2.83).*

*Proof.* Since countable intersections of sets of full measure are of full measure, to prove Proposition 2 it suffices to show that for a fixed  $k, m$  as above, the set  $\{\alpha \in \mathbb{R}^d | \alpha \cdot k \neq 0 \text{ and } F_{k,m}(\alpha) \text{ satisfies (2.83)}\}$  is of full measure.

Because the set of  $\Omega$ 's which satisfy (2.83) is of full measure on  $\mathbb{R}^{d-1}$  and the linear map  $B_k$  is differentiable and surjective, the preimage of the set of  $\Omega$ 's that satisfy (2.83) under  $B_k$  is also of full measure in the hyperplane  $\Gamma = \{\gamma \mid \gamma \cdot k - m = 0\}$ . Denote the set of preimages as  $\Gamma'$ . Then any nonzero scaling of an element of  $\Gamma'$  will give an  $\alpha$  we want, which also form a full measure set in  $\mathbb{R}^d$ .  $\square$

### 1.3 Function spaces and linear estimates

The main tool that we will use to construct perturbation theories is the solution of cohomology equations, which are standard in perturbation theory and in KAM theory. See [19]. In this paper, we will only need very elementary estimates.

We denote

$$D_\rho = \{\theta \in \mathbb{C}^d / \mathbb{Z}^d \mid |\operatorname{Im}(\theta_i)| < \rho\}$$

and denote the Fourier expansion of a periodic mapping  $v(\psi, \eta)$  on  $D_\rho$  by

$$v(\psi, \eta) = \sum_{k \in \mathbb{Z}^d} v_k e^{2\pi i k \cdot (\psi, \eta)},$$

where  $\cdot$  is the Euclidean scalar product in  $\mathbb{C}^d$  and  $v_k$  are the Fourier coefficients.

We denote by  $\mathcal{A}_\rho$  the Banach space of analytic functions on  $D_\rho$  which are real for real argument and extend continuously to  $\overline{D_\rho}$ . We make  $\mathcal{A}_\rho$  a Banach space by endowing it with the supremum norm:

$$\|v\|_\rho = \sup_{(\psi, \eta) \in \overline{D_\rho}} |v(\psi, \eta)|.$$

These Banach spaces of analytic functions are the same spaces as in [21].

We will consider equations of the form

$$v(\psi + \Omega, \eta) - v(\psi, \eta) = \phi(\psi, \eta), \tag{1.18}$$

where  $\psi \in \mathbb{T}^{d-1}$ .

To simplify our notations, we will denote  $v(\psi + \Omega)$  and  $v(\psi - \Omega)$  as  $v_+$  and  $v_-$ , respectively. Similar notations will be used for other functions. We also use  $T$  to represent the translation operators, i.e.,  $T_\Omega v(\psi) = v(\psi + \Omega)$ .

**Lemma 1.** Let  $\phi \in \mathcal{A}_\rho(\mathbb{T}^d)$  be such that

$$\int_{\mathbb{T}^{d-1}} \phi(\psi, \eta) d\psi = 0, \quad (1.19)$$

for all  $\eta$ .

Assume that  $\Omega$  satisfies the assumption (2.83).

Then, for a fixed  $\eta$ , there exists a unique solution  $v_\eta$  of (2.9) which satisfies

$$\int_{\mathbb{T}^{d-1}} v(\psi, \eta) d\psi = 0. \quad (1.20)$$

The solution  $v \in \mathcal{A}_{\rho'}$  for any  $\rho' < \rho$  and we have

$$\|v\|_{\rho'} \leq C(d, \tau) v^{-1} (\rho - \rho')^{-\tau} \|\phi_\eta\|_\rho.$$

Furthermore, any distribution solution of (2.9) differs from the solution claimed before by a constant.

If  $\phi$  is such that it takes real values for real arguments, so does  $v$ .

If we consider now the dependence in  $\eta$ , we have that  $v \in \mathcal{A}_{\rho'}(\mathbb{T}^d)$  and

$$\|v\|_{\rho'} \leq C(\rho, \rho') \|\phi\|_\rho.$$

*Proof.* We note that, as it is well known that obtaining  $v$  solving (2.9) for given  $\phi$  is very explicit in terms of Fourier coefficients. If

$$\phi(\psi, \eta) = \sum_{k \neq 0} \hat{\phi}_k(\eta) e^{2\pi i k \cdot \psi} = \sum_{k \neq 0, m} \hat{\phi}_{k,m} e^{2\pi i (k \cdot \psi + m\eta)}$$

then,  $v$  is given by

$$v(\psi, \eta) = \sum_{k \neq 0} \hat{\phi}_k(\eta) (e^{2\pi i k \cdot \Omega} - 1)^{-1} e^{2\pi i k \cdot \psi} = \sum_{k \neq 0, m} \hat{\phi}_{k,m} (e^{2\pi i k \cdot \Omega} - 1)^{-1} e^{2\pi i (k \cdot \psi + m\eta)}.$$

Using Cauchy estimates for the Fourier coefficients  $|\hat{\phi}_{k,m}| \leq \exp(-2\pi\rho(|k| + |m|))\|\phi\|_\rho$  and that  $|e^{2\pi k \cdot \Omega} - 1|^{-1} \leq C \text{dist}(k \cdot \Omega, \mathbb{Z})^{-1}$  and the assumption (2.83), we obtain that

$$\begin{aligned} \|v\|_{\rho'} &\leq C \sum_{k \neq 0, m} \exp(-2\pi\rho(|k| + |m|))\|\phi\|_\rho \text{dist}(k \cdot \Omega, \mathbb{Z})^{-1} \|e^{2\pi i(k \cdot \psi + m\eta)}\|_{\rho'} \\ &= C \sum_{k \neq 0, m} \exp(-2\pi\rho(|k| + |m|))\|\phi\|_\rho \text{dist}(k \cdot \Omega, \mathbb{Z})^{-1} \exp(2\pi\rho'(|k| + |m|)). \end{aligned}$$

□

□

In KAM theory, by assuming Diophantine assumptions stronger than (2.83), one gets that one can take  $C(\rho, \rho') = C|\rho - \rho'|^{-\sigma}$  and this can be used to show convergence of the KAM scheme. See [2].

#### 1.4 Lindstedt series for quasi-periodic solutions with resonant frequencies

The goal of this section is to study (1.13) perturbatively when the non-linear term is small. Hence, we will write (1.13) with a small parameter  $\varepsilon$

$$v(\psi + \Omega, \eta) + v(\psi - \Omega, \eta) - 2v(\psi, \eta) + \varepsilon W((\psi, \eta) + \beta v(\psi, \eta)) + \lambda(\eta) = 0. \quad (1.21)$$

We will find  $v(\psi, \eta), \lambda(\eta)$  solving (1.21) and (2.3) in the sense of formal power series in  $\varepsilon$ . In this paper, we will not consider the problem of whether these series converge or represent a function. This will be studied in more details in [2].

Since one may want to find solution that correspond to  $\lambda = 0$  (or  $\lambda = \lambda^*$  with  $|\lambda^*|$  small), it is important for us to keep track of  $\frac{\partial \lambda}{\partial \eta}(\eta, \varepsilon)$  in order to solve  $\lambda(\eta, \varepsilon) = 0$  by implicit function theorem.

Following the standard perturbative procedure we will write

$$\begin{aligned} v &= \sum_{n=0}^{\infty} \epsilon^n v^n, \\ \lambda &= \sum_{n=0}^{\infty} \epsilon^n \lambda^n. \end{aligned} \tag{1.22}$$

Here  $\epsilon^n$  indicates a power of  $\epsilon$ , but  $v^n$  and  $\lambda^n$  are coefficients of  $\epsilon^n$ , not powers of  $v$  or  $\lambda$ .

The standard method of perturbation expansion is to substitute (1.22) in (1.21) and equate powers of  $\epsilon$  on both sides. This will get a system of infinitely many equations for the  $v^n, \lambda^n$ .

Of course, carrying out this procedure for  $n \leq N$  will require that  $\Omega$  satisfies some Diophantine properties as well as some differentiability assumptions.

As usual in Lindstedt theories, cases of  $n = 0$  and  $n = 1$  will be qualitatively different from all the others, and we will need to discuss them separately.

Equating the coefficients of  $\epsilon^0$  in (1.21) we obtain

$$v^0(\psi + \Omega, \eta) + v^0(\psi - \Omega, \eta) - 2v^0(\psi, \eta) + \lambda^0(\eta) = 0. \tag{1.23}$$

Hence, if  $\Omega$  satisfies the Diophantine condition (2.8) we see that  $v^0$  is constant,  $\lambda^0 = 0$  and imposing (2.3) we obtain  $v^0 = 0$ .

Matching coefficients of  $\epsilon^1$  in both sides of (1.21) we obtain

$$v^1(\psi + \Omega, \eta) + v^1(\psi - \Omega, \eta) - 2v^1(\psi, \eta) + W(\psi, \eta) + \lambda^1(\eta) = 0. \tag{1.24}$$

We see that, using the theory in Section 2.3.3, to have analytic  $v^1$  solving (1.24), it is necessary and sufficient to have

$$\lambda^1(\eta) = - \int_{\mathbb{T}^{d-1}} W(\psi, \eta) d\psi. \tag{1.25}$$

Then,  $v^1, \lambda^1$  can be determined uniquely up to a constant from (1.24). In fact, in Fourier series, the equation for  $v^1, \lambda^1$  is

$$v_k^1 2(\cos(2\pi k\Omega) - 1) = -W_k - \delta_{0,k} \lambda^1, \quad (1.26)$$

where  $\delta_{0,k}$  is the Kronecker delta. In particular, the constant in  $v^1$  is determined by the normalization (2.3).

Proceeding to higher order follows the same pattern. We see that matching the terms of order  $\epsilon^n$  in (1.21) we obtain

$$v^n(\psi + \Omega, \eta) + v^n(\psi - \Omega, \eta) - 2v^n(\psi, \eta) + R^n(\psi, \eta) + \lambda^n(\eta) = 0, \quad (1.27)$$

where  $R^n$  is a polynomial expression in  $v^1, \dots, v^{n-1}$  with coefficients which are derivatives with respect to  $\psi$  of  $W((\psi, \eta) + \beta v(\psi, \eta))$ . This polynomial can be computed explicitly because it is given by

$$R^N = \frac{1}{(N-1)!} \frac{d^{N-1}}{d\epsilon^{N-1}} W\left((\psi, \eta) + \beta \sum_{n=0}^{N-1} v^n(\psi, \eta)\right) \Big|_{\epsilon=0} \quad (1.28)$$

and these are well known formulae. We also note that, from the algorithmic point of view there are efficient ways to compute  $R^N$  using methods of “automatic differentiation” [22, 23].

Since  $R^n$  can be computed explicitly, (1.27) can be solved the same way as (1.24).

We have therefore established

**Lemma 2.** *Assume that  $\Omega \in \mathcal{D}(v, \tau)$  as defined in (2.8) and that  $W : \mathbb{T}^d \rightarrow \mathbb{C}$  is an analytic function.*

*Then, we can find formal power series solutions in  $\epsilon$  of the form (1.22) solving the equation (1.21).*

*Each of the terms  $v^j(\psi, \eta)$  is analytic in complex neighborhoods of the torus.*

If  $W$  takes real values for real values, then so do the  $v, \lambda$ .

#### 1.4.1 The auxiliary equation

Now, we turn to the problem of studying the equation

$$\lambda(\eta, \epsilon) = \lambda^*. \quad (1.29)$$

We expect to obtain a solution  $\eta^*(\epsilon)$  provided that (1.29) satisfies some non-degeneracy conditions.

Having solution of (1.29) to order 1 in  $\epsilon$ , amounts to

$$\lambda^1(\eta) = 0.$$

That is, we need to find  $\eta$  such that

$$\int_{\mathbb{T}^{d-1}} W((\psi, \eta) + \beta v(\psi, \eta)) d\psi = 0. \quad (1.30)$$

**Theorem 1.** *The equation (1.30) has always two solutions.*

*Proof.* Since

$$\int_{\mathbb{T}^{d-1}} W((\psi, \eta) + \beta v(\psi, \eta)) d\psi = \int_{\mathbb{T}^{d-1}} (\partial_\alpha V)(B^{-1}(\psi, \eta) + \alpha v(\psi, \eta)) d\psi,$$

if we integrate again with respect to  $\eta$  we obtain

$$\int_{\mathbb{T}} \int_{\mathbb{T}^{d-1}} W((\psi, \eta) + \beta v(\psi, \eta)) d\psi d\eta = \int_{\mathbb{T}^d} (\partial_\alpha V)(B^{-1}(\psi, \eta) + \alpha v(\psi, \eta)) d\psi d\eta = 0. \quad (1.31)$$

Hence the function of  $\eta$  given by  $\int_{\mathbb{T}^{d-1}} W((\psi, \eta) + \beta v(\psi, \eta)) d\psi$  is a continuous periodic function of  $\eta$  with zero average. Therefore, it has at least two zeros. We also note that there are open sets of perturbations where there are 4, 6,  $\dots$  zeros.  $\square$

Denote one of these solutions of (1.30) as  $\eta^*$ .

A sufficient condition that ensures that we can solve the equation (1.29) to all orders is that

$$\frac{\partial}{\partial \eta} \lambda(\eta, \epsilon) \Big|_{\eta=\eta^*, \epsilon=0} \neq 0. \quad (1.32)$$

More explicitly,

$$\int_{\mathbb{T}^d} \frac{\partial}{\partial \eta} (\partial_\alpha V)(B^{-1}(\psi, \eta) + \alpha v(\psi, \eta)) d\psi \neq 0. \quad (1.33)$$

Then, the implicit function theorem for power series [24, 25] gives us that we can indeed find  $\eta^*(\epsilon)$ .

Similarly, we can solve the equation  $\lambda(\eta) = \lambda^*$  provided that  $|\lambda^*|$  is sufficiently small.

Therefore, we have established

**Theorem 2.** *Assume that  $\Omega \in \mathcal{D}(v, \tau)$  as defined in (2.83), that  $W$  is an analytic function, and that (1.33) holds, we can find formal power series  $\eta_\epsilon$  in  $\epsilon$  so that  $v_{\eta_\epsilon}$  is the solution of (1.21).*

Clearly, since the function  $\lambda^n(\eta)$  are bounded, if  $\lambda^*$  – the physical force – is large enough, there is no solution. This has a clear physical meaning. If we increase the external force but keep it small, the system can react by changing the transversal phase. If the force increases beyond a threshold, the system cannot react by adapting the phase. Hence, the equilibrium breaks down. In this paper, we are not considering the dynamics of the model, only the equilibria (our models for the energy include only the potential energy of the configuration and not any kinetic energy). One can, however, expect that, if there was some dynamics, the equilibria considered here could slide.

Of course, the sufficient condition (1.33) is far from being necessary and there are many other conditions that are enough.

**Proposition 3.** *Assume that  $\Omega \in \mathcal{D}(v, \tau)$  as defined in (2.8), that  $W((\psi, \eta) + \beta v(\psi, \eta))$  is an analytic function, and that (1.33) holds.*

Assume that  $\eta^*$  is such that for some  $m \in \mathbb{N}$  we have

$$\begin{aligned}\lambda^i(\eta^*) &= 0, \quad i = 1, \dots, 2m \\ \lambda^{2m+1}(\eta^*) &\neq 0.\end{aligned}\tag{1.34}$$

Then, we can find formal power series  $\eta_\epsilon$  in  $\epsilon$  so that  $v(\psi, \eta_\epsilon)$  is the solution of (1.21).

The proof is again an application of the implicit function theorem for power series.

## 1.5 A dynamical interpretation of the equilibrium equations of Frenkel-Kontorova models

In this section, we present a dynamical interpretation of the equilibrium equations (1.4) in Frenkel-Kontorova models.

Even if the dynamical interpretation is possible for finite range interactions, we see that adding another small interaction of longer range is a singular perturbation (even the dimension of the phase space changes). Whereas, for the methods in this paper, adding a small term in the longer range is a regular perturbation of the same order.

A straightforward way of transforming the equilibrium equation

$$x_{n+1} + x_{n-1} - 2x_n + \epsilon \partial_\alpha V(x_n \alpha) + \lambda = 0 \quad \forall n \in \mathbb{Z}\tag{1.35}$$

into a dynamical system is setting

$$\begin{aligned}y_n &= (x_n, x_{n-1}) \\ y_{n+1} &= (2y_n^1 - y_n^2 - \partial_\alpha V(\alpha y_n^1) - \lambda, y_n^1).\end{aligned}\tag{1.36}$$

However, (1.36) is not very useful because we have to consider it as a map of  $\mathbb{R}^2$  and the term  $\partial_\alpha V(\alpha y_n^1)$  does not make apparent that it is periodic in  $\alpha y_n^1$ .

A more natural formulation is obtained by observing that the equation (1.4) is equivalent

to the system on  $\mathbb{T}^d \times \mathbb{R}$

$$\begin{aligned} p_{n+1} &= p_n - \partial_\alpha V(q_n) - \lambda \\ q_{n+1} &= q_n + \alpha p_{n+1}, \end{aligned} \tag{1.37}$$

where  $q_n \in \mathbb{T}^d$ ,  $p_n \in \mathbb{R}$ . (Just multiply (1.4) by  $\alpha$  and use the substitution  $p_n = x_n - x_{n-1}$ ,  $q_n = \alpha x_n$ . Note that (1.4) is equivalent to

$$(x_{n+1} - x_n) - (x_n - x_{n-1}) + \partial_\alpha V(\alpha x_n) + \lambda = 0$$

hence, we obtain the first equation.)

Note that, even if (1.36) and (1.37) are equivalent, the variables in (1.37) are more natural. Of course, (1.37) has more variables than (1.36). The extra variables in (1.37) correspond to the internal phases of the material. From the physical point of view, sampling orbits in (1.37) can be considered as sampling different regions in the material.

We will write the mapping (1.37) as

$$(p_{n+1}, q_{n+1}) = F_{\varepsilon, \lambda}(p_n, q_n). \tag{1.38}$$

Note that (1.37) is typographically very similar to the standard map [26] or to analogues introduced for volume preserving maps. Nevertheless, there are significant differences (besides the different dimensions).

A very crucial difference between (1.38) and the generic volume preserving maps is that  $q_{n+1} - q_n$  is always a multiple of  $\alpha$  (see (1.37)). So that the two dimensional leaves

$$\mathcal{M}_{q_0} = \{(p, q_0 + \alpha t) \mid p, t \in \mathbb{R}\} \tag{1.39}$$

are preserved. Note that each of the leaves  $\mathcal{M}_{q_0}$  is dense in the  $d + 1$  dimensional phase space.

The mapping (1.37) clearly preserves the volume form  $dp \wedge dq_1 \wedge \dots \wedge dq_d$  since it is the composition of

$$\begin{aligned} p_{n+1} &= p_n - \partial_\alpha V(q_n) - \lambda \\ q_{n+1} &= q_n \end{aligned} \tag{1.40}$$

and

$$\begin{aligned} p_{n+1} &= p_n \\ q_{n+1} &= q_n + \alpha p_{n+1}. \end{aligned} \tag{1.41}$$

We recall that, in our context, a volume preserving map is exact when  $F^*(pdq_1 \wedge dq_2 \wedge \dots \wedge dq_d) = pdq_1 \wedge dq_2 \wedge \dots \wedge dq_d + dP$  where  $P$  is  $d - 1$  form.

Indeed, (1.38) is an exact volume preserving map if and only if  $\lambda = 0$ , since it is easy to observe that, when  $\lambda = 0$ , both (1.40) and (1.41) are exact.

When  $\varepsilon = 0$ ,  $\lambda = 0$ , the map (1.37) is integrable. The codimension-one tori given by  $p = \text{cte.}$  are invariant and the motion in them is a rotation.

The volume preserving KAM theory leads us to expect that for  $\epsilon \ll 1$ ,  $\lambda = 0$ , the tori in which the frequency of the motion is Diophantine survive. We also expect that the tori with resonance, breaks down into lower dimensional tori. The lower dimensional tori can survive for  $|\lambda| \ll 1$  (depending on  $\epsilon$ ).

In this paper we have quantitative (but formal and non-rigorous) prediction of these phenomena based on perturbative expansions. We hope that some of them may be either verified by rigorous results or explored numerically.

### 1.5.1 On the global geometry of the constraints given by (1.39)

Integrable systems with constraints have been studied extensively in geometric mechanics. Nevertheless, the systems we consider here have some unusual properties that we would like to highlight.

It is customary to classify the constraints in holonomic when the distributions are integrable (in the sense that they foliate the phase space with a smooth quotient) and non-holonomic when the distributions are not integrable and they violate the hypothesis of Frobenius Theorem [27, 28, 29].

The constraints (1.39) escape this dichotomy. They are locally integrable (they do satisfy the hypothesis of Frobenius Theorem and are locally given by invariant manifolds that give rise to a foliation) but nevertheless, the manifolds are dense, so that they do not give a nice quotient manifold.

Hence, even if we have holonomic constraints locally (and the infinitesimal results about holonomic systems are applicable), some global aspects such as symplectic reduction [30, 31, 32] cannot be applied to (1.37).

We note that maps with these paradoxical properties have appeared several times in the literature. In the mathematical literature, they have appeared as “reparameterization of linear flows”[33, 34]. Besides the theoretical interest of these maps, they also appear naturally in many applied problems [35, 36, 37].

### 1.5.2 Lyapunov exponents and phonon localization

In this section we study the so called *phonon gap* around the equilibria of (1.10) given by a hull function.

Let us start by recalling some standard definitions. The main idea is that sound waves are defined by the propagation of infinitesimal disturbances around an equilibrium equation.

If we linearize around an equilibrium solution  $x = \{x_n\}_{n \in \mathbb{Z}}$ , we obtain the dynamics of the infinitesimal perturbations  $\xi_n$  is given by

$$\ddot{\xi}_n = \xi_{n+1} + \xi_{n-1} - 2\xi_n + (\partial_\alpha)^2 V(\alpha x_n) \xi_n \equiv (\mathcal{L}_x \xi)_n. \quad (1.42)$$

It is clear that the propagation properties of sound waves will be affected by the spectral properties of the operator  $\mathcal{L}_x$ .

Note that the operator  $\mathcal{L}$  is a one-dimensional Schrödinger operator with a position dependent potential. The dependence will be given by the dynamics of the  $x_n$ . In particular, for the solutions given by a hull function, we will be considering quasi-periodic potentials.

The mathematical theory of the spectrum of quasi-periodic Schrödinger operators is well developed [38, 39]. In particular, it is known that the spectrum is independent of the  $\ell^p$  space in which it is considered, and, more important for us, that the spectrum can be characterized by the existence of approximate eigenfunctions. In the dynamical interpretation in this section, the spectrum corresponds to the Lyapunov exponents of the solution [40].

In the case of (1.37), we can study the Lyapunov spectra for any orbit using the geometric constraints (1.39).

**Proposition 4.** *Let  $x_n$  be an orbit of the mapping given by (1.37). Assume that Osledets Theorem applies to it. Then,  $d - 1$  Lyapunov exponents are zero. Also, the sum of all the Lyapunov exponents is zero.*

*Proof.* Consider  $\tilde{F}$ , the lift of the map  $F$  in (1.38).

Let  $s$  be a vector perpendicular to  $\alpha$ . It is a simple computation to show that:

$$\tilde{F}(\tilde{M}_{q_0+s}) = \tilde{M}_{q_0} + s.$$

Then it is clear that the  $d - 1$  vectors in the directions perpendicular to  $s$  do not grow.

The fact that the sum of the Lyapunov exponents for orbits of a volume preserving map is zero is well known since the sums of the Lyapunov exponents is the rate of growth of the determinant of iterates of the map. □

Of course, the dynamical system (1.37) is straightforward to implement numerically and allows study of statistical properties of depinning.

**CHAPTER 2**

**KAM THEORY FOR RESONANT QUASI-PERIODIC EQUILIBRIA IN  
QUASI-PERIODIC MEDIA**

**2.1 Introduction**

The goal of this paper is to develop a KAM theory for the functional equation:

$$v(\psi + \Omega, \eta) + v(\psi - \Omega, \eta) - 2v(\psi, \eta) + W((\psi, \eta) + \beta v(\psi, \eta)) + \lambda = 0 \quad (2.1)$$

where  $W : \mathbb{T}^d \rightarrow \mathbb{R}$ ,  $\Omega \in \mathbb{R}^{d-1}$ ,  $\beta \in \mathbb{R}^d$  are given,  $\psi$  is a variable in  $\mathbb{T}^{d-1}$  and we can think of  $\eta \in \mathbb{T}$  as a parameter. We are to find  $v : \mathbb{T}^{d-1} \times \mathbb{T}^1 \rightarrow \mathbb{R}$  as a function of  $(\psi, \eta)$  and  $\lambda \in \mathbb{R}$  as a function of the parameter  $\eta$ . Since we think of  $\eta$  as a parameter, we will write  $v_\eta(\psi) = v(\psi, \eta)$ . We will refer to (2.1) as the “equilibrium equation”. Later, when it cannot lead to confusion we will suppress the subindex.

The equation (2.1) was derived in the paper [1] as the equation is satisfied by hull functions of quasi-periodic equilibria in Frenkel-Kontorova models of deposition on quasi-crystals when the frequency of the equilibrium solution is resonant with the frequencies of the substratum. The variable  $\eta$  is an angle which has the meaning of a transversal phase.

Roughly, the model describes particles interacting with their neighbors and with a substratum which is quasi-periodic. The configuration describing the state of the system is parameterized by the hull function  $v$ . We try to place the particles with a frequency (inverse of the density of particles) which resonates with the frequencies of the medium.  $\Omega$  represents the *intrinsic frequencies*. Since the medium is resonating with the frequency of the configuration, the positions of the particles are parameterized by  $d - 1$  angles, i.e. they cover densely a  $d - 1$  dimensional torus which is indexed by  $\eta$ . The  $W$  represents the forces of the particles with the substratum and the  $\lambda$  is an external force. The main

motivation for our study is that, when there are external forces weaker than the potential, the non-resonant smooth solutions disappear. In the case of periodic media, it is known that many of the solutions that survive constant external forces are resonant. See [19] for a quantitative numerical study in periodic media. In this paper we will show that indeed, in quasi-periodic media, the solutions with resonant forces may exist when there is an external constant force. Note that, the configurations we construct differ from a constant frequency by a bounded corrector even if there are external fields.

To avoid repetitions, we refer to the paper [1] for the discussion of the physical motivations (there are several physical motivations for the Frenkel-Kontorova model) and for a formal analysis and for references to the literature. From the strictly logical point of view, this paper and [1] are completely independent even if they are motivated by the same physical problem. They also rely on very different techniques since [1] is concerned with physical derivations, formal expansions and the present paper uses hard analysis.

The main goal of this paper is to develop a KAM theory for the equation (2.1), but we will have to add a one dimensional extra parameter to it.

The main source of the difficulty to implement a Newton method for equation (2.1) – as needed in KAM theory – is that the equation (2.33) (the linearization of the equilibrium equation (2.1)) is not easily analyzable in a way that leads to tame estimates. We will deal with this problem by adding an extra auxiliary equation which implies that (2.33) can be solved with tame estimates.

It may seem paradoxical that solving two equations is simpler than solving just one, but this is common place in numerical analysis, when one introduces preconditioners. The addition of an extra equation that allows to solve the linearization is similar in spirit to the introduction of the reducibility in KAM theory [21]. Nevertheless, our auxiliary equation is very different from the one in reducibility.

### 2.1.1 The method of adding extra parameters to equations

The main observation that allows us to develop a KAM theory is that if we are allowed to adjust a one dimensional parameter in the potential, then the linearized equilibrium equation admits a very nice structure (it can be factorized into two first order equations and the factorization allows to develop an iterative procedure which is quadratically convergent). The role of the extra parameter will be discussed in greater depth in Section 2.2.

Hence, in Section 2.1.1, we will add an extra parameter to the left hand side of (2.1) to obtain the modified equilibrium equation (2.2) such that its linearization can be factorized. Then, we supplement (2.2) with another equation (2.4) in Section 2.2 (we call it *the factorization equation*) which encodes that the linearization of the equilibrium equation can be solved. The physical and mathematical implication of the parameters will be discussed in Section 2.2.

#### *The modified equilibrium equation*

For each fixed  $\eta \in \mathbb{T}^1$  we will look for a function  $v(\cdot, \eta) : \mathbb{T}^{d-1} \rightarrow \mathbb{R}$  and for numbers  $\lambda, \sigma$  in such a way that we have

$$\begin{aligned} & \mathcal{E}[v, \sigma, \lambda](\psi, \eta) \\ & \equiv v(\psi + \Omega) + v(\psi - \Omega) - 2v(\psi) + W((\psi, \eta) + \beta v(\psi)) + v(\psi)\sigma + \lambda \\ & = 0. \end{aligned} \tag{2.2}$$

In the rest of the paper, we will call this modified equation (2.2) the equilibrium equation. The equation (2.2) has a symmetry that makes the solutions not unique (this corresponds to a gauge symmetry related to the choice of origin of the phase in the original problem). Hence, to obtain local uniqueness, we supplement (2.2) with the following normalization:

$$\int_{\mathbb{T}^{d-1}} v(\psi) d\psi = 0. \tag{2.3}$$

We consider  $\mathcal{E}$  as a functional that given a function  $v$  and two numbers  $\sigma, \lambda$  produces another function given by the second line in (2.2). And we treat the equation (2.2) as searching for zeros of the functional  $\mathcal{E}$ .

Since  $v, \sigma, \lambda$  all depend on the parameter  $\eta$ , for convenience, we will write  $v_\eta$  when we need to emphasize the fact that  $v$  depends on  $\eta$ , and similarly for all the other functions. We will also obtain  $\sigma, \lambda$  as a function of  $\eta$  (and maybe of frequency  $\Omega$ , but we will not discuss dependence on  $\Omega$  in this paper).

## 2.2 Remarks on the role of parameters

The equations we will solve involve several parameters ( $\lambda$  external force,  $\eta$  internal phase,  $\Omega$  intrinsic frequency,  $\sigma$  the counterterm of the potential) as well as the functions  $v_\eta, c_\eta$ . For the mathematical methods used in this paper, it is more convenient to fix  $\eta$  and  $\Omega$  and obtain all the others as functions of  $\eta, \Omega$ . Of course if the potential depends on other parameters, we will also obtain that  $\lambda, \sigma, v, c$  are functions of  $\eta, \Omega$  and the parameters determining the potential. (The perturbative work of [1] considered mainly the dependence of the results on the parameters of the potential using formal perturbation expansions).

In Section 2.6.1 we will show that the dependence of these parameters on the solution on  $\eta, \Omega$  (and the parameters of the potential) is smooth and that we can find the jets of the relation between them using formal perturbation theories.

This allows to analyze several different physical situations by using only the finite dimensional implicit function theorem.

Depending on the physical problem, we may impose the value of one of these variables and determine the others. For example, if we are imposing an external force we may want to fix  $\lambda$  or if the material is constrained to have a certain density, we may fix  $\Omega$ .

It is important to notice that, once we have established the KAM theorem, eliminating some variables in terms of the others is just an application of the finite dimensional implicit function theorem. Hence, we can accommodate several physical situations by just applying

the finite dimensional implicit function theorem. Note that the results in Section 2.6.1 give explicit formulas for the jets of the above functions, so that it is quite easy to verify the hypothesis of many finite dimensional implicit function theorems [41].

Two subtle points appear: A technical point of a mathematical nature is that  $\Omega$ , since it is required to be Diophantine, ranges over a complicated closed set. This is, by now well understood since one can use the Whitney regularity theory in these sets. See the discussion in Section 2.6.1. Another complicated problem is the physical meaning of the parameter  $\sigma$ , which seems to be necessary for the mathematical treatment presented by us, but which did not appear in the perturbative treatment in [1]. It seems heuristically plausible (but we do not consider the problem rigorously) that, for small potentials the parameter  $\sigma$  can be eliminated by modifying the parameter  $\Omega$ . Note that  $\Omega$  ranges over a  $d - 1$  dimensional Cantor set of large measure. It seems possible that when the set of  $\Omega$  has large density, moving  $\Omega$  can set the  $\sigma = 0$ .

In the following remarks, we make some notes on the dependence on parameters.

**Remark 4.** *Variants of the idea of adding external parameters and then setting them to zero, has appeared in many guises. In perturbative expansions in Physics, it is called the method of counterterms [42, 43]. In differential equations, it is called Cesari's alternative method (Chapter IX of [44], [45]). Closer to us, in KAM theory, it was introduced in [21]. It was realized in [46, 47, 48, 49] that it provided a good way to deal with degenerate problems. A very systematic treatment of dependence on parameters (including parameters taking values in nowhere dense sets) appears in [50].*

**Remark 5.** *The exact form of the counterterm added is not that important. We could have put other counterterms  $\sigma F(v)$  for almost any function  $F \neq 0$ .*

*The way of thinking geometrically of the counterterms is that there is codimension 1 set of potentials for which the solutions move differentiably with respect to parameters. The counterterm is a projection that moves to keep the problem in this manifold. We could have taken any other family of corrections to the codimension one manifold where the solutions*

are found. We refer to Section 2.6 for a precise formulation and more details.

**Remark 6.** Even if we could consider (2.2) as a functional equation for each value of  $\eta$ , we will show in the next section that the symmetries of the equation involve mixing the  $\psi$  and  $\eta$  dependence. Relatedly, we note that the equation (2.2) for a fixed value of  $\eta$  does not have a variational principle.

It will be important to mention that, because  $\beta$  has components both in the  $\psi$  and the  $\eta$  directions, the equation (2.2) cannot be considered just as a parameterized version of the equations considered in [5].

**Remark 7.** The parameter  $\sigma$  is certainly needed by the method presented here. It is, in principle, possible, that there could be other method that does not have this restriction, but we suspect that this is the case. That is, unless one chooses the parameter  $\sigma$ , no equilibria of the form required are found.

As we discussed, the fact that the difference equation can be factorized is very similar to putting the linearized equation in divergence form. It is well known that even in 1-D, not all equations are in divergence form and one may have to adjust some parameters. This is the mathematical origin of the parameter  $\sigma$ . The divergence form is well known to lead to good quantitative homogenization estimates. See [51] for the case of second order elliptic operators.

Notice that if we choose nonlinearities with certain symmetries, they may force the parameter  $\sigma$  to be zero.

The physical interpretation of the counterterm  $\sigma$  is that the factorization of the equation for a fixed frequency  $\Omega$  are only true for a codimension-1 family of potentials. If we allow the frequency  $\Omega$  to vary (over a Cantor set of large measure satisfying the appropriate Diophantine conditions), heuristically, we expect that there is a  $(d-2)$ -dimensional Cantor set of Diophantine  $\Omega$ 's that lead to  $\sigma = 0$ . Of course, as the external forcing and the potential change, the set of  $\Omega$  which leads to equilibrium may change and even disappear. In the periodic case, [19] has very precise conjectures backed by numerical evidence.

*In the physical situation of deposition of materials (see [1] for a discussion of the Physics of the models), the natural interpretation is that if we apply an external force to the system, it will rearrange itself so that the internal frequency  $\Omega$  is among the resonant ones. The actual  $\Omega$  finally chosen will depend on how the force is turned on and, of course, on the initial conditions. Notice that, as we have said, we expect that there will be several equilibria (as well as metastable states).*

*In [1], it is shown that if we perform perturbation expansions from an integrable case (no potential), the counterterm  $\sigma$  vanishes to all orders in perturbation theory in the size of the potential. As indicated before, we expect that it does not vanish for a fixed  $\Omega$  so that this could be some effect beyond all orders, presumably exponentially small,*

*The factorization equation*

For the KAM treatment of the equilibrium equation (2.2), we will find it useful to supplement (2.2) with another equation which we call the factorization equation

$$\mathcal{F}[v, \sigma, c](\psi, \eta) \equiv [-c(\psi) + 2 - \partial_\beta W((\psi, \eta) + \beta v_\eta(\psi)) - \sigma] c(\psi + \Omega) - 1 = 0. \quad (2.4)$$

The equation (2.4) should be considered as a functional equation for functions  $v_\eta, c : \mathbb{T}^{d-1} \rightarrow \mathbb{R}$  and number  $\sigma$  when  $\eta$  is fixed. The dependence on  $\eta$  will be studied later.

The equation (2.4) gives a condition which ensures that the linearization of the equilibrium equation (2.2) has a nice structure which allows to implement a Newton method with tame estimates (namely, that it factorizes into two first order difference equations). See Section 2.5.2 for a discussion of (2.4) as a tool for solving (2.2).

The equation (2.4) is hard to solve exactly, but we will be able to develop a quasi-Newton method for (2.4).

The main idea of the paper is that, even if we do not know how to carry out a KAM theory for the equilibrium equation (2.2) alone, we can carry out a KAM procedure for

the pair of equations (2.2) and (2.4). As discussed in Section 2.2, similar things (a functional equation supplemented by another auxiliary one that makes the associated linearized equation solvable) have happened in classical problems in KAM theory [21, 52].

**Remark 8.** *Notice that both the equilibrium equation (2.2) and the factorization equation (2.4) are coupled because  $v$  is an unknown in both equations.*

*Nevertheless, it is heuristically useful to think of the two equations (2.2) and (2.4) as an upper diagonal system. Heuristically, the main equation is (2.2) and (2.4) is an auxiliary equation.*

*This heuristic is further justified because the perturbative treatment of the pair (2.2) and (2.4) has a skew product structure. See Section 2.6.1.*

*More relevantly, when we develop a KAM scheme looking at the linearization, (see Section 2.5.3 for a detailed treatment), we will see that the two linearizations are not upper diagonal but the coupling is only through the fact that  $\sigma$  appears in both equations. As it turns out the dependence on  $\sigma$  is affine and there are methods (introduced in [53]) to transform these equations into upper triangular (studying separately terms that depend linearly in  $\sigma$  and terms that are constant in  $\sigma$ ).*

#### *Comparison of the method in this paper with the application of reducibility*

The method of adding an extra equation so that the linearization of the equilibrium equation is solvable, has already appeared in KAM theory.

In the theory of perturbation of lower dimensional elliptic tori, the classical treatment is to try to reduce the linearized equation to an equation with constant coefficients [21, 54]. This requires extra non-resonance conditions and, in principle extra parameters. See, in particular [55, 56, 57], which study the problem of breakdown of resonant tori in Hamiltonian systems.

In the present case, the situation is completely different in the details (since we do not seek reducibility but rather factorization into two second order equations) as well as in

the concepts (in [21], the parameters are related to initial conditions or the characteristic numbers of the linearized equation). Hence the parameter count of the present method is very different from what one could expect from reducibility. Also the reducibility equations have a very different geometric meaning from the factorization equations.

The factorization method has analogies in higher dimensional systems and in elliptic PDE [58, 59]. One can think of factorization as an analogue of putting the PDE in divergence form. The transformation to divergence form is achieved in [58, 59] for elliptic operators taking advantage of an identity (which is analogous to the Ward identities in gauge theory). Here, on the other hand, we have to do a KAM theorem to obtain an auxiliary function that gives the factorization.

The present method gives an a-posteriori theorem. As an (almost) automatic consequence of the a-posteriori format, we obtain smooth dependence on parameters, and justify the perturbation theory. The method of proof leads to efficient numerical algorithms (low storage requirements, low operation count per step, quadratical convergence).

### 2.2.1 Properties of the equilibrium equations (2.2) and its associated factorization equation

#### (2.4)

Before embarking on the hard analysis, in this section, we derive some identities and symmetries of the equations which are only soft analysis. This section can be skipped by readers interested only in the KAM methods.

Many of the symmetries and elementary properties derived for the equilibrium equation in [1] lift straightforwardly to the factorization equation. Surprisingly, the formal perturbation theory developed here for the pair (2.2) and (2.4) is more efficient than the perturbation theory for (2.1) alone developed in [1]. The perturbation theory developed in [1] was only for perturbation around integrable solutions, but the perturbation theory for the pair (2.2) and (2.4) is developed around any solution of both equations (2.2) and (2.4). See Section 2.6.

The expansions around zero found in [1] are a particular case of the expansions found here since the linearization of the equilibrium equation around zero admits a trivial factorization.

*The symmetries of the equilibrium equations (2.2).*

We note that the symmetries for the equilibrium equation found in [1] extend to the factorization equation.

We have that if  $v_\eta, \sigma(\eta), \lambda(\eta)$  is a solution of (2.2), for any function  $\iota(\eta)$  so is:

$$\begin{aligned}\tilde{v}_\eta(\psi) &= v_{\eta+\iota(\eta)\beta_\eta}(\psi + \iota(\eta)\beta_\psi) + \iota(\eta), \\ \tilde{\sigma}(\eta) &= \sigma(\eta + \iota(\eta)\beta_\eta), \\ \tilde{\lambda}(\eta) &= \lambda(\eta + \iota(\eta)\beta_\eta) - \iota(\eta) \sigma(\eta + \iota(\eta)\beta_\eta).\end{aligned}\tag{2.5}$$

Here we use  $\beta_\psi$  to denote the first  $d - 1$  components of  $\beta$  and  $\beta_\eta$  to denote the last component of  $\beta$ .

Since the symmetry (2.5) involves changes of arguments, given a  $v_\eta$ , finding the  $\iota(\eta)$  that accomplishes the normalization involves solving the implicit equation

$$I(\eta + \beta_\eta \iota(\eta)) + \iota(\eta) = 0\tag{2.6}$$

where  $I(\eta) \equiv \int_{\mathbb{T}^{d-1}} v_\eta(\psi) d\psi$ .

Applying the finite dimensional implicit function theorem, we can solve (2.6) if  $I$  and its derivative with respect to  $\iota(\eta)$  are both small. In contrast, in the non-resonant case treated in [5], the normalization of the function  $v$  could always be solved explicitly.

As we will prove in Section 2.5, the solutions of (2.2) that satisfy the normalization (2.3) will be locally unique.

## 2.3 Preliminaries

To formulate the KAM results (as well as to make quantitative the Lindstedt series) we need to define precisely the norms of analytic functions. In this section, we collect the definitions and some standard properties of spaces of analytic functions.

In Section 2.3.1, we collect several standard definitions of spaces and present some preliminary results on these spaces. In Section 2.3.2 we present definitions of the Diophantine properties we will use in this paper. In Section 2.3.3 we present well known estimates for cohomology equations, which are the basis of the KAM procedure. Besides the customary constant coefficient equations, we study first order cohomology equations with non-constant coefficients in Section 2.3.4, which were also studied in [60].

To be consistent with the applications later, we will be dealing mainly with functions of  $d-1$  variables in this section. Of course,  $d$  is a dummy variable and the results are valid for any dimension. Of course, the names of the variables in the lemmas are arbitrary dummy variables, but we choose them to be indicative of the uses we will give them later. Some lemmas will be used in the proof for several functions.

### 2.3.1 Spaces of functions we will use

We will use a variation on the same spaces of analytic functions which have been used very often in KAM theory since [21]. We will use the same notations as in [20, 61, 5, 6].

We denote by

$$D_\rho \equiv \{ \psi \in \mathbb{C}^{d-1} / \mathbb{Z}^{d-1} \mid |\operatorname{Im}(\psi_j)| < \rho \}.$$

We denote the Fourier expansion of a periodic function  $v(\psi)$  on  $D_\rho$  by

$$v(\psi) = \sum_{k \in \mathbb{Z}^{d-1}} \hat{v}_k e^{2\pi i k \cdot \psi},$$

where  $\cdot$  is the Euclidean scalar product in  $\mathbb{C}^{d-1}$  and  $\hat{v}_k$  are the Fourier coefficients of  $v$ .

We denote by  $\mathcal{A}_\rho$  the Banach space of analytic functions on  $D_\rho$  which are real for real argument and extend continuously to  $\overline{D_\rho}$ . We make  $\mathcal{A}_\rho$  a Banach space by endowing it with the supremum norm:

$$\|v\|_\rho = \sup_{\psi \in \overline{D_\rho}} |v(\psi)|.$$

The spaces of analytic functions  $\mathcal{A}_\rho$  are the same spaces as in [21] and that some of their elementary and well known properties used in the argument were discussed in [21, 62]. Notably:

- Interpolation inequalities (Hadamard three circle theorem):

$$\|v\|_{\theta\rho+(1-\theta)\rho'} \leq \|v\|_\rho^\theta \|v\|_{\rho'}^{1-\theta}. \quad (2.7)$$

- Cauchy inequalities:

$$\|D^l v\|_{\rho-\delta} \leq C(l, d) \delta^{-l} \|v\|_\rho,$$

$$|\hat{v}_k| \leq e^{-2\pi |k| \rho} \|v\|_\rho.$$

- The regularity of the composition:

**Proposition 5.** *Let  $f$  be an analytic function in a domain  $\mathcal{D} \subseteq \mathbb{C}$ ,  $v \in \mathcal{A}_\rho$ . Assume  $v(\mathbb{T}_\rho^d) \subseteq \mathcal{D}$ ,  $\text{dist}(v(\mathbb{T}_\rho^d), \mathbb{C} - \mathcal{D}) \geq \xi > 0$ . Then,*

(1)  $f \circ v \in \mathcal{A}_\rho$ ;

(2) If  $\|\tilde{v}\|_\rho < \frac{\xi}{2}$ , we have

$$\|f(v + \tilde{v}) - f(v) - f'(v)\tilde{v}\|_\rho \leq C\|\tilde{v}\|_\rho^2.$$

The cohomology equations we will have to consider are different from those studied before and we will present the results in Section 2.3.4.

**Remark 9.** *The method of proof works also for spaces of functions with finite differentiability. Indeed, KAM theory is often formulated as an abstract implicit function theorem for the functional  $\mathcal{E}$  acting on spaces of functions that satisfy some mild properties [63, 64]. (The paper [65] presents a Nash Moser implicit function theorem well suited for the method in this paper.)*

*In particular, the method in this paper works as well when  $v$  is considered in Sobolev spaces of high enough regularity. For simplicity, we will not formulate the finite differentiable version of the results.*

### 2.3.2 Diophantine condition

We will require that  $\Omega$  satisfies the Diophantine condition in  $\mathbb{R}^{d-1}$ :

$$|k \cdot \Omega - m| \geq \kappa |k|^{-\tau} \quad \forall k \in \mathbb{Z}^{d-1} - \{0\}, m \in \mathbb{Z}. \quad (2.8)$$

Here  $\kappa, \tau$  are positive numbers.

We denote by  $\mathcal{D}(\kappa, \tau)$  the set of  $\Omega$  which satisfy (2.8). We also denote  $\mathcal{D}(\tau) = \cup_{\kappa>0} \mathcal{D}(\kappa, \tau)$ .

It is well known that the set  $\mathcal{D}(\tau)$  with  $\tau > d - 1$  is of full  $d - 1$  dimensional Lebesgue measure in  $\mathbb{R}^{d-1}$ .

### 2.3.3 Cohomology equations

It is standard in KAM theory to solve for  $v$  given  $\phi$  with zero average in such a way that:

$$v(\psi + \Omega) - v(\psi) = \phi(\psi), \quad (2.9)$$

where  $\Omega \in \mathcal{D}(\kappa, \tau)$ .

We will use equations similar to (2.9) frequently with some fixed frequency  $\Omega$ . To simplify our notations, we will denote  $v(\psi + \Omega)$  and  $v(\psi - \Omega)$  as  $v_+(\psi)$  and  $v_-(\psi)$ , respectively. Similar notations will be used for other functions. We also use  $T$  to represent the translation

operators, i.e.  $[T_\Omega v](\psi) = v(\psi + \Omega)$ .

Optimal estimates for (2.9) for Diophantine frequencies were proved in [66, 67]. The crucial point of these estimates is that the solution is bounded in smaller domains and that there are bounds on the solution in the smaller domains. These estimates have large constants if the loss of domain is small, but the constants can be chosen to be a power of the domain loss (tame estimates). See (2.12).

Tame estimates (and hence Diophantine conditions) are used in the convergence proofs and in the KAM theory developed here.

**Lemma 3.** *Let  $\phi \in \mathcal{A}_\rho(\mathbb{T}^{d-1})$  be such that*

$$\int_{\mathbb{T}^{d-1}} \phi(\psi) d\psi = 0. \quad (2.10)$$

*Assume that  $\Omega \in \mathcal{D}(\kappa, \tau)$ .*

*Then, there exists a unique solution  $v$  of (2.9) which satisfies*

$$\int_{\mathbb{T}^{d-1}} v(\psi) d\psi = 0. \quad (2.11)$$

*The solution  $v$  is in  $\mathcal{A}_{\rho'}$  for any  $0 < \rho' < \rho$ , and*

$$\|v\|_{\rho'} \leq C(d, \tau) \kappa^{-1} (\rho - \rho')^{-\tau} \|\phi\|_\rho. \quad (2.12)$$

*Furthermore, any distribution solution of (2.9) differs from the solution claimed before by a constant.*

*If  $\phi$  is such that it takes real values for real arguments, so does  $v$ .*

*Similarly if we consider analytic functions  $\phi \in \mathcal{A}_\rho(\mathbb{T}^d)$  satisfying  $\int_{\mathbb{T}^{d-1}} \phi(\psi, \eta) d\psi = 0$ , then for each  $\eta$ , we can solve*

$$v(\psi + \Omega, \eta) - v(\psi, \eta) = \phi(\psi, \eta). \quad (2.13)$$

The solution  $v \in \mathcal{A}_\rho(\mathbb{T}^d)$  is analytic in  $(\psi, \eta)$  and we have

$$\|v\|_{\rho'} \leq C(d, \tau) \kappa^{-1} (\rho - \rho')^{-\tau} \|\phi\|_\rho. \quad (2.14)$$

We note that, as it is well known that obtaining  $v$  solving (2.9) for given  $\phi$  is very explicit in terms of Fourier coefficients. If

$$\phi(\psi) = \sum_{k \neq 0} \hat{\phi}_k e^{2\pi i(k \cdot \psi)}$$

then,  $v$  is given by

$$v(\psi) = \sum_{k \neq 0} \hat{\phi}_k (e^{2\pi i k \cdot \Omega} - 1)^{-1} e^{2\pi i(k \cdot \psi)}.$$

The above formula for the solution makes it clear that if  $\phi$  is real for real values of its arguments, so is  $v$ . Note also that if the function  $\phi$  is discretized in terms of  $N$  Fourier coefficients, the computation of the Fourier coefficients of  $v$  takes only  $N$  operations.

The above formula also makes it clear how to obtain the tame estimates (with a worse exponent than the one obtained in [66, 67]) for Diophantine frequencies. It suffices to use the triangle inequality in all the terms, Cauchy inequalities for the Fourier coefficients and the elementary  $|e^{2\pi i k \cdot \Omega} - 1|^{-1} \leq C \text{dist}(k \cdot \Omega, \mathbb{Z})^{-1}$ . This line of argument also gives the results under the assumption (2.83).

#### 2.3.4 Cohomology equations with non-constant coefficients

In this section we consider a generalization of the above theory for equations with non-constant coefficients. These equations have also been called *twisted cohomology equations* in [60]. Our strategy is similar to that of [60], but we will need more details about the dependence of the solutions and of intermediate constructions on the coefficients, hence we will present full details.

We will be considering equations of the form

$$a(\psi)v(\psi + \Omega) - b(\psi)v(\psi) = \lambda + \phi(\psi) \quad (2.15)$$

where  $\psi \in \mathbb{T}^{d-1}$  and  $a, b$  are fixed functions in  $\mathcal{A}_\rho$ .

We consider that  $\phi \in \mathcal{A}_\rho$  is the known data of the equation and  $\lambda \in \mathbb{R}$ ,  $v \in \mathcal{A}_{\rho-\delta}$  are the unknowns we seek for. We will refer to (2.15) as “twisted cohomology equations”.

We will show that, given some non-degeneracy conditions in  $a$  and  $b$ , we can obtain estimates for  $\lambda$  and  $v$ . The idea, already present in [60], is that we can rewrite the equation (2.15) into a constant coefficient equation. We will go through the procedure in details because we will need rather detailed estimates on the effect of  $a$  and  $b$ .

**Lemma 4.** *Suppose  $\|a - 1\|_\rho < r < 1$ ,  $\|b - 1\|_\rho < r < 1$  and that  $\Omega$  satisfies the Diophantine condition (2.8). Then there exist positive real valued functions  $\gamma_a, \gamma_b \in \mathcal{A}_{\rho-\delta/2}$  and real numbers  $\bar{a}, \bar{b}$  such that*

$$\begin{aligned} a(\psi) &= \bar{a} \frac{\gamma_a(\psi + \Omega)}{\gamma_a(\psi)}, \\ b(\psi) &= \bar{b} \frac{\gamma_b(\psi)}{\gamma_b(\psi + \Omega)}. \end{aligned} \quad (2.16)$$

*In addition, for the twisted cohomology equation (2.15), there exist a unique solution  $\lambda \in \mathbb{R}$  and  $v \in \mathcal{A}_{\rho-\delta}$  for (2.15) satisfying the normalization*

$$\int_{\mathbb{T}^{d-1}} v d\psi = 0 \quad (2.17)$$

*such that*

$$|\lambda| \leq \frac{\|\phi\|_\rho \|\gamma_a(\gamma_b)_+\|_{\rho-\delta/2}}{\int_{\mathbb{T}^{d-1}} \gamma_a(\gamma_b)_+ d\psi} \quad (2.18)$$

$$\|\gamma_a \gamma_b v\|_{\rho-\delta} \leq C \delta^{-\tau} \|(\lambda + \phi) \gamma_a(\gamma_b)_+\|_\rho \quad \forall \delta > 0.$$

Therefore,

$$\|v\|_{\rho-\delta} \leq C \|\gamma_a\|_{\rho} \|1/\gamma_a\|_{\rho-\delta} \|\gamma_b\|_{\rho} \|1/\gamma_b\|_{\rho-\delta} \delta^{-\tau} \|(\lambda + \phi)\|_{\rho} \quad \forall \delta > 0. \quad (2.19)$$

*Proof.* To show (2.16), it suffices to observe that, taking logarithms, (2.16) is equivalent to:

$$\begin{aligned} (\log a)(\psi) &= \log(\bar{a}) + \log(\gamma_a)(\psi + \Omega) - \log(\gamma_a)(\psi) \\ (\log b)(\psi) &= \log(\bar{b}) + \log(\gamma_b)(\psi) - \log(\gamma_b)(\psi + \Omega) \end{aligned} \quad (2.20)$$

which are cohomology equations with constant coefficients. Applying Lemma 3, we get solutions  $\gamma_a, \gamma_b \in \mathcal{A}_{\rho-\delta/2}$ ,  $\bar{a}, \bar{b} \in \mathbb{R}$  and estimates

$$\begin{aligned} \|\log \gamma_a\|_{\rho-\delta/2} &\leq C(d, \tau, \kappa) \delta^{-\tau} \|\log a - \log \bar{a}\|_{\rho}, \\ \|\log \gamma_b\|_{\rho-\delta/2} &\leq C(d, \tau, \kappa) \delta^{-\tau} \|\log b - \log \bar{b}\|_{\rho}. \end{aligned} \quad (2.21)$$

Once we solve the constant coefficient cohomology equation (2.20) for  $\log a, \log b, \log \gamma_a, \log \gamma_b$  we obtain  $a, b, \gamma_a, \gamma_b$  by taking exponentials. This ensures that they are positive for real values of the argument. We refer to  $\bar{a}, \bar{b}$  as the average coefficients of the cohomology equation.

Once we have the solution of (2.16), we realize that the equation (2.15) is equivalent to

$$\bar{a}(\gamma_a \gamma_b v)_+ - \bar{b}(\gamma_a \gamma_b v) = (\lambda + \phi) \gamma_a (\gamma_b)_+ \quad (2.22)$$

which is a cohomology equation with constant coefficients. Let us denote  $m = \gamma_a \gamma_b v$  for simplicity.

When  $\bar{a} = \bar{b}$ , we can solve (2.22) using Lemma 3 and get estimates (2.18).

Note if  $\bar{a} \neq \bar{b}$ , the equation (2.22) is easier to solve since no small divisors appear.

- If  $\bar{a} > \bar{b}$ , then (2.22) is equivalent to

$$m_+ - \frac{\bar{b}}{\bar{a}}m = \frac{\lambda + \phi}{\bar{a}}\gamma_a(\gamma_b)_+,$$

namely,  $m_+ = \frac{\lambda + \phi}{\bar{a}}\gamma_a(\gamma_b)_+ + \frac{\bar{b}}{\bar{a}}m$ .

Therefore,

$$m(\psi) = \sum_{n=0}^{\infty} \left(\frac{\bar{b}}{\bar{a}}\right)^n \frac{\lambda + \phi(\psi - (n+1)\Omega)}{\bar{a}} \gamma_a(\psi - (n+1)\Omega) \gamma_b(\psi - n\Omega)$$

is a solution of (2.22). Hence,  $\|m\|_{\rho} \leq C(\bar{a}, \bar{b}) \|(\lambda + \phi)\gamma_a(\gamma_b)_+\|_{\rho}$ .

- If  $\bar{a} < \bar{b}$ , then (2.22) is equivalent to

$$\frac{\bar{a}}{\bar{b}}m_+ - m = \frac{\lambda + \phi}{\bar{b}}\gamma_a(\gamma_b)_+,$$

namely,  $m = \frac{\bar{a}}{\bar{b}}m_+ - \frac{\lambda + \phi}{\bar{b}}\gamma_a(\gamma_b)_+$ .

Therefore,

$$m(\psi) = - \sum_{n=0}^{\infty} \left(\frac{\bar{a}}{\bar{b}}\right)^n \frac{\lambda + \phi(\psi + n\Omega)}{\bar{b}} \gamma_a(\psi + n\Omega) \gamma_b(\psi + (n+1)\Omega)$$

is a solution of (2.22). Hence,  $\|m\|_{\rho} \leq C(\bar{a}, \bar{b}) \|(\lambda + \phi)\gamma_a(\gamma_b)_+\|_{\rho}$ .

□

**Remark 10.** Note that when  $\bar{a} \neq \bar{b}$ , the solutions could be estimated on the same domain and they do not involve any small divisors. But the estimates depend on  $\bar{a}, \bar{b}$  and indeed blow up as  $\bar{a}$  gets close to  $\bar{b}$ . To get estimates uniform in  $\bar{a}, \bar{b}$ , we need to use the Fourier method presented here and, hence assume small divisor conditions and incur loss of domains.

*In this paper, we will only use the general estimates that apply uniformly in  $\bar{a}, \bar{b}$  since most of the cases of interest for us happen in the regime when  $\bar{a} \approx \bar{b}$ .*

*In the paper [53] one encounters a very similar situation, but there it is natural to start in situations when  $\bar{a}$  is different from  $\bar{b}$  and the paper presents the improved estimates in this case.*

The choice of the parameter  $\lambda$  so as to achieve the normalization deserves some discussion. In the case  $\bar{a} = \bar{b}$  we see that we have to choose  $\lambda$  in such a way that the right hand side of (2.22) has zero average. In this case, however, we can choose the average of the solution of (2.22) arbitrarily.

In the case  $\bar{a} \neq \bar{b}$ , given any  $\lambda$ , the solution of (2.22) will be unique. Furthermore, the solution will be an affine function of  $\lambda$  and, hence, so will be its average.

We see that the derivative of the average of the solution with respect to  $\lambda$  is

$$\frac{d}{d\lambda} \langle m \rangle = \frac{\langle \gamma_a(\gamma_b)_+ \rangle}{\bar{a} - \bar{b}}.$$

In summary, in the equal average coefficient case, the equation requires adjusting one parameter to be solvable, but it gives back one free parameter of solutions. In the different average coefficient case, we do not require any parameter to ensure the solutions, but the solution is unique.

In both cases, the solutions of twisted cohomology equations require as many parameters as they give back. This allows us to discuss the solutions of the equations which factorize into twisted cohomology equations and they require as many parameters as they give back.

**Remark 11.** *It will be important for subsequent applications that the estimates (2.18) are formulated in terms of  $\gamma$ . We could have attempted to formulate them in terms of  $a$ , but this is not practical for subsequent applications. On the other hand, we have formulated the normalization condition (2.17) in a way that it is independent of  $\gamma$ . This will be important*

in our iterative scheme because  $\gamma$  will change from step to step.

In subsequent applications, we will be using Lemma 4 when the  $a, b$  are changing. It will be important for us to track the changes of  $\gamma_a, \gamma_b$  when we change  $a, b$ . See estimates (2.69).

## 2.4 The KAM theorem

In this section, we will state precisely the main result of this paper.

### 2.4.1 Statement of the main result

For the following theorem, we will fix the parameter  $\eta$  and omit the subscript  $\eta$ .

We denote  $\langle g \rangle$  the average of some function  $g$  and  $\tilde{g} = g - \langle g \rangle$ . We also use the notation:

$$\mathcal{L} = T_\Omega + T_{-\Omega} - 2 + \partial_\beta W((\psi, \eta) + \beta v) + \sigma.$$

In this section as well as in the subsequent section on proofs, we will consider  $\eta$  fixed but we will not write subindices on the variables considered.

**Theorem 3.** *Let  $\alpha \in \mathbb{R}^d$  such that  $\alpha \cdot j \neq 0$ ,  $j \in \mathbb{Z}^d \setminus \{0\}$  and  $\omega \in \mathbb{R}$  be such that  $\omega\alpha$  is resonant. Let  $W$  be an analytic function defined in a domain  $\mathcal{D} \subset \mathbb{C}^d / \mathbb{Z}^d$ . Take  $\rho > 0$  and  $0 < s < \rho/2$ .*

*Denote:*

$$\mathcal{E}(v, \sigma, \lambda) = v_+ + v_- - 2v + W((\psi, \eta) + \beta v) + \sigma v + \lambda, \quad (2.23)$$

$$\mathcal{F}(v, \sigma, c) = (-c + 2 - \partial_\beta W((\psi, \eta) + \beta v) - \sigma)c_+ - 1. \quad (2.24)$$

*We assume:*

(H1) *Initial guesses: Let  $(v^0, c^0, \sigma^0, \lambda^0)$  be an approximate solution such that  $\|\mathcal{E}[v^0, \sigma^0, \lambda^0]\|_\rho \leq \epsilon$  and  $\|\mathcal{F}[v^0, \sigma^0, c^0]\|_\rho \leq \epsilon$ .*

(H2) *Diophantine properties: There exists a matrix  $B \in SL(d, \mathbb{Z})$ ,  $\Omega \in \mathbb{R}^{d-1}$ ,  $L \in \mathbb{Z}^d$  such that  $B\omega\alpha = (\Omega, 0) + L$  with*

$$|l \cdot \Omega - n| \geq \kappa |l|^{-\tau} \quad \forall l \in \mathbb{Z}^{d-1} - \{0\}, n \in \mathbb{Z}.$$

(H3) *Non-degeneracy conditions:*

$$\|c^0 - 1\|_\rho < M_1 < 1,$$

$$|\sigma^0| < M_2 < 1,$$

$$\|W_{v^0}\|_{C^2(\mathcal{D})} < M_3 < 1$$

$$\|v^0\|_\rho < m < 1,$$

where  $W_{v^0}$  is short for  $W((\psi, \eta) + \beta v^0)$ ,  $M_1 + M_2 + M_3 < 1$  and  $m$  depends on  $d, \tau, \kappa, M_i, s$ .

(H4) *Composition condition: Denote*

$$\mathcal{R}_{v^0} = \{(\psi, \eta) + \beta v^0(\psi), (\psi, \eta) \in \mathbb{T}_\rho^d\}.$$

We assume  $\mathcal{R}_{v^0} \subset \mathcal{D}$  and  $\text{dist}(\mathcal{R}_{v^0}, \partial\mathcal{D}) \geq 2\xi > 0$ , where  $\xi$  depends on  $d, \tau, \kappa, M_i, s, |\beta|_1$ .

Let  $\rho' = \rho - s - \delta < \rho - s$ . Let  $\epsilon$  be such that

$$\epsilon \leq \epsilon^* \delta^{4\tau},$$

where  $\epsilon^*$  depends on  $d, \tau, \kappa, M, s, |\beta|_1$  and will be specified in the proof.

Then, there exist functions  $v^*, c^* \in \mathcal{A}_{\rho'}$  and numbers  $\sigma^*, \lambda^* \in \mathbb{R}$  such that

$$\begin{aligned} \mathcal{E}[v^*, \sigma^*, \lambda^*] &= 0, \\ \mathcal{F}[v^*, \sigma^*, c^*] &= 0. \end{aligned} \tag{2.25}$$

In addition,

$$\begin{aligned}
\|v^0 - v^*\|_{\rho'} &\leq C\delta^{-4\tau}\epsilon, \\
|\lambda^0 - \lambda^*| &\leq C\delta^{-2\tau}\epsilon, \\
|\sigma^0 - \sigma^*| &\leq C\delta^{-2\tau}\epsilon, \\
\|c^0 - c^*\|_{\rho'} &\leq C\delta^{-4\tau}\epsilon,
\end{aligned} \tag{2.26}$$

where  $C$  depends on  $d, \tau, \kappa, M, s, |\beta|_1$ . In the rest of the paper, we will use  $C$  to denote any constant depending on these parameters.

We also have local uniqueness: Suppose  $(v_1, \sigma_1, \lambda_1, c_1)$  and  $(v_2, \sigma_2, \lambda_2, c_2)$  satisfying

$$\mathcal{E}[v_1, \sigma_1, \lambda_1] = \mathcal{E}[v_2, \sigma_2, \lambda_2] = 0, \tag{2.27}$$

$$\mathcal{F}[v_1, \sigma_1, c_1] = \mathcal{F}[v_2, \sigma_2, c_2] = 0, \tag{2.28}$$

and the normalization condition

$$\int_{\mathbb{T}^{d-1}} v_1 d\psi = \int_{\mathbb{T}^{d-1}} v_2 d\psi = 0. \tag{2.29}$$

If

$$\max\{\|v_2 - v_1\|_{3\rho/2}, |\sigma_2 - \sigma_1|, |\lambda_2 - \lambda_1|\} < \epsilon^* \rho^{4\tau} \tag{2.30}$$

then, we have

$$(v_1, c_1, \sigma_1, \lambda_1) = (v_2, c_2, \sigma_2, \lambda_2). \tag{2.31}$$

Finally, we have that the solution depends on the parameter  $\eta$  analytically.

The Theorem 3 is in an ‘‘a-posteriori’’ format. Given an approximate solution which satisfies some non-degeneracy condition, we establish that there is a true solution nearby.

For the experts in KAM theory, we note that we have two parameters  $s, \delta$  measuring the domain loss. The parameter  $s$  measures the domain loss in the first step and the parameter

$\delta$  measures the domain loss in the subsequent steps. The first step sets up several quantities which affect subsequent steps and are estimated in a different way from the other steps. The steps after the first are all very similar, and the estimates are very similar to the standard Nash-Moser scheme, even if the iterative step is very different.

To produce the approximate solution, we can use a variety of methods.

In the case that  $W$  is small, we can take as approximate solution  $(v^0, c^0, \sigma^0, \lambda^0) = (0, 1, 0, 0)$  (the solution corresponding to  $W = 0$ ) and then (H1) just becomes smallness condition on  $W$ .

We can use the result of a Lindstedt series as approximate solutions. Then, we obtain a validation of the Lindstedt procedure, and a consequence for the (complex) differentiability of the solutions and the convergence of Lindstedt series (see Section 2.6). See also [1].

Even if we will not discuss it in this paper, one could take as an approximate solution the outcome of a numerical computation and Theorem 3 gives a validation of the numerical result (provided that we check a few “condition numbers”). Indeed, the proof of Theorem 3 leads to an efficient algorithm, which if implemented numerically would produce efficiently numerical solutions. See Section 2.5.4.

## 2.5 Proof of Theorem 3

### 2.5.1 Outline of the proof

The proof of Theorem 3 is based on a quadratically convergent iterative method. The convergence of the method will be established by a Nash-Moser argument. Here we give an outline of the proof.

The linearization of the equilibrium equation is a linear second order difference equation. We will solve this linearized equilibrium equation using that it factorizes into two first order difference equations. In our case, we cannot write down the factorization in closed form (as in [5, 20]). So we will impose an auxiliary equation for the coefficients of the factorized equation. We will call this equation the factorization equation. We will not need

to solve exactly the factorization equation at each step, but we will require that there is an approximate solution of the factorization equation with an accuracy comparable to the accuracy of the approximate solution of the equilibrium equation. Then, we will derive an iterative method that improves both of the equilibrium equation and the factorization equation. This is reminiscent of the procedure to study an elliptic torus and its reducibility at the same time. See [21, 68]. Note without the parameter  $\sigma$ , we cannot find coefficients satisfying the factorization equation.

We have the difficulty that the equilibrium equation and the factorization equation are coupled. We do not know how to establish convergence if we solve one equation after another. We will derive a way to solve the two coupled linearized equations simultaneously, taking advantage of the fact that the coupling appears only in terms that are affine in the correction to the parameter  $\hat{\sigma}$ .

After we factorize the linearized equilibrium equation, we will face three twisted cohomology equations (difference equations with non-constant coefficients), two for the linearized equilibrium equation and one for the linearized factorization equation. We will solve them using the technique in Section 2.5.2. This completes one step of iteration.

One small technical complication is that the first step is estimated in a different way from the subsequent steps. In the first step of the iteration, we compute some auxiliary functions related to factorization (the auxiliary functions  $\gamma$  related to the twisted cohomology equation) and estimate them from the original data. In subsequent steps, even if we compute the same auxiliary functions, we do not estimate them from the data but we estimate the change on the auxiliary functions induced by the (rather small) changes in the approximate solution.

Under some minor non-degeneracy conditions, we can repeat the process indefinitely. Finally, we will prove that the iterative procedure converges with suitably chosen domains under the analytic norm. This is very standard in KAM theory.

The local uniqueness will be obtained in Section 2.5.8 by a very simple argument. (See

[61]). It suffices to observe that the linearized equation properly normalized admits unique solutions and then use Hadamard's three circle theorem to the identity obtained through the Taylor theorem with remainder.

We also note that the main part of Theorem 3 has what is called "a-posteriori" format in numerical analysis. We show that if there is an approximate enough solution that satisfies some non-degeneracy conditions, then, there is a true solution nearby. It is well known that this a-posteriori format leads to smooth dependence on parameters, bootstrap of regularity and several other consequences.

Finally, the analyticity with respect to parameters (we will use either  $\epsilon$  or  $\eta$  as parameters) will be a corollary of the existence of the perturbative expansions (see Section 2.6.1). Using the a-posteriori format of Theorem 3 and the local uniqueness, it follows that the solution is complex differentiable in the parameters. Hence, it is analytic on the parameters. Furthermore, since the perturbative expansions are the Taylor expansions of an analytic function they converge.

We note that the iterative process described above leads to an efficient algorithm, which we have formulated in Section 2.5.4, but we have not implemented.

### 2.5.2 Motivation for the iterative step

Our goal in this section is to devise a procedure that given an approximate solution produces another approximate solution with much smaller error and not much worse non-degeneracy conditions. This procedure is done for the equilibrium and factorization equations simultaneously.

*The equilibrium equation*

We consider the initial guess  $(v^0, \sigma^0, \lambda^0)$  which solves equation (2.2) with a small error  $e$ , where  $\|e\|_\rho < \epsilon$ , i.e.

$$v_+^0 + v_-^0 - 2v^0 + W((\psi, \eta) + \beta v^0) + \sigma^0 v^0 + \lambda^0 = e. \quad (2.32)$$

The Newton procedure for the approximate solutions of the equilibrium equation (2.32) requires to find an update  $(\hat{v}, \hat{\sigma}, \hat{\lambda})$  satisfying

$$\hat{v}_+ + \hat{v}_- - 2\hat{v} + \partial_\beta W_{v^0} \hat{v} + \hat{\sigma} v^0 + \sigma^0 \hat{v} + \hat{\lambda} = -e, \quad (2.33)$$

where we denote  $\partial_\beta W = \beta \cdot \nabla W$  for simplicity and we use  $W_v$  to indicate  $W((\psi, \eta) + \beta v)$ .

*The factorization equation*

The equation (2.33) – the Newton step for the invariance equation (2.1) is not easy to solve directly. Nevertheless, we add to it another equation that expressed the fact that (2.33) can be factorized into two first order difference equations with non-constant coefficients. If we accomplish this, we can solve (2.33) using the theory of twisted cohomology equations developed in Section 2.3.4.

In this section, we will show how this factorization can be accomplished just by introducing a parameter.

Therefore we want that the operator  $\mathcal{L}$  (recall that we denote  $\mathcal{L} = T_\Omega + T_{-\Omega} - 2 + \partial_\beta W_{v^0} + \sigma$ ) is factorized into two first order operators:

$$\mathcal{L} = \mathcal{A}_+ \mathcal{A}_-, \quad (2.34)$$

where

$$\mathcal{A}_+ = a(\psi)T_\Omega - b(\psi) \quad (2.35)$$

$$\mathcal{A}_- = c(\psi) - d(\psi)T_{-\Omega} \quad (2.36)$$

and  $a, b, c, d$  are the new unknowns.

A direct calculation shows

$$\mathcal{A}_+\mathcal{A}_-\hat{v} = a(\psi)c_+(\psi)\hat{v}_+ - [a(\psi)d_+(\psi) + b(\psi)c(\psi)]\hat{v} + b(\psi)d(\psi)\hat{v}_-. \quad (2.37)$$

Hence we want to choose  $a, b, c, d$  satisfying the following equations

$$\begin{aligned} a(\psi)c_+(\psi) &= 1, \\ -[a(\psi)d_+(\psi) + b(\psi)c(\psi)] &= -2 + \partial_\beta W_{v^0} + \sigma^0, \\ b(\psi)d(\psi) &= 1. \end{aligned} \quad (2.38)$$

Note that the problem of factorization has always many solutions. If  $\mathcal{A}_+\mathcal{A}_-$  is a solution and  $g$  is any invertible function, then  $\tilde{\mathcal{A}}_+\tilde{\mathcal{A}}_-$  is also a solution, where

$$\begin{aligned} \tilde{\mathcal{A}}_+ &= \mathcal{A}_+g, \\ \tilde{\mathcal{A}}_- &= g^{-1}\mathcal{A}_-. \end{aligned} \quad (2.39)$$

We can use this non-uniqueness to impose some extra normalization condition without loss of generality. In this paper, we will take the normalization

$$b(x) = 1. \quad (2.40)$$

With condition (2.40) we can simplify the system (2.38) to (after eliminating  $a$ ):

$$(-c + 2 - \partial_\beta W_{v^0} - \sigma^0)c_+ = 1. \quad (2.41)$$

This is how the operator  $\mathcal{F}$  comes into play. Note it is a non-linear, non-local equation which we will have to solve iteratively. By assumption (H1), we can solve this equation with an error  $f$  using some initial guess  $c^0$ , i.e.

$$(-c^0 + 2 - \partial_\beta W_{v^0} - \sigma^0)c_+^0 - 1 = f \quad (2.42)$$

and we have  $\|f\|_\rho < \epsilon$ .

Then the Newton procedure for (2.42) requires solving the following equation for  $\hat{c}$  – the Newton correction for  $c$ :

$$-c_+^0 \hat{c} + (-c^0 + 2 - \partial_\beta W_{v^0} - \sigma^0) \hat{c}_+ - c_+^0 \hat{\sigma} - \partial_\beta \partial_\beta W_{v^0} c_+^0 \hat{v} = -f. \quad (2.43)$$

Then  $c + \hat{c}$  would be a more accurate solution.

We replace  $\mathcal{L}$  with  $\mathcal{A}_+ \mathcal{A}_-$  in the original equilibrium equation (2.33) to get

$$\mathcal{A}_+ \mathcal{A}_- \hat{v} + \hat{\sigma} v^0 + \hat{\lambda} = -e. \quad (2.44)$$

**Remark 12.** *Note that the equation (2.44) is slightly different from (2.33), so the  $(\hat{v}, \hat{\sigma}, \hat{\lambda}, \hat{c})$  we find is not exactly the solution of the linearized equation of (2.2). But the only difference between (2.44) and (2.33) is a term  $f \hat{v} (c_+^0)^{-1}$ , which we will show is quadratic in  $e, f$  (since  $\hat{v}$  will be of the order of  $e$ ).*

**Remark 13.** *To obtain quadratic convergence, the full Newton step will have to improve both the equilibrium and the factorization equation at the same time. (A moment's reflection shows that improving one equation and then the other does not lead to quadratic conver-*

gence.) We will prove that our quasi-Newton procedure (using (2.44) instead of (2.33) as well as (2.43)) converges quadratically to a solution of (2.2) – and as a byproduct to the factorization equation.

In the following section, we will develop a method to solve (2.44) and (2.43) simultaneously. In Section 2.5.6 we will obtain estimates for the size of the error. Then, we will show in Section 2.5.7 that they lead to an improved solution and that the process can be iterated and converges to a solution.

### 2.5.3 Solving the linearized equations

Our goal in this section is to solve (2.44) and (2.43) simultaneously.

The difficulty arises because the equations (2.44) and (2.43) are coupled (the unknown  $\hat{\sigma}$  appears in both of them). Observe that since  $\hat{\sigma}$  appears in an affine way, we can guess that the solutions will be affine in  $\hat{\sigma}$ . This allows to uncouple the equations.

When we find the corrections  $(\hat{v}, \hat{\sigma}, \hat{\lambda}, \hat{c})$ , we can write down the updated solution of the equilibrium equation (2.2) and the factorization equation (2.42):

$$(v^1, \sigma^1, \lambda^1, c^1) = (v^0 + \hat{v}, \sigma^0 + \hat{\sigma}, \lambda^0 + \hat{\lambda}, c^0 + \hat{c}), \quad (2.45)$$

which can be used in the next iterative step. We will show that the improved solution (2.45) is indeed more approximate (in a smaller domain). Then the procedure can be repeated indefinitely and converges to a solution if the errors are small enough.

Now we write

$$\hat{v} = A + \hat{\sigma}B, \quad (2.46)$$

$$\hat{\lambda} = G + \hat{\sigma}D, \quad (2.47)$$

where  $A$  and  $B$  are functions,  $G$  and  $D$  are numbers. All these quantities will be determined shortly.

Then the equation (2.44) for all values of  $\hat{\sigma}$  is equivalent to:

$$\mathcal{A}_+ \mathcal{A}_- A + G = -e, \quad (2.48)$$

$$\mathcal{A}_+ \mathcal{A}_- B + D = -v^0. \quad (2.49)$$

The Newton equation for factorization (2.43) after substitution (2.48) and (2.49) becomes

$$-c_+^0 \hat{c} + (-c^0 + 2 - \partial_\beta W_{v^0} - \sigma^0) \hat{c}_+ + (-c_+^0 - \partial_\beta \partial_\beta W_{v^0} c_+^0 B) \hat{\sigma} = \partial_\beta \partial_\beta W_{v^0} c_+^0 A - f. \quad (2.50)$$

The equation (2.50) will determine  $\hat{\sigma}$  as a compatibility condition and, then determine  $\hat{c}$ . Since the previous equations (2.48), (2.49) gave the solutions for any value of  $\hat{\sigma}$ , we obtain the solutions for all the unknowns. Now, we turn to give details and to obtain estimates.

The Newton step improving simultaneously the invariance and factorization equations consists in solving (2.48), (2.49), (2.50). Notice that this system has an upper triangular structure, we can solve (2.48), (2.49) for  $A, B, G, D$  and then solve (2.50) for  $\hat{c}$  and  $\hat{\sigma}$ . Once we have  $\hat{\sigma}$ , we can determine  $\hat{v}$  and  $\hat{\lambda}$  using (2.46) and (2.47).

To solve (2.48) and (2.49), we observe that each of them can be obtained by solving two cohomology equations with non-constant coefficients. We can find the zero average solution of (2.48) and (2.49). In fact,  $G$  is determined so that  $A$  has zero average and  $D$  is determined so that  $B$  has zero average. This ensures that  $\langle \hat{v} \rangle = 0$ .

We note that the choice of the constants in the solution of two consecutive twisted cohomology equations is a simple extension of the arguments developed at the end of Section 2.3.4.

In the case that  $\mathcal{A}_+, \mathcal{A}_-$  both have different average coefficients, we see that the average of the solution as a function of  $G$  is the composition of two affine functions, hence affine and if the linear part of each of them is not zero, we obtain that the composition of the two affine functions has non-zero derivative.

In the case that  $\mathcal{A}_+$  has equal average coefficient, but  $\mathcal{A}_-$  does not, we choose  $G$  so that

$\mathcal{A}_+$  is solvable and choose the average of its solution so that the solution of  $\mathcal{A}_-$  satisfies the normalization.

In the case that  $\mathcal{A}_+$  has different average coefficient but  $\mathcal{A}_-$  has the same average coefficient, we choose  $G$  so that the solution produced by  $\mathcal{A}_+$  satisfies the compatibility conditions for  $\mathcal{A}_-$ . Then, the solution of  $\mathcal{A}_-$  is defined up to a constant which can be chosen in a unique way to satisfy the normalization condition.

In the case that both  $\mathcal{A}_+, \mathcal{A}_-$  have the same average coefficients—which is the case that appears in standard KAM theory—we choose  $G$  so that  $\mathcal{A}_+$  is solvable. Then, we use the free parameter of the solution of  $\mathcal{A}_-$  to ensure the solvability of  $\mathcal{A}_-$  and use the free constant in the solution of  $\mathcal{A}_-$  to adjust the normalization.

Therefore, we obtain the solution of (2.48). Similar procedure can be done for (2.49).

Now that we have solved (2.48) and (2.49) we turn to solving (2.50). As long as

$$\int_{\mathbb{T}^{d-1}} \left( -c_+^0 - \partial_\beta \partial_\beta W_{v^0} c_+^0 B \right) d\psi \neq 0, \quad (2.51)$$

which can be proved under some non-degeneracy conditions on the initial guesses, equation (2.50) is a twisted cohomology equation. Provided that  $-c_+^0$  and  $-c^0 + 2 - \partial_\beta W_{v^0} - \sigma^0$  are away from zero, we can apply Lemma 4 to solve (2.50) after  $A$  and  $B$  are found.

To make the procedure clear, we will write the full algorithm in Section 2.5.4. In Section 2.5.5, we will carefully estimate the errors after one iterative step to show that the errors of the equilibrium and the factorization equations are both reduced quadratically after performing the corrections in the iterative step. Finally, we will prove the convergence rigorously in Section 2.5.7.

#### 2.5.4 Formulation of the iterative step

**Algorithm 1.** (1) Given initial guesses  $v^0, \sigma^0, \lambda^0, c^0$ , set  $a^0 = (c_+^0)^{-1}$ .

(2) Calculate the errors  $e = \mathcal{E}(v^0, \sigma^0, \lambda^0)$  and  $f = \mathcal{F}(v^0, \sigma^0, c^0)$ .

(3) Find  $\gamma_{a^0}$  and  $\bar{a}^0$  satisfying

$$\log a^0 = \log \bar{a}^0 + \log(\gamma_{a^0})_+ - \log(\gamma_{a^0})_-.$$

Also find  $\gamma_{c^0}$  and  $\bar{c}^0$  satisfying

$$\log c^0 = \log \bar{c}^0 + \log(\gamma_{c^0})_+ - \log(\gamma_{c^0})_-.$$

(4) Compute  $\bar{a}_+, \bar{b}_+, \gamma_{a_+}, \gamma_{b_+}$  (the average coefficients and the auxiliary functions) for  $\mathcal{A}_+$  and  $\bar{a}_-, \bar{b}_-, \gamma_{a_-}, \gamma_{b_-}$  for  $\mathcal{A}_-$ .

(5a) If  $\bar{a}_+ \neq \bar{b}_+, \bar{a}_- \neq \bar{b}_-$ , compute

$$\alpha = -\mathcal{A}_+^{-1} \mathcal{A}_-^{-1} e, \beta = -\mathcal{A}_+^{-1} \mathcal{A}_-^{-1} \mathbf{1}.$$

Set  $G = -\frac{\langle \alpha \rangle}{\langle \beta \rangle}$ . Set  $A = \alpha + G\beta$ .

(5b) If  $\bar{a}_+ = \bar{b}_+, \bar{a}_- \neq \bar{b}_-$ , choose  $G = -\langle e \rangle$ . Set  $\tilde{\alpha} = -\mathcal{A}_+^{-1}(e + G)$  and  $\langle \tilde{\alpha} \rangle = 0$ . Set  $\beta_1 = \mathcal{A}_-^{-1} \tilde{\alpha}, \beta_2 = -\mathcal{A}_-^{-1} \mathbf{1}$ . Set  $A = \beta_1 - \beta_2 \frac{\langle \beta_1 \rangle}{\langle \beta_2 \rangle}$ .

(5c) If  $\bar{a}_+ \neq \bar{b}_+, \bar{a}_- = \bar{b}_-$ , choose  $\alpha_1 = -\mathcal{A}_+^{-1} e, \alpha_2 = -\mathcal{A}_+^{-1} \mathbf{1}$ . Set  $G = \frac{\langle \alpha_1 \rangle}{\langle \alpha_2 \rangle}$ . Set  $A = \mathcal{A}_-^{-1}(\alpha_1 - G\alpha_2)$  and  $\langle A \rangle = 0$ .

(5d) If  $\bar{a}_+ = \bar{b}_+, \bar{a}_- = \bar{b}_-$ , choose  $G = -\langle e \rangle$ . Set  $\alpha = \mathcal{A}_+^{-1}(e - \langle e \rangle)$  and  $\langle \alpha \rangle = 0$ . Set  $A = \mathcal{A}_-^{-1} \alpha$  and  $\langle A \rangle = 0$ .

(6) Find  $B$  and  $D$  in a similar way as we found  $A$  and  $G$ . Also set  $\langle B \rangle = 0$ .

(7) Find  $\hat{\sigma}$  and  $\hat{c}$  by solving (2.50).

(8) Set  $\hat{v} = A + \hat{\sigma}B$  and  $\hat{\lambda} = G + \hat{\sigma}D$ .

(9) Update  $v, \lambda, \sigma$  and  $c$  and repeat the steps.

**Remark 14.** *When we apply repeatedly the iterative steps to obtain estimates, it would be advantageous in Step 3 to use the information we have on  $\gamma_a$  computed in the previous steps, because it leads to better estimates. In the first step, we can only use Cauchy estimates on the initial data. See Section 2.5.1.*

**Remark 15.** *The iterative method described above achieves quadratic convergence (see Section 2.5.7). It only entails performing algebraic operations among functions, composing them, taking derivatives and solving the cohomology equations.*

*If we discretize a function by the values of the point in a grid of  $N$  points and (redundantly)  $N$  Fourier coefficients, we note that each of the operations above requires  $N$  operations either in the grid representation or in the Fourier space representation. If we obtain either the Fourier or the real space representation for a function, we can obtain the other representation using the FFT algorithm that requires  $N \log(N)$  operations.*

*Hence the method in Section 2.5 achieves quadratic convergence but no matrix inversion (or storage) is required. It only requires  $O(N)$  storage and  $O(N \log(N))$  operations per step.*

*This has already been observed in [69] in the periodic case (both for short range and for long range interactions) and [5] for the quasi-periodic non-resonant case. Numerical implementations in the non-resonant quasi-periodic case were carried out in [7]. We have not implemented the above algorithm, but we think it would be interesting to do so.*

### 2.5.5 Estimates on the corrections

Denote  $V^0 = -c^0 + 2 - \partial_\beta W_{\nu^0} - \sigma^0$ . In the first step, we argue as follows. From (2.21), it is clear that all the quantities  $\|\gamma_{c^0}\|_{\rho-\delta/4}$ ,  $\|\gamma_{c^0}^{-1}\|_{\rho-\delta/4}$ ,  $\|\gamma_{(c^0)^{-1}}\|_{\rho-\delta/4}$ ,  $\|\gamma_{(c^0)^{-1}}^{-1}\|_{\rho-\delta/4}$ ,  $\|\gamma_{\nu^0}\|_{\rho-\delta/4}$  and  $\|\gamma_{\nu^0}^{-1}\|_{\rho-\delta/4}$  are bounded by some constant which depends only on  $d, \tau, \kappa, M, s$ . We denote the bound by  $E$ .

In subsequent steps, we will just assume that we have the bounds  $E$  for the above auxiliary quantities. These bounds will be derived from the bounds in the first step.

Apply the estimate (2.19) of twisted cohomology equations for equations (2.48) and (2.49), also recall the averages of  $A$  and  $B$  both vanish we have

$$\|A\|_{\rho-\delta/2} \leq CE^4 \delta^{-2\tau} \|\tilde{e}\|_{\rho} = C\delta^{-2\tau} \|\tilde{e}\|_{\rho}, \quad (2.52)$$

$$\|B\|_{\rho-\delta/2} \leq CE^4 \delta^{-2\tau} \|\tilde{v}^0\|_{\rho} = C\delta^{-2\tau} \|\tilde{v}^0\|_{\rho}, \quad (2.53)$$

$$|G| \leq CE^4 \|e\|_{\rho} \leq C\epsilon, \quad (2.54)$$

$$|D| \leq CE^4 \|v^0\|_{\rho} \leq C. \quad (2.55)$$

Choose  $m$  small, we can make  $\|B\|_{\rho-\delta/2} < 1$ . Then

$$\begin{aligned} \|(-c_+^0 - \partial_{\beta}\partial_{\beta}W_{v^0}c_+^0B)^{-1}\|_{\rho-\delta/4} &= \|(c_+^0)^{-1}(1 + \partial_{\beta}\partial_{\beta}W_{v^0}B)^{-1}\|_{\rho-\delta/4} \\ &\leq (1 - M_1)^{-1}(1 - M_3)^{-1}. \end{aligned} \quad (2.56)$$

This guarantees that  $\int_{\mathbb{T}^{d-1}} (-c_+^0 - \partial_{\beta}\partial_{\beta}W_{v^0}c_+^0B) d\psi \neq 0$ . Therefore the cohomology equation (2.50) is solvable. Moreover, we note that, if the constants  $M$  remain uniformly bounded in the iteration, we obtain that the constants entering in the estimates of the twisted cohomology equations remain uniformly bounded.

The estimate for (2.50) gives

$$\begin{aligned} |\hat{\sigma}| &\leq C(\|A\|_{\rho-\delta/2} + \|f\|_{\rho}) \\ &\leq C\delta^{-2\tau}\epsilon + C\epsilon \\ &\leq C\delta^{-2\tau}\epsilon, \end{aligned} \quad (2.57)$$

and

$$\begin{aligned} \|\hat{c}\|_{\rho-\delta} &\leq CE^4 \delta^{-\tau} (\|A\|_{\rho-\delta/2} + \|f\|_{\rho}) \\ &\leq C\delta^{-3\tau}\epsilon. \end{aligned} \quad (2.58)$$

From (2.46), we have the estimate

$$\begin{aligned} \|\hat{v}\|_{\rho-\delta/2} &\leq \|A\|_{\rho-\delta/2} + |\hat{\sigma}|\|B\|_{\rho-\delta/2} \\ &\leq C\delta^{-4\tau}\epsilon. \end{aligned} \tag{2.59}$$

Also, from the estimates for  $G, D$  and  $\sigma$ , we have

$$|\lambda| \leq C\epsilon + C\delta^{-2\tau}\epsilon \leq C\delta^{-2\tau}\epsilon. \tag{2.60}$$

### 2.5.6 Estimates on the improved error

Next we estimate the new error for both equilibrium and factorization equations after one iteration step.

We need the Assumption (H4) to make sure the compositions can be done in appropriate domains. Recall that  $\|W_{v^0}\|_{C^2(\mathcal{D})} < M_3$ . Also note  $\hat{v}$  is relatively smaller than  $v^0$ . From (2.60), we see that as long as  $\epsilon$  is small enough the range of  $v + \hat{v}$  is inside the domain of  $W$ . So we can choose proper  $\xi$  such that  $\text{dist}(\mathcal{R}_{v^0}, \partial\mathcal{D}) \geq \xi > 0$ .

For the subsequent iterative step, we note that if  $\delta^{-4\tau}\epsilon$  is small enough,  $\|\hat{v}\|_{\rho-\delta}$  will also be small. So that under smallness condition on  $\delta^{-4\tau}\epsilon$ , we can ensure that  $v + \hat{v}$  is well inside the domain of definition of  $W$ . The linear estimates are valid for all  $\delta$ 's, but in order to ensure that we can apply the non-linear estimates, we have to choose  $\delta$ 's (the domain loss) in such a way that  $\delta^{-4\tau}\epsilon$  is small.

It is standard in KAM theory (and we will do it later in Section 2.5.7) that one can choose domain losses  $\delta_n$  in such a way that the composition condition is met, such that  $\delta_n$ 's go to zero fast enough, so there is still a domain left. Therefore, the composition will remain in the proper domain for all iterative steps and the procedure will converge in a non-trivial domain.

Using the Taylor expansions (see Proposition 5) and the equations (2.32),(2.33) and

(2.42),(2.43) for the initial guesses, we have:

$$\begin{aligned}
& \mathcal{E}[v^0 + \hat{v}, \sigma^0 + \hat{\sigma}, \lambda^0 + \hat{\lambda}] \\
&= \mathcal{E}[v^0, \sigma^0, \lambda^0] + \hat{v}_+ + \hat{v}_- - 2\hat{v} + \hat{\sigma}v^0 + \sigma^0\hat{v} + \hat{\sigma}\hat{v} + \hat{\lambda} - W_{v^0} + W_{v^0 + \hat{v}} \\
&= e + \mathcal{A}_+ \mathcal{A}_- \hat{v} - f\hat{v} - (\partial_\beta W_{v^0} + \sigma^0)\hat{v} + \hat{\sigma}v^0 + \sigma^0\hat{v} + \hat{\sigma}\hat{v} + \hat{\lambda} \\
&\quad - W_{v^0} + W_{v^0 + \hat{v}} \\
&= -f\hat{v} + \hat{\sigma}\hat{v} + (W_{v^0 + \hat{v}} - W_{v^0} - \partial_\beta W_{v^0}\hat{v}),
\end{aligned} \tag{2.61}$$

and

$$\begin{aligned}
& \mathcal{F}[v^0 + \hat{v}, \sigma^0 + \hat{\sigma}, c^0 + \hat{c}] \\
&= \mathcal{F}[v^0, \sigma^0, c^0] + [-(c^0 + \hat{c}) + 2 - \partial_\beta W_{v^0 + \hat{v}} - (\sigma^0 + \hat{\sigma})]\hat{c}_+ \\
&\quad + [-\hat{c} - \partial_\beta W_{v^0 + \hat{v}} + \partial_\beta W_{v^0} - \hat{\sigma}]c_+^0 \\
&= [-\hat{c} - (\partial_\beta W_{v^0 + \hat{v}} - \partial_\beta W_{v^0}) - \hat{\sigma}]\hat{c}_+ \\
&\quad - [(\partial_\beta W_{v^0 + \hat{v}} - \partial_\beta W_{v^0})c_+^0 - \partial_\beta \partial_\beta W_{v^0} c_+^0 \hat{v}].
\end{aligned} \tag{2.62}$$

Take  $0 < \delta < \rho$ , we have

$$\begin{aligned}
& \|\mathcal{E}[v^0 + \hat{v}, \sigma^0 + \hat{\sigma}, \lambda^0 + \hat{\lambda}]\|_{\rho-\delta} \\
&\leq \|f\hat{v}\|_{\rho-\delta} + \|\hat{\sigma}\hat{v}\|_{\rho-\delta} + \|W_{v^0 + \hat{v}} - W_{v^0} - \partial_\beta W_{v^0}\hat{v}\|_{\rho-\delta} \\
&\leq \|f\|_{\rho-\delta}\|\hat{v}\|_{\rho-\delta} + \|\hat{\sigma}\|_{\rho-\delta}\|\hat{v}\|_{\rho-\delta} + C\|\hat{v}\|_{\rho-\delta}^2.
\end{aligned} \tag{2.63}$$

Also,

$$\begin{aligned}
& \|\mathcal{F}[v^0 + \hat{v}, \sigma^0 + \hat{\sigma}, c^0 + \hat{c}]\|_{\rho-\delta} \\
&\leq (\|\hat{c}\|_{\rho-\delta} + C\|\hat{v}\|_{\rho-\delta} + \|\hat{\sigma}\|_{\rho-\delta})\|\hat{c}\|_{\rho-\delta} + C\|\hat{v}\|_{\rho-\delta}^2\|c^0\|_{\rho-\delta}.
\end{aligned} \tag{2.64}$$

Now it is clear the new errors are quadratic in  $f, \hat{v}, \hat{\sigma}, \hat{c}$ , multiplied by the domain loss

to a negative power. This is what are called ‘‘tame estimates’’ in KAM theory.

The final estimates for both equilibrium and factorization equations on the updated solutions are

$$\|\mathcal{E}[v^0 + \hat{v}, \sigma^0 + \hat{\sigma}, \lambda^0 + \hat{\lambda}]\|_{\rho-\delta} \leq C\delta^{-8\tau}\epsilon^2 \quad (2.65)$$

and

$$\|\mathcal{F}[v^0 + \hat{v}, \sigma^0 + \hat{\sigma}, c^0 + \hat{c}]\|_{\rho-\delta} \leq C\delta^{-8\tau}\epsilon^2. \quad (2.66)$$

Therefore we get updates for  $c$ ,  $v$ ,  $\sigma$  and  $\lambda$  which reduce the error of both the equilibrium equation and the factorization equation quadratically under the condition that all the bounds we derived before still hold for all iterative steps. We can prove the convergence following the standard procedure, which we give in the following.

### 2.5.7 Proof of convergence

The main effect of the iterative step is to reduce the error in (2.44) and (2.43). But it could also deteriorate the constants in the non-degeneracy assumptions when it improves the solution.

Therefore the first goal of this section is to show that the constants in non-degeneracy assumptions of the solution do not deteriorate much and that the deterioration can be estimated by the error. In this case, as we will see, the convergence can be proved by choosing suitable domains (this is the choice we will do first) for each iterative step as is standard in KAM theory.

We will use subscript  $n$  to denote the quantities  $\rho$ ,  $\delta$  and  $\epsilon$  after application of the iterative step  $n$  times, while we use superscript  $n$  for  $v$ ,  $c$ ,  $\sigma$ ,  $\lambda$  and  $B$ . We take

$$\rho_0 = \rho, \rho_1 = \rho - s - \delta_0, \delta_n = \delta_0 \cdot 2^{-n} \quad \text{and} \quad \rho_{n+1} = \rho_n - \delta_n. \quad (2.67)$$

Denote  $\epsilon_n = \|\mathcal{E}(v^n, \delta^n, \lambda^n)\|_{\rho_n}$  and  $\tilde{\epsilon}_n = \|\mathcal{F}(v^n, \sigma^n, c^n)\|_{\rho_n}$ . We will prove the following holds for all iterative steps by induction.

**(B1)** All the quantities  $\|v^n\|_{\rho_n}, \|c^n - 1\|_{\rho_n}, |\sigma^n|, \|W_{v^0}\|_{\rho_n}, \|B^n\|_{\rho_n}, \|\gamma_{c^n}\|_{\rho_n}, \|\gamma_{c^n}^{-1}\|_{\rho_n}, \|\gamma_{v^n}\|_{\rho_n}, \|\gamma_{v^n}^{-1}\|_{\rho_n}$ , and  $\|(-c_+^0 - \partial_\beta \partial_\beta W_{v^0} c_+^0 B)^{-1}\|_{\rho_n}$  are still bounded uniformly in  $n$ . To be precise, for any quantity  $A^0 < E$ , we will prove  $|A^n - A^{n-1}| < E \cdot 2^{-n}$ , therefore,  $A^n < 2E$  for any  $n$ .

**(B2)** Denote  $\mathcal{R}_{v^n} = \{(\psi, \eta) + \beta v^n, (\psi, \eta) \in \mathbb{T}_{\rho_n}^d\}$ . Then  $\text{dist}(\mathcal{R}_{v^n}, \partial \mathcal{D})$  is also bounded by  $\xi$ .

**(B3)**  $\epsilon_{n+1} \leq (C\epsilon_0)^{2^{n+1}}, \quad \tilde{\epsilon}_{n+1} \leq (C\tilde{\epsilon}_0)^{2^{n+1}}$ .

Note that as a consequence of (B3), and the choices of  $\delta_n$ , we obtain that the composition assumption holds if  $\epsilon_0$  is small enough.

The first step is already shown in Section 2.5.5. Now we assume the first  $n$  steps are proved.

We first prove (B1). We only prove the bound

$$\|\gamma_{c^n} - \gamma_{c^{n-1}}\|_{\rho_n - \delta/4} < E \cdot 2^{-n}. \quad (2.68)$$

The proof of the other bounds is similar (up to changing the symbols).

From (2.21), we have

$$\|\log \gamma_{c^n} - \log \gamma_{c^{n-1}}\|_{\rho_n - \delta_n/4} \leq C\delta_n^{-\tau} \|\log c^n - \log c^{n-1}\|_{\rho_n}. \quad (2.69)$$

From estimate (2.58) for  $\hat{c}$ , we have

$$\|\hat{c}^n\|_{\rho_n} \leq C\delta_n^{-3\tau} \epsilon_n. \quad (2.70)$$

As a result, we have

$$\|\log c^n - \log c^{n-1}\|_{\rho_n} \leq C\delta_n^{-3\tau} \epsilon_n. \quad (2.71)$$

Combining (2.69) and (2.71), we have

$$\|\log \gamma_{c^n} - \log \gamma_{c^{n-1}}\|_{\rho_n - \delta_n/4} \leq C \delta_n^{-4\tau} \epsilon_n. \quad (2.72)$$

Therefore we have (using that  $\gamma_{c^{n-1}}$  are uniformly bounded)

$$\|\gamma_{c^n} - \gamma_{c^{n-1}}\|_{\rho_n - \delta_n/4} \leq C \delta_n^{-4\tau} \epsilon_n. \quad (2.73)$$

Note for (B2), we only need bounds for  $v^n$ , which is easy to prove.

Now recall  $\epsilon_n < (C\epsilon_0)^{2^n}$ . Therefore if we choose  $\epsilon_0$  such that  $\delta^{-4\tau} \epsilon_0$  is small enough, we can guarantee (2.68) (i.e. (B2)). (B3) can be shown as follows

$$\begin{aligned} \epsilon_n &\leq C \delta_{n-1}^{-8\tau} \epsilon_{n-1}^2 \\ &= C \delta_0^{-8\tau} (2^{8\tau})^{n-1} \epsilon_{n-1}^2 \\ &\leq (C \delta_0^{-8\tau})^{1+2+\dots+2^{n-1}} (2^{8\tau})^{(n-1)+(n-2)\cdot 2+\dots+1\cdot(n-1)} \epsilon_0^{2^n} \\ &\leq (C \delta_0^{-8\tau} 2^{8\tau} \epsilon_0)^{2^n} \\ &= (C 2^{8\tau} \epsilon_0)^{2^n}. \end{aligned} \quad (2.74)$$

Similar estimates also hold for  $\tilde{\epsilon}_n$ .

### 2.5.8 Proof of local uniqueness

Suppose we have two solutions  $(v_1, \sigma_1, \lambda_1, c_1)$  and  $(v_2, \sigma_2, \lambda_2, c_2)$  of both the equilibrium and the factorization equations, which also satisfy the non-degeneracy conditions. We have

$$\mathcal{E}[v_1, \sigma_1, \lambda_1] = \mathcal{E}[v_2, \sigma_2, \lambda_2] = 0. \quad (2.75)$$

Then we can write

$$\begin{aligned}\mathcal{E}[v_2, \sigma_2, \lambda_2] &= \mathcal{E}[v_1, \sigma_1, \lambda_1] + D\mathcal{E}[v_1, \sigma_1, \lambda_1] \cdot (v_2 - v_1, \sigma_2 - \sigma_1, \lambda_2 - \lambda_1) + R^2 \\ &= D\mathcal{E}[v_1, \sigma_1, \lambda_1] \cdot (v_2 - v_1, \sigma_2 - \sigma_1, \lambda_2 - \lambda_1) + R^2 = 0,\end{aligned}\tag{2.76}$$

where  $R^2$  is the Taylor remainder for  $\mathcal{E}$ .

Another way to read this identity (2.76) is to say that  $v_1 - v_1, \lambda_2 - \lambda_1, \sigma_2 - \sigma_1$  is a solution of the equation

$$\mathcal{A}_+ \mathcal{A}_-(v_2 - v_1) + (\sigma_2 - \sigma_1)v_1 + (\lambda_2 - \lambda_1) = -R^2.\tag{2.77}$$

Similarly, we have

$$-(c_1)_+(c_2 - c_1) + (-c_1 + 2 - \partial_\beta W_{v_1} - \sigma_1)(c_2 - c_1) + (c_1)_+(\sigma_2 - \sigma_1) - \partial_\beta \partial_\beta W_{v_1}(c_1)_+(v_2 - v_1) = -\tilde{R}^2.\tag{2.78}$$

We have shown in Section 2.5.5 that the solutions of (2.77) and (2.78) satisfying the normalization condition are unique and satisfy the bounds (2.57) and (2.59). So we have

$$\|v_2 - v_1\|_{\frac{\rho}{2}} + \|c_2 - c_1\|_{\frac{\rho}{2}} + |\sigma_2 - \sigma_1| \leq C\rho^{-4\tau}\|R^2\|_\rho \leq C\rho^{-4\tau}(\|v_2 - v_1\|_\rho + \|c_2 - c_1\|_\rho + |\sigma_2 - \sigma_1|)^2.\tag{2.79}$$

Since  $\|v_2 - v_1\|_\rho, \|c_2 - c_1\|_\rho$  and  $|\sigma_2 - \sigma_1|$  are all small, we have

$$\begin{aligned}\|v_2 - v_1\|_{\frac{\rho}{2}} &\leq C\rho^{-4\tau}\|v_2 - v_1\|_\rho^2 \\ &\leq C\rho^{-4\tau}\|v_2 - v_1\|_{\frac{\rho}{2}}\|v_2 - v_1\|_{\frac{3\rho}{2}}.\end{aligned}\tag{2.80}$$

The last inequality uses the interpolation inequality (2.7).

Therefore, as long as  $\rho^{-4\tau}\|v_2 - v_1\|_{\frac{3\rho}{2}}$  is sufficiently small (depending on the properties of the auxiliary function  $c$  in the factorization equation), we have  $\|v_1 - v_2\|_{\frac{\rho}{2}} = 0$ , which also implies  $\sigma_2 = \sigma_1$  and  $\lambda_2 = \lambda_1$ .

## 2.6 Consequences of Theorem 3 and its proof

### 2.6.1 Perturbative series around any solution of invariance and factorization

In this section we present methods to compute formal power series expansions. In Section 2.6.2 we will show that, under Diophantine conditions on the frequency, they converge on a sufficiently small domain.

Assume:

**A0** We are given a family of interaction potentials  $W^\mu$  indexed by an external parameter  $\mu$  which can be complex. We assume that  $W^\mu$  is analytic in both its arguments  $\psi, \eta$  and the parameter  $\mu$ .

**A1** For some parameter  $\mu_0$  we have a solution  $v^0, \sigma^0, \lambda^0$  of (2.2). We assume that  $v^0 \in \mathcal{A}_\rho$  for some  $\rho > 0$ .

**A2** The operator  $\mathcal{L}_{v^0}$ , the linearization of the equilibrium equation factorizes at  $\mu_0$  into two first order operators.

Our goal is to find a perturbative expansion of the solutions of (2.2) in formal power series of  $\mu - \mu_0$ . Later, we will show that these perturbative expansions are convergent following an argument of [21] which is made much easier by the a-posteriori format of Theorem 3. See Section 2.6.2. We seek

$$\begin{aligned} v^\mu &= v^0 + \sum_{n>0} (\mu - \mu_0)^n v^n \\ \sigma^\mu &= \sigma^0 + \sum_{n>0} (\mu - \mu_0)^n \sigma^n \\ \lambda^\mu &= \lambda^0 + \sum_{n>0} (\mu - \mu_0)^n \lambda^n \end{aligned} \tag{2.81}$$

in such a way that, when we substitute it in (2.2) and expand (formally) in powers of  $(\mu - \mu_0)^n$  we obtain that the coefficients of same powers match.

Note that this generalizes the standard Lindstedt series, which is a particular case of the expansion in the case that the family is just  $W^\mu = \mu W$  and that we expand near  $\mu_0 = 0$ .

If we substitute (2.81) in (2.2), expand in powers of  $\mu - \mu_0$ , the coefficient of order  $n$  has the form:

$$v_\eta^n(\psi + \Omega) + v_\eta^n(\psi - \Omega) + v_\eta^n(\psi)(-2 + \partial_\beta W^{\mu_0}(\psi, \eta)) + \sigma^0 v_\eta^n + \sigma^n v_\eta^0 + \lambda^n = R_n \quad (2.82)$$

where  $R_n$  is a polynomial expression in  $v^0, \dots, v^{n-1}$ .

The main observation is that the equation (2.82) is precisely the Quasi-Newton equations (2.44) which can be solved by factorization. Note that we get the perturbative series to all orders only assuming that  $W^\mu$  factorizes at  $\mu = \mu_0$  and the expansion series we get has  $\sigma = 0$  to all orders.

We note that to solve the cohomology equations and obtain analytic solutions, as shown in [1], it suffices to assume

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sup_{|\tilde{k}| \leq N, m \in \mathbb{Z}} \left| \ln |\tilde{k} \cdot \Omega - m| \right| = 0, \quad (2.83)$$

which is weaker than Diophantine and, indeed weaker than Brjuno conditions.

The conditions (2.83) are equivalent to the fact that for any  $\epsilon > 0$

$$\left| \tilde{k} \cdot \Omega - m \right|^{-1} \leq C_\epsilon \exp(\epsilon |k|).$$

Since the solution of the cohomology equations are obtained by multiplying the Fourier coefficients by the small divisors, the estimates imply that we can loose as little domain as desired. To obtain quantitative estimates on the norms, we would need to assume a specific form of the dependence on  $\epsilon$  of  $C_\epsilon$ . These quantitative estimates are crucial for the convergence problems, but are not needed for the study of the existence of the perturbative expansions.

We have, therefore established the following:

**Lemma 5.** *Under the assumptions **A0**, **A1** and that  $\Omega$  satisfies the weak Diophantine conditions (2.83).*

*Then, we can find formal power series as in (2.81) such that for any  $N \in \mathbb{N}$  and any  $\rho'$ ,  $0 < \rho' < \rho$ , we have*

$$\left\| \mathcal{E}_\mu \left[ \sum_{n \leq N} v^n (\mu - \mu_0)^n, \sum_{n \leq N} \lambda^n (\mu - \mu_0)^n \right] \right\|_{\rho'} \leq C_{N, \rho'} |\mu - \mu_0|^{N+1}.$$

*Furthermore, it is possible to find a formal power series that satisfies the normalization*

$$\langle v_\eta^n \rangle = 0 \quad n = 1, \dots, N.$$

*We refer to it as the “normalized perturbative expansion”.*

*This normalized perturbative expansion is unique.*

Similarly, we can obtain existence of perturbation expansions for both the equilibrium and the factorization equations. In analogy with (2.81), we seek expansions

$$\begin{aligned} v^\mu &= v^0 + \sum_{n>0} (\mu - \mu_0)^n v^n & \lambda^\mu &= \lambda^0 + \sum_{n>0} (\mu - \mu_0)^n \lambda^n \\ c^\mu &= c^0 + \sum_{n>0} (\mu - \mu_0)^n c^n & \sigma^\mu &= \sigma^0 + \sum_{n>0} (\mu - \mu_0)^n \sigma^n \end{aligned} \quad (2.84)$$

in such a way that the equilibrium and factorization equations are solved.

The equations for order  $n$  are

$$\begin{aligned} v_+^n + v_-^n + (-2 + \partial_\beta W_{v^0}^{\mu_0} + \sigma^0) v^n + v^0 \sigma^n + \lambda^n &= R_n \\ -c_+^0 c^n + (-c^0 + 2 - \partial_\beta W_{v^0}^{\mu_0} - \sigma^0) c_+^n - c_+^0 \sigma^n - \partial_\beta \partial_\beta W_{v^0}^{\mu_0} c_+^0 v^n &= \tilde{R}_n. \end{aligned} \quad (2.85)$$

From the proof of the KAM theorem, it's clear these can be solved to all orders assuming

that  $W^\mu$  factorizes at  $\mu = \mu_0$ . The series we get do not have  $\sigma = 0$ , which is different from the series when we do not require the factorization for all orders.

We have, therefore established the following:

**Lemma 6.** *Under the assumptions **A0**, **A1**, **A2** and that  $\Omega$  satisfies the quantitative conditions.*

*Then, we can find formal power series as in (2.84) such that for any  $N \in \mathbb{N}$  and any  $\rho'$ ,  $0 < \rho' < \rho$ , we have*

$$\left\| \mathcal{O}_\mu \left[ \sum_{n \leq N} v^n (\mu - \mu_0)^n, \sum_{n \leq N} \sigma^n (\mu - \mu_0)^n, \sum_{n \leq N} \lambda^n (\mu - \mu_0)^n \right] \right\|_{\rho'} \leq C_{N, \rho'} |\mu - \mu_0|^{N+1}$$

and

$$\left\| \mathcal{F}_\mu \left[ \sum_{n \leq N} v^n (\mu - \mu_0)^n, \sum_{n \leq N} \sigma^n (\mu - \mu_0)^n, \sum_{n \leq N} c^n (\mu - \mu_0)^n \right] \right\|_{\rho'} \leq C_{N, \rho'} |\mu - \mu_0|^{N+1}.$$

*Furthermore, it is possible to find a formal power series that satisfies the normalization*

$$\langle v_\eta^n \rangle = 0 \quad n = 1, \dots, N.$$

*We refer to it as the “normalized perturbative expansion”. This normalized perturbative expansion is unique.*

The above results could be interpreted in a more geometric way. We have proved convergence for the perturbative expansion involving also the counterterms that ensure the factorization. Given a potential  $W$  small, the main result shows that we can find a locally unique counterterm  $\sigma$ , which is a functional on  $W$  so that the equation factorizes. The set  $\{W(v) + \sigma(W)v\}$  can be interpreted as a codimension 1 manifold (the factorization manifold) in the space of potentials.

The perturbative expansions in Lemma 4 can be interpreted as the perturbative expansions for a path of potentials indexed by  $\epsilon$  but requiring that  $W$  stays on the factorization

manifold.

In this geometric interpretation, the condition (2.51) that we can solve the factorization by adjusting  $\sigma$  saying that the direction (in the space of potentials) given by  $\sigma v$  are transversal to the factorization manifold  $F$ . Notice that this is in very close analogy with second order differential equations being writable in divergence form.

### 2.6.2 Convergence of Lindstedt series for the equilibrium and the factorization equations

In this section, we are going to show that the a-posteriori format of the main Theorem and the uniqueness it concludes imply automatically the convergence of the perturbation series developed in Section 2.6.1.

**Theorem 4.** *Assume that the conditions of Lemma 6 hold and that  $\Omega$  is Diophantine. Then, the normalized formal series obtained in Lemma 6 is convergent.*

Note that a particular case of the above result is the convergence of the Lindstedt series starting from the case  $V = 0$  when the frequency is Diophantine.

We need the frequency to be Diophantine because, as we will see, the proof uses repeatedly the KAM theorem. It seems quite possible that for the frequencies that satisfy (2.83) but not (2.8), for many perturbations, it is possible to obtain perturbative expansions to all orders, which nevertheless do not converge.

*Proof.* Without loss of generality, we assume that  $v^0$  satisfies (2.3).

Using the KAM theorem (Theorem 3), we obtain that for all  $\mu$  in a small ball centered on  $\mu_0$  there exists a (unique) normalized solution. (It suffices to note that  $v^0$  is a sufficiently approximate solution for all  $\mu$  close to  $\mu_0$ .)

Now, given any  $\tilde{\mu}$  in this small ball, we can obtain a perturbative expansion in powers of  $\mu - \tilde{\mu}$ .

We consider the first term of the expansion  $v_{\tilde{\mu}}^1$ . We remark that it will be uniformly bounded in  $\|\cdot\|_{\rho'}$ .

We note that because

$$\|\mathcal{E}_\mu[v_\mu^0 + (\mu - \tilde{\mu})v_\mu^1, \lambda_\mu^0 + (\mu - \tilde{\mu})\lambda_\mu^1]\|_{\rho'} \leq C|\mu - \tilde{\mu}|^2$$

we can apply the KAM theorem (note that the non-degeneracy conditions of the KAM theorem are satisfied with uniform bounds when the ball is considered small enough) and obtain that there is a normalized solution  $v_\mu^*, \lambda_\mu^*$  of (2.2) for any value of  $\mu$  in a ball around  $\tilde{\mu}$  and that it satisfies

$$\begin{aligned} \|v_\mu^* - v_\mu^0 + (\mu - \tilde{\mu})v_\mu^1\|_{\rho''} &\leq C|\mu - \tilde{\mu}|^2 \\ \|\lambda_\mu^* - \lambda_\mu^0 + (\mu - \tilde{\mu})\lambda_\mu^1\|_{\rho''} &\leq C|\mu - \tilde{\mu}|^2. \end{aligned} \tag{2.86}$$

Using the uniqueness obtained in the KAM theorem we obtain that  $v_\mu^* = v_\mu^0, \lambda_\mu^* = \lambda_\mu^0$ . Hence, (2.86) means that  $v_\mu^1$  is the derivative at  $\mu = \tilde{\mu}$  of the mapping that to  $\mu$  associates  $v_\mu^0, \lambda_\mu^0$  if we give  $v$  the topology in  $\mathcal{A}_{\rho''}$ .

We recall that the Cauchy-Goursat theorem shows that any complex function which is differentiable at every point, is analytic [62]. This argument also works for functions taking values in Banach spaces. Alternatively, it is not difficult to show that the mapping  $\mu \mapsto v_\mu^1$  is continuous (a quick way is to show that the graph of the map is closed because of the uniqueness and that, since it is uniformly bounded, it is compact by Montel's theorem [62]).

Once we have that the function is analytic, we know its Taylor series converges, but the Taylor series has to be the one given by the formal series expansion.  $\square$

Notice as a corollary of the dependence on parameters we can obtain that the solution is analytic in the parameter  $\eta$ .

Since in the physical applications  $\eta \in \mathbb{T}^1$  is important to discuss the periodicity in  $\eta$  of the solutions thus obtained, we remark that, if we start with an approximate solution which is periodic in  $\eta$ , we will obtain a solution which is also periodic in  $\eta$ .

This can be seen in two ways. One can observe that, applying Theorem 3 we can obtain

solutions in small enough intervals of  $\eta$ . They will be analytic in these small intervals and therefore they give a global analytic solution. Furthermore, we observe that if the approximate solution corresponding to  $\eta = 1$  is close to the solution corresponding to  $\eta = 0$ , they have to agree because of uniqueness. Hence, we obtain that the solution is periodic.

We could also argue that, the proof is based on an iterative step and that, by examining the proof, all the steps preserve the periodicity in  $\eta$  of the approximate solutions. Hence, the KAM procedure that we describe for a fixed  $\eta$  lifts to a procedure for periodic functions of  $\eta$ .

The lifting of the problem to a space of functions of  $\eta$  also gives a direct proof of smooth dependence on parameters.

## CHAPTER 3

### TRANSITION STATE THEORY WITH QUASI-PERIODIC FORCING

The goal of this chapter is to develop and implement efficient algorithms for a model studying the transition state theory in chemical reactions.

#### 3.1 The Model

We consider an oscillating double-well potential model

$$\begin{aligned}\dot{x} &= v \\ \dot{v} &= -\gamma v - V'(x - \epsilon_1 E(t))\end{aligned}\tag{3.1}$$

where  $\epsilon_1$  is the strength of oscillation.  $V(x) = -\frac{1}{2}x^2 + \mu x^4$ .  $E(t) = A \sin t + B \sin(\omega t + \phi)$ .

Note that we allow that the oscillation of the substratum to be quasi-periodic. The quasi-periodic motion seems to be a novelty compared to previous papers [70, 71], which only consider periodic.

#### 3.2 Numerical Calculations of Transition State

We consider the extended equations, which are autonomous

$$\begin{aligned}\dot{\theta} &= (1, \omega) \\ \dot{x} &= v \\ \dot{v} &= -\gamma v - V'(x - \epsilon_1 E(\theta))\end{aligned}\tag{3.2}$$

Note that, for  $\epsilon_1 = 0$ , the set  $\Lambda_0 = \{x = 0, v = 0, \theta \in \mathbb{T}^2\}$  is a normally hyperbolic invariant manifold (NHIM). The Fenichel theory ensures that this NHIM persists for small  $\epsilon_1$ .

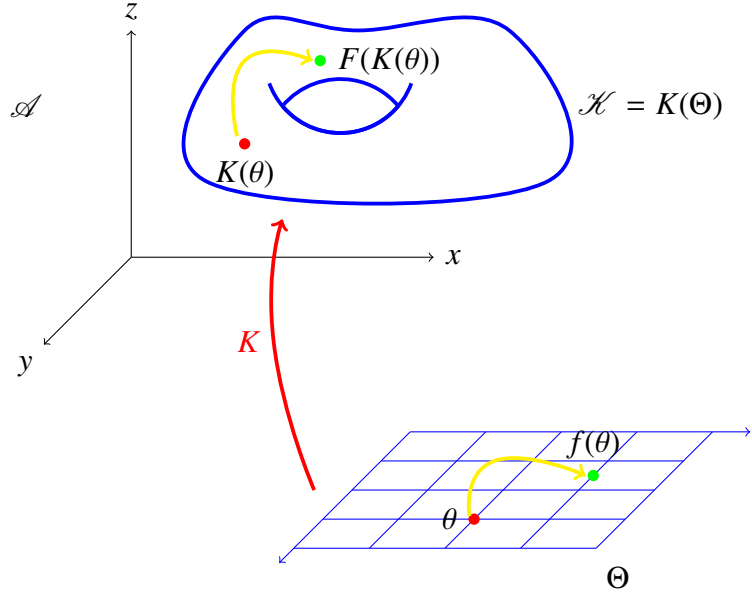


Figure 3.1: Invariant Manifold Parameterized by  $K$  with internal dynamics  $f$

The goal of this section is to implement and run a very efficient numerical method to compute the quasi-periodic transition state.

We adapt the parameterization method for quasi-periodic manifolds and their state/unstable directions introduced in [72, 73, 74] and developed more fully in [75].

Let  $\mathcal{A}$  be a manifold (the *ambient space*). An injective immersion  $K : \Theta \rightarrow \mathcal{A}$  of a manifold  $\Theta$  into  $\mathcal{A}$  defines a submanifold  $\mathcal{H} = K(\Theta)$ . We say that  $\mathcal{H}$  is parameterized by  $K$ , and that  $\Theta$  is its *model manifold*.

Let  $F : \mathcal{A} \rightarrow \mathcal{A}$  be a diffeomorphism. A submanifold  $\mathcal{H} \subset \mathcal{A}$  parameterized by  $K : \Theta \rightarrow \mathcal{A}$  is  $F$ -invariant if there exists a diffeomorphism  $f : \Theta \rightarrow \Theta$  such that

$$F \circ K = K \circ f \tag{3.3}$$

The meaning of the invariance equation (3.3) is sketched in Figure 3.1

### 3.2.1 The invariance and reducibility equations

The algorithm is based on finding an embedding

$$(id, K) : \mathbb{T}^2 \rightarrow \mathbb{T}^2 \times \mathbb{R} \times \mathbb{R} \quad (3.4)$$

in such a way that its range is invariant.

Let

$$F : \mathbb{T}^2 \times \mathbb{R}^2 \rightarrow \mathbb{R}^2 \quad (3.5)$$

be the time-one map of the equation 3.2 projected to the  $(x, v)$  space.

If  $K$  parameterizes an invariant manifold for  $F$ , it must satisfy

$$F(\theta, K(\theta)) - K(\theta + \omega) = 0. \quad (3.6)$$

Now suppose we have an approximate NHIM parameterized by  $K$  and we also have an approximate invariant frame  $P : \mathbb{T}^2 \rightarrow SL_2(\mathbb{R})$  reducing the dynamics to diagonal:

$$F(\theta, K(\theta)) - K(\theta + \omega) = E(\theta) \quad (3.7)$$

$$P(\theta + \omega)^{-1} D_2 F(\theta, K(\theta)) P(\theta) - \Lambda(\theta) = E_{red}(\theta) \quad (3.8)$$

where  $E$  and  $E_{red}$  are the errors for the approximation.  $E(\theta)$  measures the error for the invariance equation and  $E_{red}(\theta)$  measures the error for the reducibility equation.

For simplicity, in the following we will omit  $\theta$  when there is no ambiguity and use the notation

$$f_+ = f(\theta + \omega) \quad (3.9)$$

$$f_- = f(\theta - \omega) \quad (3.10)$$

for any function  $f$ .

### 3.2.2 Newton's Method

We formulate a Newton's method for (3.7) and (3.8). As we will see, it turns out to be more efficient to solve both equations than to solve just (3.7). The unknowns are  $K, P, \Lambda$ . We look for updates  $\Delta K, \Delta P$  and  $\Delta \Lambda^{S,U}$ . We also denote  $\Delta K = P\xi$  and  $\Delta P = PQ$ .

The linearization of the invariance equation gives

$$D_2F(\theta, K)\Delta K - \Delta K_+ = -E \quad (3.11)$$

multiply  $P_+^{-1}$  on the left and use the reducibility equation, we have

$$\Lambda\xi - \xi_+ = \eta \quad (3.12)$$

This splits in the stable and unstable direction as

$$\begin{aligned} \Lambda^S \xi^S - \xi_+^S &= \eta^S \\ \Lambda^U \xi^U - \xi_+^U &= \eta^U \end{aligned} \quad (3.13)$$

which can be written as two contractions

$$\begin{aligned} \xi^S &= \Lambda_-^S \xi_-^S - \eta_-^S \\ \xi^U &= (\Lambda^U)^{-1}(\xi_+^U + \eta^U) \end{aligned} \quad (3.14)$$

We can solve (3.14) by simple iteration or by solving for the Fourier coefficients.

To find updates of  $P$  and  $\Lambda$ , we first define

$$\tilde{E}_{red} = P_+^{-1}D_2F(\theta, K + \Delta K)P - \Lambda \quad (3.15)$$

Then a linearization of the reducibility equation gives

$$\Lambda Q - Q_+ \Lambda - \Delta \Lambda = -\tilde{E}_{red}. \quad (3.16)$$

Writing (3.16) in block form, we have:

$$\begin{aligned} \Lambda^S Q^{SS} - Q_+^{SS} \Lambda^S &= -\tilde{E}_{red}^{SS} + \Delta \Lambda^S \\ \Lambda^S Q^{SU} - Q_+^{SU} \Lambda^U &= -\tilde{E}_{red}^{SU} \\ \Lambda^U Q^{US} - Q_+^{US} \Lambda^S &= -\tilde{E}_{red}^{US} \\ \Lambda^U Q^{UU} - Q_+^{UU} \Lambda^U &= -\tilde{E}_{red}^{UU} + \Delta \Lambda^U \end{aligned} \quad (3.17)$$

Note the solution to (3.16) is not unique. Geometrically, only the direction of the column vectors of  $P$  matters. So we only update the stable and unstable frame in the complementary direction and choose  $Q^{SS} = 0$  and  $Q^{UU} = 0$ . As a consequence, we will choose  $\Delta \Lambda^S = \tilde{E}_{red}^{SS}$  and  $\Delta \Lambda^U = \tilde{E}_{red}^{UU}$ .

Then (3.16) can be written as two contractions

$$\begin{aligned} Q^{SU} &= (\Lambda_-^S Q_-^{SU} + (\tilde{E}_{red}^{SU})_-)(\Lambda_-^U)^{-1} \\ Q^{US} &= (\Lambda^U)^{-1} (Q_+^{US} \Lambda_S - E_{red}^{US}) \end{aligned} \quad (3.18)$$

which can be solved using simple iteration or by solving for the Fourier coefficients.

### 3.2.3 Some Remarks

It is interesting to compare this numerical method with the non-stationary normal form. The first remark is that the method requires to deal only with functions of two variables (takes surfaces of reduction, only require one variable functions). In contrast the non-stationary normal form requires to deal with four variable functions, which is much more costly since the computational requirements grow exponentially fast with the dimension (the ‘‘curse of dimensionality’’).

Notice also that we implemented a Newton method to solve the equation(3.4), which allows a very fast convergence up to machine precision.

### 3.2.4 Numerical Results for the Invariant Manifolds

Here we calculated the NHIM for the quasi-periodic potential  $U$  with  $E(t) = \sin(2\pi t) + 2 \sin(2\pi\omega t)$  where  $\omega = \frac{\sqrt{5}+1}{2}$ . We used a continuation method with  $\epsilon_1 = 0$  and continued to  $\epsilon_1 = 1.0$  with an increment=0.1. We have used a Macbook Air with 1.4 GHz Intel Core i5 and 4GB memory using 1024 Fourier modes, the continuation method run in 45 seconds and provided accuracy which we believe is only a few units of roundoff error. The NHIM projected to the phase space is shown in Figure 3.2. The NHIM in  $(\theta, x, v)$  space is shown in Figure 3.3. The angle between stable and unstable spaces is shown in Figure 3.4.



Figure 3.2: Invariant Torus in phase space

Parameters:  $A = 1, B = 2, \epsilon_1 = 1, \mu = 1, \omega = \frac{\sqrt{5}+1}{2}, \phi = \frac{\pi}{2}$

Once we have computed accurately the NHIM and their invariant bundles, it is easy to provide transversally to the NHIM which is away from the stable/unstable manifolds and

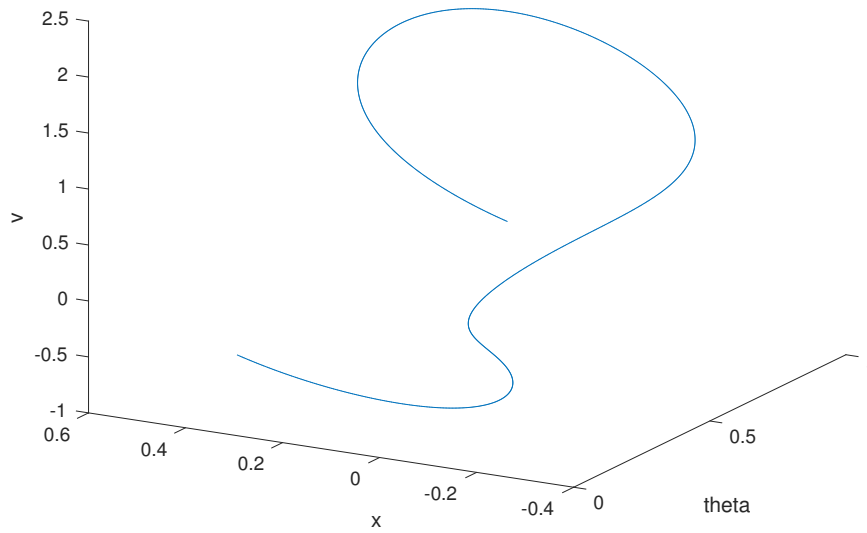


Figure 3.3: Invariant Torus, 3D  
 Parameters:  $A = 1, B = 2, \epsilon_1 = 1, \mu = 1, \omega = \frac{\sqrt{5}+1}{2}, \phi = \frac{\pi}{2}$

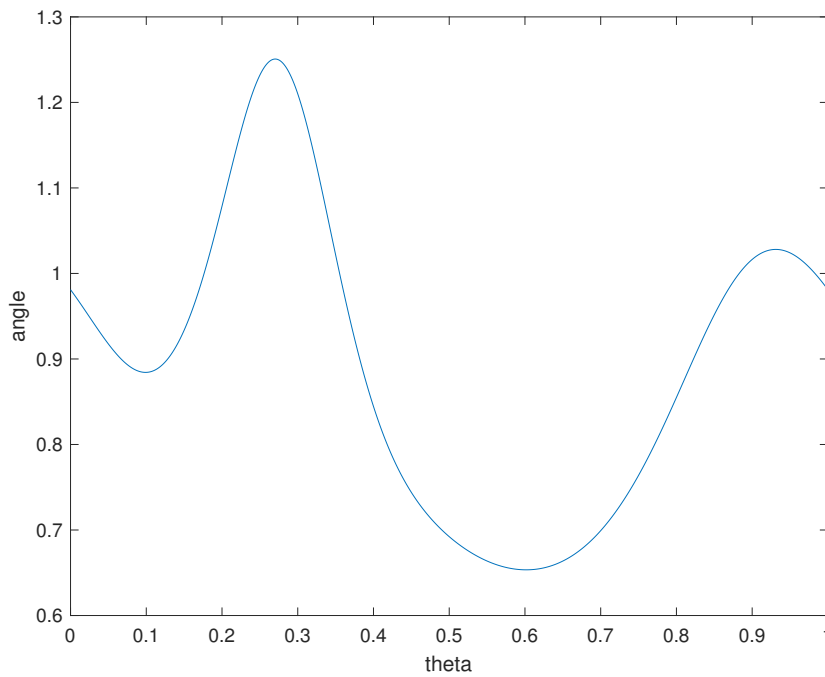


Figure 3.4: Angle between stable/unstable spaces  
 Parameters:  $A = 1, B = 2, \epsilon_1 = 1, \mu = 1, \omega = \frac{\sqrt{5}+1}{2}, \phi = \frac{\pi}{2}$

hence, provide a surface which can be considered of no recrossing.

### 3.3 Computation of Stable and Unstable Manifolds of Transition States

The next interesting question is to calculate the stable and unstable manifolds of the invariant tori.

We first consider the stable manifolds. Again, we seek a parameterization:

$$W(\theta, s) : \mathbb{T}^2 \times \mathbb{R}^1 \rightarrow \mathbb{T}^2 \times \mathbb{R}^2. \quad (3.19)$$

The invariance equation for the parameterization of the stable manifold is:

$$F(\theta, W(\theta, s)) = W(\theta + \omega, \Lambda^s s). \quad (3.20)$$

Here  $\Lambda^s$  parameterize the contraction on stable bundle.

#### 3.3.1 Evolve the flow along curves

The main problem we have to face in a numerical implementation is how to compute  $F(\theta, W(\theta, s))$  when we are given  $W(\theta, s)$ .

In principle this is possible using the theory of equations of variation to arbitrary orders [76]. A more efficient way already used in [77] is to propagate curves through the differential equation. If we fix  $\theta = \theta_0$ , we can think of (3.2) as an ODE in the space of polynomials. We consider a curve of initial conditions:

$$(x, v)(s) = W(\theta_0, s) \equiv (W_x(\theta_0, s), W_v(\theta_0, s)) = \sum_n W_n(\theta_0) s^n. \quad (3.21)$$

Then, the curve of initial conditions evolve according to

$$\begin{aligned}
\frac{d}{dt}\theta &= (1, \omega) \\
\frac{d}{dt}W_x(\theta_0, s, t) &= W_v(\theta_0, s, t) \\
\frac{d}{dt}W_v(\theta_0, s, t) &= -\gamma W_v(\theta_0, s, t) - V'(W_x - \epsilon_1 E(\theta))
\end{aligned} \tag{3.22}$$

The way to think of equations (3.22) is as an ODE in the space of polynomials in  $s$ .  $t$  is the time under which we are evolving and  $\theta_0$  is treated as a parameter.

The solutions of (3.22) can be computed very efficiently in our case. Note that the right hand side of the equation (3.2) are algebraic expansions in the variables  $x, v$ . Therefore the equation (3.22) have a right hand side which is an algebraic expansion on the polynomials of  $W_x, W_v$ .

Therefore, once we implemented algebraic operations (sum, multiplication, etc.) on polynomials, we can implement the right hand side of (3.22) and pass it to a standard integration method (e.g. a RK integrator). The time one map of the extended system gives the map

$$\theta_0, W(\theta_0, s) \rightarrow F(\theta_0, W(\theta_0, s)) \tag{3.23}$$

which is the core of the evaluation of the invariance equation (3.20).

After we can evaluate (3.2), the Newton method presented in Section 3.3.3 can proceed.

The Newton method would be doubling the order of the correct coefficients at each step. Then, it is efficient to run the calculation of  $F$  with a number of coefficients  $2^L$  where  $L$  is the number of truncation steps.

It is very fortunate that the ignored terms of higher degree do not affect the terms of lower degree in subsequent steps (since the product of a high degree term and a lower degree polynomial is always higher degree). Note that the implementation of polynomial operations involves truncation in the multiplication (the product of two polynomials of degree  $d$  is a polynomial of higher degree). So that the truncation does not affect the

accuracy of the computed low degree terms.

**Remark 16.** *A practical remark is that if we make a scaling*

$$\tilde{W}(\theta, s) = W(\theta, \Lambda^s s), \quad (3.24)$$

*Then, we obtain an equivalent parameterization. Nevertheless the numerical behavior of  $\tilde{W}$  may be very different from that of  $W$ .*

*The reason is that  $\tilde{W}^n = \Lambda^{s,n} W^n$ . Hence for certain  $\Lambda^s$ 's, it could well happen that  $\tilde{W}^n$  has coefficients that differ very widely in size. This makes the computation of algebraic expansions of  $\tilde{W}$  very prone to round off error and it should be avoided.*

*In practice, once one runs a preliminary calculation, and then determines a suitable  $\Lambda^s$  which makes the coefficients of  $\tilde{W}$  to be of roughly consistent size. This ensures that the numerical calculation is as stable to round off error as possible.*

**Remark 17.** *Note that one could also overload the propagation operator and take the initial condition to be  $K(\theta)$  a trigonometric polynomial  $K(\theta)$ .*

**Remark 18.** *The calculation of the time one map for  $N$  values of  $\theta$  is very easy to parallelize. So that the calculation of the  $N$  points of the trajectory is easy to do.*

Once we know how to compute  $F(\theta, W(\theta, s))$  as polynomials in  $s$ , we have several algorithms to solve the invariance equation (3.20).

### 3.3.2 The order by order method

If we expand in powers of  $s$  and equate same order powers, we have that (3.20) is equivalent to a sequence of equation

$$D_2 F(\theta, K(\theta)) W_n(\theta) = \Lambda^{s,n} W_n(\theta + \omega) + R_n \quad (3.25)$$

where  $R_n = -[F(W_{<n})]_n$  is an expansion involving only the terms of orders lower than  $n$ .

The only unknown in (3.25) is the function  $W_n(\theta)$ .  $K(\theta) = W(\theta, 0)$  is the parameterization of the invariant manifold we calculated in Section 3.2. The  $\Lambda^s$  is computed in Section 3.2 already and the  $R_n$  is available through the propagation algorithm.

The equation for  $W_n$  (3.25) can be solved recursively

$$\begin{aligned}
W_n(\theta) &= \Lambda^{s,n}[D_2F(\theta, W_0(\theta))]^{-1}W_n(\theta + \omega) + R_n(\theta) \\
&= R_n(\theta) + \Lambda^{s,n}D_2F(\theta + \omega, W_0(\theta + \omega))^{-1}R_n(\theta + \omega) \\
&\quad + \Lambda^{s,2n}[D_2F(\theta + \omega, W_0(\theta + \omega))]^{-1}[D_2F(\theta + 2\omega, W_0(\theta + 2\omega))]^{-1}R_n(\theta + 2\omega) \\
&\quad + \dots
\end{aligned} \tag{3.26}$$

It is easy to show that the series (3.26) converges uniformly for  $n \geq 2$ . Indeed, we know from (3.8) that

$$\| [D_2F(\theta + j\omega, W_0(\theta + j\omega)) \cdots D_2F(\theta, W_0(\theta))]^{-1} \| \leq C\Lambda^{s,-n} \tag{3.27}$$

Therefore the factors in the general term of (3.26) decrease exponentially for  $n \geq 2$ .

### 3.3.3 Reducibility Method

We can also use the reducibility equation (3.8). Multiplying (3.25) by  $P^{-1}(\theta + \omega)$  and writing  $W_n = PV_n$ , we have

$$\Lambda^s V_n(\theta) = \Lambda^{s,n} V_n(\theta + \omega) + P^{-1}(\theta + \omega) R_n(\theta) - E_{red} V_n(\theta) \tag{3.28}$$

The equation (3.29) (order  $n$  reduced) can be solved iteratively or matching Fourier coefficients.

We can also use the reducibility equation (3.8). Multiplying (3.25) by  $P^{-1}(\theta + \omega)$  and

writing  $W_n = PV_n$ , we have

$$\Lambda V_n(\theta) = \lambda^n V_n(\theta + \omega) + P^{-1}(\theta + \omega)R_n(\theta) - E_{red}V_n(\theta) \quad (3.29)$$

The equation (3.29) (order  $n$  reduced) can be solved iteratively or matching Fourier coefficients.

In component form, we have

$$\begin{aligned} V_n^s(\theta) &= (\lambda^s)^{n-1} V_n^s(\theta + \omega) + (\lambda^s)^{-1} P^{-1}(\theta + \omega) R_n(\theta) \\ V_n^u(\theta) &= (\lambda^s)^n (\lambda^u)^{-1} V_n^u(\theta + \omega) + (\lambda^u)^{-1} P^{-1}(\theta + \omega) R_n(\theta) \end{aligned} \quad (3.30)$$

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