EQUILIBRIUM QUASI-PERIODIC CONFIGURATIONS WITH RESONANT FREQUENCIES IN QUASI-PERIODIC MEDIA I: PERTURBATIVE EXPANSIONS

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Abstract. We consider 1-D quasi-periodic Frenkel-Kontorova models (describing, for example, deposition of materials in a quasi-periodic substrate).

We study the existence of equilibria whose frequency (i.e. the inverse of the density of deposited material) is resonant with the frequencies of the substrate.

We study perturbation theory for small potential. We show that there are perturbative expansions to all orders for the quasi-periodic equilibria with resonant frequencies. Under very general conditions, we show that there are at least two such perturbative expansions for equilibria for small values of the parameter.

We also develop a dynamical interpretation of the equilibria in these quasi-periodic media. We show that the dynamical system has very unusual properties. Using these, we obtain results on the Lyapunov exponents of the resonant quasi-periodic solutions.

In a companion paper, we develop a rather unusual KAM theory (requiring new considerations) which establishes that the perturbative expansions converge when the perturbing potentials satisfy a one-dimensional constraint.

Quasi-periodic Frenkel-Kontorova models, resonant frequencies, equilibria, quasicrystals, Lindstedt series, counterterms
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1. Introduction

The goal of this paper is to study resonant quasi-periodic solutions in quasi-periodic Frenkel-Kontorova models.

These Frenkel-Kontorova models [FK39] are widely studied models of phenomena in one-dimensional quasi-crystals. The main interpretation we will use is the deposition of materials over a quasi-periodic substratum. Other interpretations (planar dislocations in 3-D crystals, spin waves) are also possible [Sel88, BK04, Sel92].

In Frenkel-Kontorova models, one considers configurations given by a sequence of real numbers (think of the position of a sequence of particles deposited on a 1-D quasi-crystal). 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., in 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 2.

In [SdlL12b, SdlL12a], 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 [SdlL12b, SdlL12a] 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 [BdlL13a]. The paper [SdlL12b], studies models with nearest neighbor interaction while [SdlL12a] studies the case of long range interactions. So far, to the best of our knowledge, there are no numerical studies of equilibria in quasi-periodic media with long range interactions. In the periodic case, numerical studies of long range interactions were conducted in [CdIL09, CdIL10a].

The goal of this paper is to start developing the theory of quasi-periodic equilibria whose frequency resonates with the frequencies of the medium.

In this paper, we use the name quasi-periodic equilibria to denote equilibria that are given by a smooth hull function. See Section 2.2. Of course, it could happen that the hull function becomes discontinuous as it has been known in the periodic Frenkel-Kontorova models since [Per79, ALD83, Mat82, Kat83]. When the hull function is discontinuous, the solutions are called quasi-automorphic in the mathematical literature. In this paper, we will not consider discontinuous hull functions.

We will study perturbative expansions for the solutions with a fixed frequency (the physical meaning of the frequency is the mean spacing, i.e. the inverse of the density). We establish the existence of Lindstedt series to all orders for the solutions of the equilibrium equations. We note that the Lindstedt series involves not only the hull function describing the equilibrium but it also involves counterterms. This is very common in perturbative expansions in statistical mechanics [Gal85].

Roughly, the counterterms are constant fields we apply to stabilize the equilibrium solution. Note however, that due to the resonance we obtain one parameter family of solutions for the perturbative expansion. We obtain a solution for each value of another number which has the physical meaning of a transversal phase. The counterterm is thus a function of the transversal phase.

In some applications, we may decide to apply the force to obtain a solution with a prescribed force. More commonly, when the external force is fixed, the system will have some equilibria (obtained by choosing the average phase) which are equilibria for the Frenkel-Kontorova model including the applied external field. In Section 3.1, we discuss how to find the average phase to match the applied external force. We will show that, under very general circumstances, for each external force, sufficiently small, we can find two average phases that match it to all orders in perturbation theory. See Proposition 2.

In [SdlL12a], it was shown that non-resonant quasi-periodic solutions exist only when the average force applied to the material vanishes. In contrast, we will show that, to all orders in perturbation theory, the quasi-periodic solutions with a resonant frequency can exist for a range of external average
forces. These resonant quasi-periodic solutions are, therefore, crucial to understand “depinning” effects. We recall that the minimal force for which there are no equilibria is called the “depinning force” (sometimes the depinning force is called the minimal force for which there are no minimizing equilibria). The application of an external force (no matter how small) makes it impossible to have any solution with non-resonant frequencies and with a continuous hull function. Nevertheless, as we show in this paper, it is possible to have quasi-periodic solutions with resonant frequencies. Hence, there are still equilibria for positive external force. In the case of Frenkel-Kontorova models, it was empirically studied that among the equilibrium configurations that persist for external forces, solutions with resonant frequencies are more “abundant”. The paper [FdlL15] contains quantitative conjugacies. We think it would be interesting to study the depinning in quasi-periodic model.

We also develop a dynamical interpretation of the equilibria in quasi-periodic media. This is a rather elementary remark, which applies to all equilibrium solutions in quasi-periodic media. We use it to discuss the possibility of phonon gaps, which dynamically correspond to Lyapunov exponents [AMB92]. We find that these solutions do not have a phonon gap – there are sliding modes – nevertheless, they can exist in the presence of external fields.

In this paper, we will not consider the question of whether the perturbative expansions developed here converge or not. In a companion paper [ZSdlL14], we will develop a KAM theory for these methods. This KAM theory is rather unusual, since it does not rely on the usual transformation theory, but requires a technique based on factorization of some auxiliary equations. It requires the use of an extra parameter. Of course, the techniques used in [ZSdlL14] are rather different from those of this paper and require hard analysis. We anticipate that the results of [ZSdlL14] show that the Lindstedt series for quasi-periodic equilibria developed in this paper converge when the potentials are chosen satisfying a constraint (in mathematical terms, we choose the potentials in a codimension one manifold in the space of potentials). We believe that this is not an artifact of the proof and that one can get exponentially small phenomena. Similar phenomena have been observed already in the study of lower dimensional tori in Hamiltonian mechanics, namely that the convergence of the perturbative expansions is affected by “normal” denominators that do not appear in the term by term solutions but which lead to exponentially small effects [IdlLZ99]. The existence of these exponentially small effects is not understood for our models.

Equilibria in quasi-periodic media with a resonant frequency have been investigated numerically in [vEFRJ99, vEFJ01, vEF02]. These papers also
studied the phonon gap and found it to vanish when there are smooth solutions (in agreement with the results here). From the mathematical point of view, the existence of solutions of all frequencies in quasi-periodic media was also considered using topological methods in \[ \text{GGP06, AP10} \].

Variational methods, which have proved very useful and deep facts in the periodic case \((d = 1\) in our notation), so far have not been developed for quasi-periodic potentials. The extension of variational methods to quasi-periodic media is not straightforward. Indeed in \[ \text{LS03} \] there are counterexamples to straightforward generalizations of the results from the periodic case to the quasi-periodic case in models similar to ours (the discrete derivative is an analogue of the second derivative). Examples which can be interpreted as geodesic flows in quasi-periodic metrics in \( \mathbb{S}^2 \) can be found in \[ \text{Fed75} \]. Of course, the fact that some features of the \( d = 1 \) case do not survive in the quasi-periodic case, does not exclude that other features do survive. It is a very interesting problem to characterize which part of the theory of minimizers goes through in the quasi-periodic case.

This paper is organized as follows:

In Section 2 we present the models we study and in Section 3 we present the definition of spaces we consider and some preliminary standard results.

In Section 4 we present systematic perturbative expansions (Lindstedt series) which we show can be defined to all orders for analytic systems. We obtain series expansions in powers of the coupling parameter for the hull function of the equilibria and for external forces that stabilize these equilibria (counterterms). Since the problem is degenerate, these series will include a free parameter that has the physical meaning of a transversal phase and the solution and the counterterm are functions of this transversal phase. For each value of the transversal phase, we obtain a series expansion of the solution and the counterterm.

As is standard in perturbative expansions, to study the physical situation when there is an external force being applied, we just need to choose the transversal phase so that the counterterm matches the force applied. This determines the transversal phase and, hence the solution.

We will show that, under very general nondegeneracy conditions, this program can be carried out and that, when the external force is small, there are two solutions in the sense of formal power series expansions. When the external force reaches a critical value, there may be no solutions. This critical value of the forces that lead to sliding can be computed perturbatively. Analogous problems in the periodic case have been considered in \[ \text{ALD83, QW15} \].

In Section 5, we present a dynamical interpretation of the equilibrium equations. This allows to compare better the KAM theory developed here
with the KAM theory for volume preserving systems and has some consequences for the study of the phonon gap. We find that, in the dynamical interpretation, the quasi-periodic solutions have always several zero Lyapunov exponents.

We point out that for the dynamical interpretation, adding longer range interactions is a singular perturbation (even the dimension of the phase space changes!). Nevertheless, for the methods of the present paper, adding a small non-local interaction is a regular perturbation. We hope to come back to this problem.

In Section 5.2 we study the phonon gap and show it vanishes while the solution remains smooth. Dynamically, this means that for the smooth solutions there are always zero Lyapunov exponents. We point out however that the dynamical systems we obtain has very unusual properties which have the origin in that the system preserves an irrational foliation.

2. Models considered and formulation of the problem

We consider models of deposition in a quasi-periodic one-dimensional medium. Other physical interpretations are possible.

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

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

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

The term \((x_{n+1} - x_n - \alpha)^2\) represents the interaction among neighboring deposited atoms. The term \(V(x_n \alpha)\) represents the interaction with the sub-stratum. 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.

The existence of external forces \(\lambda\) is a very important novelty with respect to the previous papers [SdlL12b, SdlL12a]. In these papers, the only possible \(\lambda\) was zero. In [SdlL12b, SdlL12a] there is a simple argument that shows 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 non-trivial \(\lambda\) and will show how to compute perturbatively the range of such \(\lambda\) for which solutions with a prescribed frequency exist. This corresponds to the physical phenomenon of pinning which is the microscopic explanation of static friction.
The fact that the interaction at position \( y \in \mathbb{R} \) is the quasi-periodic function \( V(y\alpha) \) models that the substratum is quasi-periodic.

Without any loss of generality, we can assume that

\[
(2) \quad k \cdot \alpha \not\in \mathbb{N} \quad \forall \ k \in \mathbb{Z}^d - \{0\}.
\]

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

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,

\[
\frac{\partial \mathcal{L}}{\partial x_n}(x) = 0 \quad \forall \ n \in \mathbb{Z}.
\]

In the model (1), the equilibrium equations are

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

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

Note that even if the energy (1) is just a formal sum, the equilibrium equations (3) are well defined equations.

It is very tempting to consider (3) 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 5. Note however that the intention of a dynamical system is very different from the minimization of energy. Initial conditions picked at random tend not to be minimizing and minimizers tend to occupy small measure in phase space.

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

\[
(4) \quad x_n = n\omega + h(n\omega \alpha),
\]

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

A configuration given by a hull function (4) satisfies the equilibrium equation (3) if and only if the hull function \( h \) satisfies

\[
(5) \quad h(n\omega\alpha + \omega\alpha) + h(n\omega\alpha - \omega\alpha) - 2h(n\omega\alpha) + \partial_\alpha V(n\omega\alpha + ah(n\omega\alpha)) + \lambda = 0.
\]

The equation (5) was considered in \[SdlL12b, SdlL12a\] when \( \omega\alpha \) is Diophantine (in particular, \( n\omega\alpha \) is dense in the torus \( \mathbb{T}^d \)). In that case, one can transform the equation (5) into an equation where \( n\omega\alpha \) is replaced by a continuous variable \( \theta \in \mathbb{T}^d \). The treatment of \[SdlL12b, SdlL12a\] was based on the study of the continuous equation.
In our case, \( n \omega \) will not be dense on the \( d \)-dimensional torus (see Section 2.3) and the equilibrium equations we will derive are somewhat different. See Section 2.4 in particular (9), for a precise formulation of these equilibrium equations.

2.3. Resonances. The goal of this paper is to study situations when \( \omega \) is such that there are \( k \in \mathbb{Z}^d - \{0\} \) and \( m \in \mathbb{Z} \) such that
\[
k \cdot \omega - m = 0. \tag{6}
\]
When (6) holds we say that \((k, m)\) is a discrete resonance for \( \omega \) and we refer to the pair \((k, m)\) as a resonance.

Remark 1. Note that these discrete resonances (6) 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 \( k \cdot \alpha \neq 0 \) \( \forall k \in \mathbb{Z}^d - \{0\} \), 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.

2.3.1. 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 \((k_1, m_1), \ldots, (k_l, m_l)\) 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).

2.3.2. Only resonances of multiplicity 1 appear in the models \( \Pi \). 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 \( \S \) one can give a dynamical interpretation of the equilibrium equations as a dynamical system in \( d + 1 \) dimension. Nevertheless, in our models only \( l = 1 \) appears independently of the number of degrees of freedom. This is, of course, sort of obvious since the resonance condition is a one-dimensional condition, but it highlights that the problem here is different from the Hamiltonian problem.
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 (2))
\[ \omega = \frac{m_1}{k_1 \cdot \alpha} = \frac{m_2}{k_2 \cdot \alpha} \]
and therefore
\[ \alpha \cdot (k_1 m_2 - k_2 m_1) = 0 \]
and, because \( \alpha \) is non-resonant (2) we have
\[ k_1 m_2 = k_2 m_1. \]
Therefore, the two resonant vectors are related. \( \square \)

2.3.3. The intrinsic frequencies. Hence, in the future we will only consider \( l = 1 \) resonances. In this case 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
\[ (7) \quad B \omega \alpha = (\Omega, 0) + L \quad \text{with} \quad \Omega \cdot \hat{k} \notin \mathbb{Z} \text{ for } \hat{k} \in \mathbb{Z}^{d-1} - \{0\}. \]
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 some future arguments we will assume that \( \Omega \) is Diophantine in \( \mathbb{R}^{d-1} \) (see (15) in Section 2.7).
We remark that even if the \( \Omega \)'s are not unique as indicated above, if one of them satisfies (15), all of them satisfy a Diophantine condition (15) with the same exponent \( \tau \) (but may be different constants \( \nu \)).
In some parts of the argument (notably the existence of Lindstedt series to all orders or the existence of perturbative expansions) we can use some other conditions weaker than the above Diophantine conditions. In particular, for the existence of formal power series to all orders it suffices that (16) holds.
The following proposition shows that the sets of frequencies we are considering are abundant.
Fix a vector \( k \in \mathbb{Z}^d \backslash \{0\}, m \in \mathbb{Z} \). For any \( \alpha \in \mathbb{R}^d \) we can find a unique \( \omega \) such that \( \alpha \cdot k \omega - m = 0 \). Then, we can find the intrinsic frequencies \( \Omega \). Hence, for any \( k, m \) we can define \( \Omega = F_{k,m}(\alpha) \).
Proposition 1. The set of \( \alpha \) for which \( F_{k,m}(\alpha) \) is Diophantine for all \( k, m \) is of full measure in \( \mathbb{R}^d \).
Proof. Since countable intersections of sets of full measure are of full measure, to prove Proposition 1 it suffices to show that for a fixed \( k, m \) as above, the set of \( \alpha \in \mathbb{R}^d \) for which \( F_{k,m}(\alpha) \) is Diophantine is of full measure.
This is easy because the set of \( \Omega \) which are Diophantine is full measure on \( \mathbb{R}^{d-1} \). The map from \( \alpha \omega \) to \( F_{k,m} \) is differentiable and surjective. Therefore
the preimage of the set of Diophantine $\Omega$ is also of full measure in the hyperplane $\Gamma = \{ \gamma \mid \gamma \cdot k - m = 0 \}$. The corresponding $\alpha$’s are just a scaling of $\alpha \omega$, which also form a full measure set in $\mathbb{R}^d$. □

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

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

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

We use the notation $B\theta = (\psi, \eta)$ where $B \in SL(d,\mathbb{Z})$ is the matrix introduced in (7) and $\psi \in \mathbb{T}^{d-1}$, $\eta \in \mathbb{T}^1$.

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.

Note that each of the sets $\{n\omega \alpha\}_{n \in \mathbb{Z}}$ has a closure which is a $d-1$ dimensional torus. This torus is invariant under the translation $T_{\omega \alpha}$. 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.

We will refer to the $\eta$ variable as the transversal phase. Note that 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 $V$.

Since the equilibrium equations in the integrable case conserve the transversal phase (this is not the case on the full equations!), we see that it will be a slow variable. In the perturbative expansions, it will be a free parameter. For each value of $\eta$ we will find a perturbative expansion for the hull function and for the counterterm. In physical applications, we will choose the transversal phase so that the counterterm $\lambda$ matches the physical values of the applied external force.

If we substitute the parameterization (8) into the equilibrium equation, we obtain that the equilibrium equation (3) is equivalent to:

$$v(n\Omega + \Omega) + v(n\Omega - \Omega) - 2v(n\Omega) + \partial_\alpha V(n\omega \alpha + \alpha v(n\Omega)) + \lambda = 0.$$  \hspace{1cm} (9)

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 (9) for continuous functions $v$ is equivalent to:

$$v(\psi + \Omega) + v(\psi - \Omega) - 2v(\psi) + W((\psi, \eta) + \beta v(\psi)) + \lambda = 0.$$  \hspace{1cm} (10)
We note that, in the subsequent treatment, we will not use the fact that $W$ has the form $W = \partial_\alpha V$.

The functional equation (10) is the centerpiece of our analysis.

**Remark 3.** It will be important to mention that, because $\beta$ has components both in the $\psi$ and the $\eta$ directions, the equation (10) cannot be considered as a parameterized version of the equations considered in [SdlL12b]. As we will see, the symmetries of the equation involve transformations that mix the dependence in $\psi$ and in $\eta$.

2.5. **The symmetries of the invariance equation (10).** The equation (10) possesses remarkable symmetries that make the solutions not unique. These symmetries lead to Ward identities. In contrast with the case of non-resonant solutions, the group of symmetries is infinite dimensional. In [dL08, SdlL12b, SdlL12a] these symmetries are used to develop a KAM method. In the companion paper [ZSdlL14], we will see that in the present case, the Ward identities do not lead to a KAM method.

The main observation is that if $(v, \lambda)$ is a solution of (10), then, for every $\iota(\eta) : \mathbb{T}^1 \to \mathbb{R}$, the pair $(\tilde{v}, \tilde{\lambda})$ is also a solution of (10) where we denote $\beta = (\beta_\psi, \beta_\eta)$ and $\tilde{v}, \tilde{\lambda}$ are defined by:

\[
\tilde{v}(\psi, \eta) = v((\psi, \eta) + \iota(\eta)\beta) + \iota(\eta),
\]

\[
\tilde{\lambda}(\eta) = \lambda(\eta + \iota(\eta)\beta_\eta).
\]

Notice that the symmetry (11) involves changing not only the argument $\psi$ but also the argument $\eta$. The subsequent arguments will use very much (11). Note also that in this case, the space of symmetries of the equation is not just a finite dimensional space but rather an infinite dimensional space of functions.

2.6. **A normalization of the solutions of the invariance equation (10).** Since 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), we indicate that it is natural to impose the normalization

\[
\int_{\mathbb{T}^1} v(\psi, \eta) \, d\psi = 0.
\]

Since the symmetry (11) involves changes of arguments, giving a $v_\eta$, finding the $\iota(\eta)$ that accomplishes the normalization is not trivial and involves solving the implicit equation

\[
I(\eta + \beta_\psi(\eta)) + \iota(\eta) = 0
\]

where $I(\eta) \equiv \int_{\mathbb{T}^1} v(\psi, \eta) \, d\psi$. 
Applying the finite dimensional implicit function theorem, we can solve (13) if \( J \) is small and its derivative is also small. In contrast, in the non-resonant case, the normalization of the function considered in [SdlL12b] could always be solved explicitly.

Actually, we will prove in a companion paper [ZSdlL14] that the solutions of (10) that satisfy the normalization (12) will be locally unique.

2.7. Diophantine condition. We will assume that \( \alpha \in \mathbb{R}^d \) is non-resonant, in the sense that

\[
\alpha \cdot k \neq 0 \quad \forall \, k \in \mathbb{Z}^d - \{0\}.
\]

We are interested in the frequency \( \omega \in \mathbb{R} \) such that (6) holds. Then, we can find a matrix \( B \in SL(d, \mathbb{Z}) \) as in (7) in such a way that \( \Omega \) satisfies Diophantine condition in \( \mathbb{R}^{d-1} \):

\[
|\hat{k} \cdot \Omega - m| \geq \nu |\hat{k}|^{-\tau} \quad \forall \, \hat{k} \in \mathbb{Z}^{d-1} - \{0\}, \, m \in \mathbb{Z}.
\]

Here \( \nu, \tau \) are positive numbers and we denote such set of \( \Omega \) by \( \mathcal{D}(\nu, \tau) \). We also denote \( \mathcal{D}(\tau) = \cup_{\nu > 0} \mathcal{D}(\nu, \tau) \).

In contrast with KAM theory, we will not need very delicate estimates on the solutions and hence, we can deal with very general Diophantine conditions. We will assume that \( \Omega \) satisfies

\[
\lim_{N \to \infty} \frac{1}{N} \max_{|\hat{k}| \leq N, m \in \mathbb{Z}} \ln |\hat{k} \cdot \Omega - m| = 0.
\]

Note that the condition (16) is much weaker than the usual Diophantine conditions and even than the Brjuno-Rüssmann conditions. The condition (16) is the natural condition in the study of existence of series to all orders.

3. Function spaces and linear estimates

The main tool that we will use to construct perturbation theories is the solution of cohomology equations.

We denote

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

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

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

These Banach spaces of analytic functions are the same spaces as in [Mos67].

### 3.0.1. Cohomology equations

We will consider equations of the form

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

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

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

for all $\eta$.

Assume that $\Omega$ satisfies the assumption (16).

Then, for a fixed $\eta$, there exists a unique solution $v_\eta$ of (17) which satisfies

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

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

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

Furthermore, any distribution solution of (17) 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

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

We note that, as it is well known that obtaining $v$ solving (17) 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

$$v(\psi, \eta) = \sum_{k \neq 0} \hat{v}_k(\eta)(e^{2\pi i k \cdot \Omega} - 1)^{-1}e^{2\pi i k \cdot \psi} = \sum_{k \neq 0, m} \hat{v}_{k,m}(e^{2\pi i k \cdot \Omega} - 1)^{-1}e^{2\pi i (k \cdot \psi + m \eta)}.$$
Using Cauchy estimates for the Fourier coefficients $|\hat{\phi}_{k,m}| \leq \exp(-2\pi \rho (|k| + |m|)) \|\phi\|_\rho$, and that $|e^{2\pi i k \cdot \Omega} - 1|^{-1} \leq C \text{dist}(k \cdot \Omega, \mathbb{Z})^{-1}$ and the assumption (16), we obtain that

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

In this paper, we will not pursue obtaining refined estimates for these solutions. This will be done in [ZSdlL14]. □

4. Lindstedt series for quasi-periodic solutions with resonant frequencies

The goal of this section is to study (10) perturbatively when the non-linear term is small. Hence, we will write (10) with a small parameter $\epsilon$

$$(20) \quad v(\psi + \Omega, \eta) + v(\psi - \Omega, \eta) - 2v(\psi, \eta) + \epsilon W((\psi, \eta) + \beta v(\psi, \eta)) + \lambda(\eta) = 0.$$  

We will find $v(\psi, \eta), \lambda(\eta)$ solving (20) and (12) in the sense of formal power series in $\epsilon$. 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 [ZSdlL14].

Since one possible goal is to solve $\lambda(\eta, \epsilon) = 0$ by implicit function theorem, as indicated in Section 4.1, it will be important for us to keep track of $\frac{\partial \lambda}{\partial \eta}(\eta, \epsilon)$ as well.

Following the standard perturbative procedure we will write

$$v = \sum_{n=0}^{\infty} \epsilon^n v^n,$$

$$\lambda = \sum_{n=0}^{\infty} \epsilon^n \lambda^n.$$  

Here $v^n$ and $\lambda^n$ are coefficients of $\epsilon^n$, not powers of $v$ or $\lambda$. Substitute (21) in (20) and equate powers of $\epsilon$.

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

Equating the coefficients of $\epsilon^0$ in (20) we obtain

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

Hence, if $\Omega$ satisfies the Diophantine condition (15) we see that $v^0$ is constant, $\lambda^0 = 0$ and imposing (12) we obtain $v^0 = 0$. 

□
Matching coefficients of $\epsilon^1$ in both sides of (20) we obtain
\begin{equation}
\psi^1(\psi + \Omega, \eta) + \psi^1(\psi - \Omega, \eta) - 2\psi^1(\psi, \eta) + \psi^1(\eta) + \lambda^1(\eta) = 0.
\end{equation}
We see that, using the theory in Section 3.0.1 to have analytic $\psi^1$ solving (23), it is necessary and sufficient to have
\begin{equation}
\lambda^1(\eta) = -\int_{\mathbb{T}^{d-1}} W(\psi, \eta) d\psi.
\end{equation}
Then, $\psi^1$, $\lambda^1$ can be determined uniquely up to a constant from (23). In fact, in Fourier series, the equation for $\psi^1$, $\lambda^1$ is
\begin{equation}
\nu^1_k 2(\cos(2\pi k \Omega) - 1) = -W_k - \delta_{0,k}\lambda^1,
\end{equation}
where $\delta_{0,k}$ is the Kronecker delta. In particular, the constant in $\psi^1$ is determined by the normalization (12).

Proceeding to higher order follows the same pattern. We see that matching the terms of order $\epsilon^n$ in (20) we obtain
\begin{equation}
\psi^n(\psi + \Omega, \eta) + \psi^n(\psi - \Omega, \eta) - 2\psi^n(\psi, \eta) + R^n(\psi, \eta) + \lambda^n(\eta) = 0,
\end{equation}
where $R^n$ is a polynomial expression in $\psi^1, \ldots, \psi^{n-1}$ with coefficients which are derivatives with respect to $\psi$ of $W((\psi, \eta) + \beta \nu(\psi, \eta))$. This polynomial can be computed explicitly because it is given by
\begin{equation}
R^N = \frac{1}{(N - 1)!} \frac{d^{N-1}}{de^{N-1}} W((\psi, \eta) + \beta \sum_{n=0}^{N-1} \nu^n(\psi, \eta)) \bigg|_{e=0}
\end{equation}
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” [Har11, BCH+06].

We have therefore established

**Lemma 2.** Assume that $\Omega \in \mathbb{D}(\nu, \tau)$ as defined in (15) and that $W: \mathbb{T}^d \to \mathbb{C}$ is an analytic function.

Then, we can find formal power series solutions in $\epsilon$ of the form (21) solving the equation (20).

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

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

4.1. **The auxiliary equation.** Now, we turn to the problem of studying the equation
\begin{equation}
\lambda(\eta, \epsilon) = 0.
\end{equation}
We expect to obtain a solution $\eta^*(\epsilon)$ provided that (28) satisfies some non-degeneracy conditions.
Having solution of (28) to order 1 in $\epsilon$, amounts to
$$\lambda^1(\eta) = 0.$$ That is, we need to find $\eta$ such that
$$\int_{\mathbb{T}^{d-1}} W((\psi, \eta) + \beta v(\psi, \eta))d\psi = 0. \tag{29}$$

**Proposition 2.** The equation (29) 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
$$\int_\mathbb{T} \int_{\mathbb{T}^{d-1}} W((\psi, \eta) + \beta v(\psi, \eta))d\eta d\psi = \int_{\mathbb{T}^{d}} (\partial_\alpha V)(B^{-1}(\psi, \eta) + \alpha v(\psi, \eta))d\psi d\eta = 0. \tag{30}$$

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, \ldots zeros. \hfill \square

Denote one of these solutions of (29) as $\eta^*$. A sufficient condition that ensures that we can solve the equation (28) to all orders is that
$$\frac{\partial}{\partial \eta} \lambda(\eta, \epsilon) \bigg|_{\eta = \eta^*, \epsilon = 0} \neq 0. \tag{31}$$

More explicitly,
$$\int_{\mathbb{T}^{d}} \frac{\partial}{\partial \eta} (\partial_\alpha V)(B^{-1}(\psi, \eta) + \alpha v(\psi, \eta))d\psi d\eta \neq 0. \tag{32}$$

Then, the implicit function theorem for power series \cite{Car95, Die71} 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

**Lemma 3.** Assume that $\Omega \in \mathcal{D}(\nu, \tau)$ as defined in (16), that $W$ is an analytic function, and that (32) holds, we can find formal power series $\eta_\epsilon$ in $\epsilon$ so that $v_{\eta_\epsilon}$ is the solution of (20).

Clearly, since the function $\lambda^\epsilon(\eta)$ 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 $\text{(32)}$ is far from being necessary and there are many other conditions that are enough.

**Lemma 4.** Assume that $\Omega \in \mathcal{D}(v, \tau)$ as defined in $\text{(15)}$, that $W((\psi, \eta) + \beta v(\psi, \eta))$ is an analytic function, and that $\text{(32)}$ holds.

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

$$\lambda^i(\eta^*) = 0, \quad i = 1, \ldots, 2m$$

$$\lambda^{2m+1}(\eta^*) \neq 0$$

Then, we can find formal power series $\eta_\varepsilon$ in $\varepsilon$ so that $v(\psi, \eta_\varepsilon)$ is the solution of $\text{(20)}$.

5. A dynamical interpretation of the equilibrium equations of Frenkel-Kontorova models

In this section, we present a dynamical interpretation of the equilibrium equations $\text{(3)}$ in Frenkel-Kontorova models.

This interpretation suggests several conjectures and methods of exploration. Nevertheless, we point out that the methods we have developed in this paper work also when the interactions have infinite range [SdlL12a] (see [dlL08, CdlL10b] for the periodic case). These infinite dimensional cases do not admit any dynamical interpretation.

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 $\text{(3)}$ into a dynamical system is setting

$$y_n = (x_n, x_{n-1})$$

$$y_{n+1} = (2y_n^1 - y_n^2 - \partial_\alpha V(\alpha y_n^1) - \lambda, y_n^1).$$

However, $\text{(34)}$ 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 (3) is equivalent to the system on $\mathbb{T}^d \times \mathbb{R}$

\[
\begin{align*}
p_{n+1} &= p_n - \partial_\alpha V(q_n) - \lambda \\
q_{n+1} &= q_n + \alpha p_{n+1},
\end{align*}
\]

(35)

where $q_n \in \mathbb{T}^d$, $p_n \in \mathbb{R}$. (Just multiply (3) by $\alpha$ and use the substitution $p_n = x_n - x_{n-1}$, $q_n = \alpha x_n$. Note that (3) 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.)

We will write the mapping (35) as

\[
(p_{n+1}, q_{n+1}) = F_{\varepsilon, \lambda}(p_n, q_n).
\]

(36)

Note that (35) is typographically very similar to the standard map [Chi79] or to analogues introduced for volume preserving maps. Nevertheless, there are significant differences (besides the different dimensions).

A very crucial difference between (36) and the generic volume preserving maps is that $q_{n+1} - q_n$ is always a multiple of $\alpha$ (see (35)). So that the two dimensional leaves

\[
\mathcal{M}_{q_0} = \{(p, q_0 + \alpha t) \mid p, t \in \mathbb{R}\}
\]

(37)

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

The mapping (35) clearly preserves the volume form $dp \wedge dq_1 \wedge \ldots \wedge dq_d$ since it is the composition of

\[
\begin{align*}
p_{n+1} &= p_n - \partial_\alpha V(q_n) - \lambda \\
q_{n+1} &= q_n
\end{align*}
\]

(38)

and

\[
\begin{align*}
p_{n+1} &= p_n \\
q_{n+1} &= q_n + \alpha p_{n+1}.
\end{align*}
\]

(39)

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

Indeed, (36) is an exact volume preserving map if and only if $\lambda = 0$, since it is easy to observe that, when $\lambda = 0$, both (38) and (39) are exact. To show that if $\lambda \neq 0$ then the mapping (36) is not exact is not very difficult and is done in detail, e.g., in [FdlL15].

When $\varepsilon = 0$, $\lambda = 0$, the map (35) is integrable. That is, the codimension-one tori given by $p = \text{cte.}$ are invariant and the motion in them survives. We call any codimension-one torus homotopic to these tori, a rotational torus.
It is easy to show that if a volume preserving map preserves a rotational torus then it is exact (see [BdlL13b]). (The converse, of course, is not true). This small remark, reproduces for the models in (35) the results of Lemma 5 in [SdlL12b]. This is remarkable because Lemma 5 in [SdlL12b] has a very different proof, which applies also to models with long range interactions whose equilibrium equations cannot be transformed into a map of the form (35). The existence of rotational tori with Diophantine frequencies for mappings close to integrable has been established by KAM theory [CS90a, CS90b, Xia92, Yoc92] for general volume preserving maps.

Nevertheless, the KAM theory developed in [SdlL12b] is very different from the KAM theory for general volume preserving maps. For volume preserving maps of general form, one does not expect the persistence of \(d\)-dimensional tori with a fixed frequency under general volume preserving perturbations, and so one needs to adjust parameters. In contrast, the papers [SdlL12b, SdlL12a] do not need to adjust parameters. This can be explained by observing that the constraints (37), make the mappings (35) very non-generic.

Similarly, the results of this paper (preservations of tori without any normal hyperbolicity) are not to be expected in the generic volume preserving case without adjustment of more parameters.

5.1. **On the global geometry of the constraints given by (37).** 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 [Sou97, Aud08, Hol11].

The constraints (37) 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 [Mey73, MW74, MW01] cannot be applied to (35).

5.2. **Lyapunov exponents and phonon localization.** In this section we study the so called phonon gap around the equilibria of (9) 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

\[
\ddot{\xi}_n = \xi_{n+1} + \xi_{n-1} - 2\xi_n + (\partial_\alpha)^2 V(\alpha x_n) \xi_n \equiv (L_x \xi)_n.
\]

It is clear that the propagation properties of sound waves will be affected by the spectral properties of the operator \( L_x \).

Note that the operator \( L \) 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 [PF92, dILH10]. 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 [AMB92].

In the case of (35), we can study the Lyapunov spectra for any orbit using the geometric constraints (37).

**Proposition 3.** Let \( x_n \) be an orbit of the mapping given by (35). Assume that Oseledets 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 (36).

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. \( \square \)

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