FAST NUMERICAL COMPUTATION OF QUASI-PERIODIC EQUILIBRIUM STATES IN 1-D STATISTICAL MECHANICS, INCLUDING TWIST MAPS

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

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

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

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

We argue that the method presented here gives a method, independent of other previous methods to compute the breakdowns. We use this method to explore the analyticity breakdown in some Frenkel-Kontorova models with extended interactions. In some ranges of parameters, we find that the breakdown presents scaling relations that, up to the accuracy of our calculations are the same as those for the standard map.

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

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Contents

1. Introduction

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

The class of models we consider (described in Section 2) is very general. The models we consider include as a particular case twist mappings of an annulus. In this case, the equilibrium states of the statistical mechanics model are orbits of the map. Hence our algorithm includes, as particular cases, the computation of KAM tori for twist maps. The computation of KAM tori for twist mappings has been studied extensively in [Mac82, Mac83, CC98, Per74, KM89, ALD83]. Other particular cases of the models considered are the Frenkel-Kontorova models of deposition of materials and of dislocations [ALD83, BK04], as well as some long range variants [CDLFM07], the XY models of magnetism and their long range variants [Mat06, BB07], models of spin waves, and monotone recurrences [Ang90].

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

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

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

These quasi-periodic equilibrium configurations have been extensively studied in twist mappings and Frenkel-Kontorova models. In particular, we call attention to [ALD83]. In that paper, it is showed that many important physical properties of the materials described by a Frenkel-Kontorova model depend on whether the function h is analytic or has discontinuities. Both alternatives happen for different values of the parameter of the model which are, apparently arbitrarily close. A great deal of effort has been devoted understanding this *breakdown of analyticity transition.* For the case of nearest neighbor interactions, this breakdown of analyticity is equivalent to the problem of breakdown of KAM tori and the onset of large scale stochasticity. See [Mei92, MF94] for reviews written with two different viewpoints.

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

The main strategy is that we derive a functional equation for h which is equivalent to the fact that the configuration $x_i = h(\omega i)$ is in equilibrium and then consider Newton methods for this equation. Since

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

We include a discussion of an implementation of the large matrix method in 3.1. This serves as a comparison with the more efficient methods which are the main novelty of this paper. Perhaps more importantly, we note that the large matrix method can be used to study models with rather long range interactions. These long-range models are somewhat similar to the hierarchical models of [Dys71], which experiment phase transitions even if they are one-dimensional. We find empirically that the large matrix method does not have any difficulty finding invariant tori. We call attention to the fact that there is no rigorous study of the existence of quasi-periodic solutions in these very long-range models.

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

Of course, even if Newton methods lead to very accurate solutions, they require rather good initial guesses. We have two alternatives: The first one is to use a continuation method from an integrable case [AG03], roughly, starting from the integrable case, whose solutions are known, we use the accurate solutions of for some parameters as initial approximations for the computation of solutions of a slightly different parameter.

A second alternative, in the models considered are ferromagnetic (or twist in the language of dynamical systems), comes from the fact that the quasi-periodic equilibria are minimizers of a variational principle which we develop in section 2.5. In these cases, we compute the minimizer using a minimization algorithm and then, polish the computation using the Newton method.

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

We also note that the computations presented here are backed by rigorous results. In [dlL08] it is shown that, given one approximate solution of the equilibrium equations, if the solution is approximate enough compared with some quality numbers computable out of the approximate solution (some non-degeneracy assumptions and some appropriate norms of the approximate solution) then, there is a true solution close to the approximate solution. Furthermore, the solution is unique in a small neighborhood.

As a first application of the method, in Section 5, we undertake a study of breakdown of analyticity transition. This transition is of great importance for the applications of the models. Since the analyticity of not of the quasi-periodic solutions determines several physical properties such as stickiness (in the Frenkel-Kontorova model) or global transport (in twist-maps).

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

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

As a byproduct of the validation of the calculations, we obtain a direct way to compute the analyticity transition. As we approach the breakdown of the analytic solutions, the norms of the function have to blow up. This gives a criterion for the breakdown of analyticity which is independent of the criterion of [Gre79] and which is applicable to extended models.

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

The scaling behavior found in these models is, up to the error of the computations reported here, is very similar to the scaling exponents found in twist mappings [Mac82, Mac83, Koc04]. Since some of the models studied here cannot be interpreted as a dynamical systems, this suggests that there should be formulations of renormalization group for models of statistical models which are not dynamical systems.

Remark 1.1. The speedup of the methods presented here comes from several identities that are derived from the variational structure of the models. This is very different from other recent algorithms for Hamiltonian systems [HdlLS08]. The algorithms presented in this paper apply for systems that do not have an interpretation as a dynamical system – much less as a Hamiltonian one –. On the other hand, the algorithms of [HdlLS08] apply to systems such as non-twist mappings that have a Hamiltonian structure but not a variational one.

Remark 1.2. In the case that the interactions satisfy some convexity properties – which are not needed by the KAM method – there are variational methods that allow to produce quasi-periodic solutions. In the case of nearest neighbor interactions, this is the celebrated Aubry-Mather theory [Mat82, Mat86, MF94, ALD83]. Extensions to systems with long range interactions (and to higher dimensional lattices, and existence of other multiple critical points) were obtained in [Ang90, CdlL98, dlLV07b, dlLV07a],

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

2. Statistical mechanics models in 1-D and their equilibrium configurations

We will consider one dimensional systems. At each integer, there is one site, whose state is described by one real variable. Hence, the configuration of the system is characterized by giving a sequence of real values (equivalently a function $x : \mathbb{Z} \to \mathbb{R}$).

As is standard in Statistical Mechanics, [Rue99] the interaction among the particles of the system is described by assigning an energy to each finite subset of sites. The total energy of a configuration of the system is the sum of all the possible energies. As it is well known, this sum is purely formal, but there are well defined ways of making sense of several quantities of interest.

We will assume that:

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

$$\mathcal{S}(\{x_n\}) = \sum_{L\in\mathbb{N}} \sum_{k\in\mathbb{Z}} H_L(x_k, ..., x_{k+L}) \tag{1}$$

(H2) The following periodicity condition holds.

$$H_L(x_k, ..., x_{k+L}) = H_L(x_k + 1, \dots, x_{k+L} + 1) \tag{2}$$

The property (2) is a rather weak periodicity condition. It is implied by the stronger property

$$H_L(x_k, ..., x_{k+L}) = H_L(x_k + \ell_0, \dots, x_{k+L} + \ell_L) \tag{3}$$

for all $\ell_i \in \mathbb{Z}$. The latter property (3) is natural when the variables x_i are angles. For example, spin variables. The weaker property (2) has appeared in many situations. It is natural when considering twist maps of the annulus [MF94] or monotone recurrences [Ang90].

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

The paper [dlL08] contains a precise formulation of decay conditions which leads to a rigorous theorem. Even if it is clear that some decay is needed (e.g. to make sense of the equilibrium equations (6)), we prefer to omit a precise statement Indeed, in section 3.1 we consider models which do not satisfy the conditions of [dlL08] and find that some numerical methods work well. We think that this deserves future investigation.

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

2.1. **Some examples of models.** Models of the form (1) include as particular cases, several models which have been proposed in the literature and which are worth to keep in mind.

- The Frenkel-Kontorova model corresponds to taking $H_0(t) = \lambda V(t)$, where λ is an arbitrary coupling constant and $V(t)$ is periodic function – a popular one is $V(\theta) = -\frac{\varepsilon}{4\pi^2}\cos(2\pi\theta)$, $H_1(x, y) = \frac{1}{2}|x - y - a|^2$, and $H_L \equiv 0$ for $L \geq 2$. This models have appeared in many context is physics (e.g. as models of deposition [ALD83], models of dislocations [FK39]), and in dynamical systems as twist maps, [Mei92, MF94].

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

  An interesting toy model which we refer as the extended Frenkel-Kontorova model (see Section 4.2) corresponds to taking H_0, H_1 as above, but we take, for $k \geq 2$

$$H_k(x_0, \dots, x_k) = \frac{A_k}{2}(x_0 - x_k)^2 \tag{4}$$

  One case, that we will consider later is $A_k = ak^{-\alpha}$, $k \geq 2$. These models are very similar to the hierarchical models of [Dys71].
- The XY model of magnetism corresponds to taking $H_0(t) = B\cos(2\pi t)$, where B is the external magnetic field. $H_1(x, y) = J\cos(2\pi(x - y))$ and $H_L \equiv 0$ for $L \geq 2$. The physical meaning of the x in the XY model that $S = (\cos(2\pi x), \sin(2\pi x))$ is the spin variable at site i.

  Note that in the Heisenberg models it is very natural to consider interactions with longer range since the spin interactions extend for several sites. Indeed [BB07, p. 600] considers adding terms of the form $a_k s_i \cdot s_{i+k}$, $b_k(s_i \cdot s_{i+k})^2$, $c_{j,k,l}[(s_i \cdot s_{i+j}) \cdot (s_{i+k} \cdot s_{i+l}) + (s_{i+j} \cdot s_{i+k}) \cdot (s_{i+k} \cdot s_i) - (s_i \cdot s_{i+k}) \cdot (s_{i+j} \cdot s_{i+l})$. The coefficients a, b, c above are expected to decrease exponentially, Computations of these coefficients are discussed in [RS63]. Models including these terms fit well into the models discussed in this paper.
- In Dynamical Systems, models of the form (1) appear as variational principles for twist mappings (again $H_L \equiv 0$ for $L \geq 2$). In this case, the physical meaning of $\mathcal{S}$ is an action. Under the assumption that $\partial_1\partial_2 H_1(x, y) \leq -c < 0$, the critical points of the action are the orbits of a twist map.
- In [Ang90], one can find a discussion of monotone recurrences. The models that can be considering as dynamical systems are finite range. Hence we can just consider that $H_L \equiv 0$ for $L \neq R$. The monotonicity comes from $\partial_i\partial_j H_J \leq 0$ for $i \neq j$, and $\partial_i\partial_{i+1} H_L \leq C < 0$. One good example of monotone recurrences is the equilibrium equation of the Extended Frenkel-Kontorova model.

  For certain choices of A_k in (4) (in particular, $A_k = 0$ for $k > R$), the equilibrium equations of this model appear as multi-step order $2R$ integration methods for ODE's.

2.2. The equilibrium equations.

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

$$\partial_{x_i} \mathcal{S}(\{x_n\}) = 0 \tag{5}$$

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

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

For models of the form (1) the Euler-Lagrange equations are:

$$\sum_{L\in\mathbb{N}} \sum_{j=0}^{L} \partial_j H_L(x_{k-j}, ..., x_{k-j+L}) = 0 \quad \forall k \in \mathbb{Z} \tag{6}$$

We call attention that, in contrast with the sums defining $\mathcal{S}$ which are merely formal, the sums involved in equilibrium equations (6) are meant to converge.

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

$$\begin{aligned} &x_{i+1} + x_{i-1} - 2x_i + \lambda V'(x_i) = 0 \\ &\sum_{k=1} A_k(x_{i+k} + x_{i-k} - 2x_i) + \lambda V'(x_i) = 0 \\ &J\left[\sin(2\pi(x_{i+1} - x_i)) - \sin(2\pi(x_i - x_{i-1}))\right] + B\sin(2\pi x_i) = 0 \end{aligned} \tag{7}$$

Remark 2.1. The equilibrium equations can be considered as a dynamical systems but this point of view has limitations.

The equation of equilibrium for the Frenkel-Kontorova model can be considered as a dynamical system in 2 dimensions. It suffices to consider the state of the system given by (x_i, x_{i-1}). Then, the equations (7), allow to determine (x_{i+1}, x_i). Indeed, this dynamical system is the well known area preserving standard map.

In the extended FK model, when $A_k = 0 \; j > R$, We can also consider it as a dynamical system in $2R$ dimensional space. It suffices to consider the state of a system given by $(x_{i+R-1}, \dots, x_{i-R})$. Then, the equilibrium equations (7), allow to determine the next state. This is a symplectic dynamical system [Ves91]. Note however that, changing A_{R+1} from zero to a small quantity, even if a small perturbation from the physical point of view, and from the point of veiw of the formalism discussed here, is a very drastic perturbation from the dynamical systems point of view. This arbitrarily small changes even change the dimension of the phase space. Some of the terms in the evolution include factors $1/A_{R+1}$.

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

For the XY model, if we want to consider (7) as defining a dynamical system, we need to extricate x_{i+1} from the equilibrium equations. This requires that $|\sin(2\pi(x_i - x_{i-1})) - B/J \sin(2\pi x_i)| < 1$. Unfortunately, this condition is not invariant under the dynamical system so that the nature of the phase space of this system is rather problematic and certainly dependes on the parameters.

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

$$x_n = h(n\omega) \tag{8}$$

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

$$h(x + e) = h(x) + e \quad \forall e \in \mathbb{Z} \tag{9}$$

and is analytic.

The function h is often called the *hull function*. The periodicity condition (9) means that h can be considered as a map of the circle to itself. We will use the notation

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

Were u is a periodic function.

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

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

$$|q\omega - p| \geq \kappa |q|^{-\tau} \qquad \forall p \in \mathbb{Z} - \{0\}, \quad q \in \mathbb{Z} \tag{10}$$

2.4. **Equilibrium equations in terms of hull functions.** For configurations of the form (8), the equilibrium equations become:

$$\begin{aligned} E[u](\theta) \equiv \sum_L \sum_{j=0}^{L} \partial_j H_L(\theta - j\omega + u(\theta - j\omega), \dots, \\ \theta + u(\theta), \dots, \theta + (L-j)\omega + u(\theta + (L-j)\omega)) \\ =0 \end{aligned} \tag{11}$$

2.5. **Percival Variational Principle.** It is easy to see that (11) is the Euler-Lagrange equation associated to the functional $\mathcal{P}$ given by the expression

$$\mathcal{P}[u] = \int_0^1 \sum_L \frac{1}{L} H_L(\theta + u(\theta), ..., \theta + L\omega + u(\theta + L\omega)). \tag{12}$$

This is an extension to the functional introduced in [Per74, Per79].

In the case that $\mathcal{P}$ satisfies some convexity properties, implied by the ferromagnetism (or the twist), the minimizers of the problem satisfy very interesting properties [Mat82, ALD83] and, in particular, they will be described by a hull function. Unfrotunately, the regularity of the minimizer may depend on the parameter.

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

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

3. Algorithms for the solution of equilibrium solutions for hull functions

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

3.1. **Straightforward Newton method.** The Newton step consists in, given u, replace it by $u+v$ where v satisfies the equation

$$E'[u]v(\theta) = -E[u](\theta). \tag{13}$$

The numerical Newton method consists in discretizing (13). If we discretize functions using N Fourier modes, $E'[u]$ is an $N \times N$ matrix. We note that $E'[u]$ is typically a dense matrix so its inversion can be performed with $O(N^3)$ operations and its storage is $O(N^2)$.

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

3.2. **Quasi-Newton method.** The Quasi-Newton method is based in the algorithms developed in [dlL08]. Given u, the improved solution is $u+v$ where v is obtained solving

$$h'(\theta)(E'[u]v)(\theta) - v(\theta)(E'[u]h')(\theta) = -h'(\theta)E[u](\theta). \tag{14}$$

Note that the equation (14) differs from the Newton step equation (13) by the term $v(\theta)(E'[u]h')(\theta)$. Using the identity

$$\frac{d}{d\theta}E[u](\theta) = E'[u]h'(\theta) \tag{15}$$

we see that (13) and (14) differ by a term whose norm can be controlled by $||E||\,||v|| \approx ||E||^2$. Hence, the iterative method based on solving (14) will also be quadratically convergent.

The advantage of (14) comes from the fact that it can can be solved very efficiently because the left hand side can be factored into a sequence of simple operators. For a detailed exposition of this factorization and estimates we refer the reader to [dlL08]. Here we summarize what we need.

Introducing the operator

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

and the new variable w related to v by $v(\theta) = h'(\theta)w(\theta)$, the equation (14) transforms into:

$$\Delta_1[(\mathcal{C}_{0,1,1} + \mathcal{G})\Delta_{-1}w] = -h'E[u]. \tag{16}$$

where

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

with

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

and

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

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

$$\varphi(\theta \pm \omega) - \varphi(\theta) = \eta(\theta) \tag{17}$$

The equation(17) can be solved observing that the operators $\Delta_{\pm 1}$ are diagonal in Fourier space. Indeed, the solution is given by:

$$\hat{\varphi}_k = \hat{\eta}_k / (\exp(\pm 2\pi i \omega k) - 1), \quad k \neq 0 \tag{18}$$

The average of φ, $\hat{\varphi}_0$ is arbitrary. The equation (17) and its solution (18) are very standard in KAM theory. Very detailed estimates can be found in [Rüs75] when ω is Diophantine, which is our hypothesis (H4). See also the exposition in [dlL01].

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

Thus, equation (16) can be solved following the next algorithm:

Algorithm 3.1. *1) Check that $\int_{\mathbb{T}} h' E[u] = 0$.*

Note that (15) *guarantees that this would be true if the evaluation was exact. Hence, the average gives a measure of the numerical error.*

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

$$\Delta_1 \varphi = -h' E[u] \tag{19}$$

Therefore, if φ is a solution for (19) *then for any $\mathcal{T} \in \mathbb{R}$ the equation $\Delta_1(\varphi + \mathcal{T}) = h'E[u]$ holds. In particular, we choose $\mathcal{T}$ such that*

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

3) We solve for w from

$$\Delta_{-1} w = (\mathcal{C} + \mathcal{G})^{-1} (\varphi + \mathcal{T}) \tag{20}$$

4) Finally we obtain the improved solution

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

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

We call attention that all teh steps are diagonal either in Fourier space or in real space. The steps in Algorithm 3.1 are of the following form:

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

$$\text{Find } \varphi(\theta) \text{ so that } \int_{\mathbb{T}} \varphi \, d\theta = 0 \text{ and } \Delta_{\pm 1}\varphi = \eta_{\pm}. \tag{21}$$

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

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

$$(\mathcal{C}_{0,1,1} + \mathcal{G})^{-1} = \left(\sum_{n \geq 0} (-\mathcal{C}_{0,1,1}^{-1} \circ \mathcal{G})^n \right) \circ \mathcal{C}_{0,1,1}^{-1} \tag{22}$$

  This gives an initial guess for a Conjugate Gradient (CGNE) method [Saa03]. Since these operators are diagonal in real space then the inversion can be performed in $O(N)$ operations once we have computed the operators. In fact, the main cost of the complete inversion procedure lies in the computation of the elements of $\mathcal{C}_{0,1,1}$ and $\mathcal{G}$.

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

$$f(\theta) = \sum_{k=-N}^{N} \hat{f}_k e^{2\pi i k \theta} \tag{23}$$

$$\hat{f}_k = \bar{\hat{f}}_{-k}. \tag{24}$$

where (24) comes from the fact that f is real on the real axis. Then, it is clear that we can store a f using either $N+1$ coefficients of the Fourier series or the values of f on a grid of $2N-1$ points.

As we discussed in section 3.2, the Newton methods involve some operators that are diagonal in Fourier Spaces (i.e., shifts, sums) and some that are diagonal in real space (i.e., sums, products, divisions, composition with transcendental functions, etc.). Therefore, sometimes it will be convenient to store a periodic function as $N+1$ Fourier coefficients, and sometimes as values on a grid of $2N-1$ points. An alternative to storing the values on a grid could be to compute the operations between periodic functions directly from the Fourier series as described in the next section.

In Sections 3.3.2,3.3.3, we discuss the operation count and storage cost of implementations using just Fourier series discretizations and in Section 3.3.4 we discuss the same issues for discretization on Fourier coefficient/grid. The accuracy and numerical stability will be discussed empirically in Section 3.5.

3.3.1. *Sobolev norms.* We define

$$\|f\|_{H^r} = \|D^r f\|_{L^2}. \tag{25}$$

Note that (25) is a norm on a space of periodic functions with zero average, which is the only case we will consider.

This norm can also be computed by

$$\|f\|_{H^r} = \left(\sum_{k \geq 0} (2\pi k)^r |f_k|^2 \right)^{\frac{1}{2}}. \tag{26}$$

Renormalization techniques (see section 5.3) will make clear that values of r greater than 3 will have to be taken into consideration when we perform computations. Different methods of computation were tested since the H^r norm (26) tends to be sensitive to round-off error in the higher frequency terms (see section 3.5). Note that (26) makes sense even if r is not an integer.

3.3.2. *Algebraic operations by manipulating Fourier coefficients.* Elementary algebraic function (sum, product and product by scalar) can be implemented using formulas for the coefficients of the result in terms of the coefficients of each of the terms. Of course, addition and subtraction are trivial, multiplication can be computed using Cauchy formula.

$$\widehat{(uv)}_k = \sum_j \hat{u}_j \hat{v}_{k-j} \tag{27}$$

Note that the straightforward implementation of (27) requires $O(N^2)$ operations. From the practical point of view, evaluations of sums such as (27) are very well optimized for almost any computer in the `cdot` function of the BLAS library.

The book [Knu81, p. 525–533] contains several groupings of (27) whose operation count is $O(N^\alpha)$ for some $\alpha < 2$. We will not consider these operations in these paper.

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

3.3.3. *Computation of the elementary transcendental functions by manipulation of Fourier coefficients.* One first idea to compute transcendental functions of a Fourier series is to use a Taylor expansion and the duplication formulas. In [Knu81], one can find an alternative that is more efficient and is also useful in the computation of Lindstedt series. Let us briefly discuss the method for the exponential and refer to [Knu81] for more details.

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

$$(n+1)E_{n+1} = \sum_{k=0}^{n}(k+1)P_{k+1}E_{n-k} \tag{28}$$

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

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

Recursion formulas in [Knu81, p. 418-514] allow us to compute sin, cos, exp of Fourier series in $O(N^2)$ steps by just manipulating Fourier series.

3.3.4. *Using Fast Fourier Transforms (FFT).* The fastest algorithm for performing algebraic operations or compositions of transcendental functions is the FFT method. We perform this operations by applying inverse FFT to our coefficients, computing the function on each grid point in real space, and the applying inverse FFT. This procedure has a cost of $O(N \log N)$. Therefore, a straightforward implementation of Algorithm 3.1 takes $O(N \log N)$ operations.

Another advantage of the FFT method is that the interactions between particles do not have to be given in terms of transcendental functions. As long as we have a method for computing the interactions in a grid of equally spaced points in the torus we can perform FFT. One algorithm that also deserves further exploration is the algorithm USFFT that can perform Fourier transforms in non-equally spaced grids [AD96, DR93]. This seems quite promising for the cases in which the function is rather differentiable.

3.4. **The efficiency of Algorithm 3.1.** Besides the operations discussed in the above section, we note that shifts, computations of derivatives and solutions of difference equations are $O(N)$ in Fourier space.

We conclude that it is possible to implement Algorithm 3.1 using only discretizations in N Fourier terms and manipulating Fourier coefficients (or using FFT to compute the derivatives).

We also note that keeping Fourier series discretizations, the storage required for Algorithm 3.1 is only $O(N)$.

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

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

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

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

$$B_n(\theta) = \frac{1}{(2\pi i)^n} \sum_{k \in \mathbb{Z} - \{0\}} \frac{1}{n^k} e^{2\pi i k\theta} \tag{29}$$

The functions B_n admit closed form expressions and their product satisfy identities (see [AS64]) we can test. Note that, by changing n, we can use B_n as models of functions with different regularities.

A remark about Newton methods. One very crucial point for our discussion is that the accuracy of the final result of a Newton method depends only on the accuracy of the evaluation of the functional equation. Provided that the iterative procedure is sensible, it will converge to an approximate solution which will solve the functional equation up to an accuracy comparable to the accuracy of the evaluation. We note

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

TABLE 1. H^r semi-norms for the error of the product of Bernoulli polynomials $B_n(\theta)B_4(\theta)$ using the Cauchy formula with 1500 coefficients.

that the rigorous results in [dlL08] show that (provided that the approximate solutions satisfy some non-degeneracy assumptions), there are true solutions.

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

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

$$B_n(\theta)B_m(\theta) = \sum_{k=0}^{n+m} \Gamma^k_{n,m} B_k(\theta). \tag{30}$$

in different Sobolev norms.

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

The conclusion that we obtain is that the direct Cauchy formula (27) gives results which are moderately more precise (a factor 2 or 3) than the FFT when the functions are moderately smooth.

An easy improvement of the FFT multiplication is

- Shift the polynomials by $1/2N$ which can be done multiplying the Fourier coefficients by an appropriate phase.
- Evaluate both in real space, so that we obtain the polynomials evaluated at $2N$ points in real space.
- Multiply them to obtain the product in $2N$ points.
- Compute the FFT to obtain $2N$ coefficients of the product
- Truncate up to order N.

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

Composition with elementary functions. The FFT method of computing $\sin(f), \cos(f), \exp(f)$ is just to evaluate the function on a grid, evaluate the function and then, compute the Fourier transform of the resulting grid of points.

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

TABLE 2. H^r semi-norms for the error of the product of Bernoulli polynomials $B_n(\theta)B_4(\theta)$ using the FFTW.

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

TABLE 3. H^r norm of the difference between the approximated composition $f\widetilde{(B_n(\theta))}$ and the exact formula $f(B_n(\theta))$ for $f = \sin, \cos, \& \exp$.

The alternative we compare with is the use of recursive formulas involving Fourier coefficients to compute the exponential and trigonometric functions discussed in [Knu81, p. 525-533].

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

4. NUMERICAL RESULTS ON THE COMPUTATION OF QUASI-PERIODIC EQUILIBRIA ON SEVERAL MODELS

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

4.1. **The XY model.** In the XY model x_i are angles describing the orientation of a spin $s_i = (\cos(2\pi x_i), \sin(2\pi x_i))$. The interaction that we consider in this model are interactions with an external field ($B = (\frac{\lambda}{2\pi}, 0)$) and exchange interactions between nearest neighbors. Since the meaning of the interactions are exchange interactions, it makes sense to consider terms which are not just nearest neighbor or, indeed that they are not just two body interactions. See, for example [BB07, p. 600].

The Euler-Lagrange equations for u are:

$$\begin{aligned} E[u](\theta) \;=\; & \sin(2\pi(\omega + u(\theta+\omega) - u(\theta)) \\ & - \sin(2\pi(\omega + u(\theta) - u(\theta-\omega))) \\ & -\tfrac{\lambda}{2\pi}\sin(2\pi(\theta + u(\theta))) = 0 \end{aligned} \tag{31}$$

The nearest neighbor interaction operator $\mathcal{C}_{0,1,1}$ appearing in Algorithm 3.1 is a multiplication operator given by

$$\mathcal{C}_{0,1,1}\eta(\theta) = -\cos(2\pi(\omega + u(\theta) - u(\theta-\omega)))h'(\theta-\omega)h'(\theta)\eta(\theta). \tag{32}$$

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

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

We show some of the $u(\theta) = h(\theta) - \theta$ obtained by the continuation method in figure 1.

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

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

It is not hard to show that the solutions of the invariance equations for the Heisenberg model are odd. Therefore, the Fourier coefficients

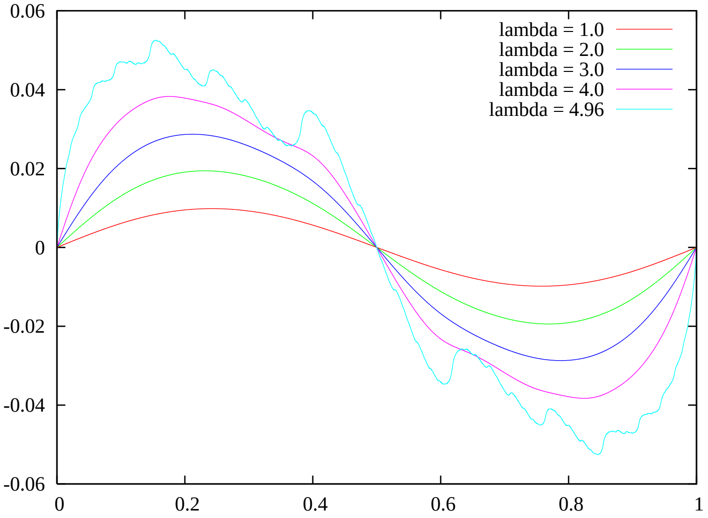

FIGURE 1. $u(\theta)$ for some values of λ.

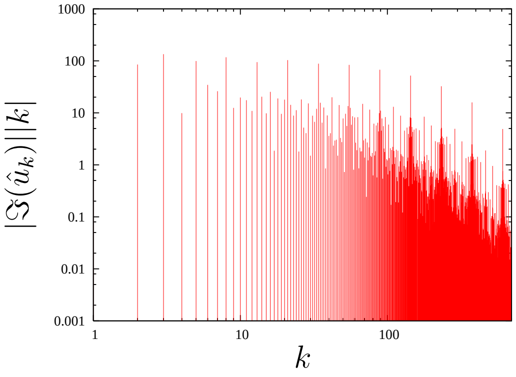

FIGURE 2. Natural logarithm of $\hat{u}_k$ versus the subindex k for $\lambda = 4.97$ in model (31).

will be purely imaginary. This is not built in in the algorithms we use, so that the size of the real part of the Fourier coefficients gives an indication of the effect of the round off and truncation error.

We note in particular that the plot of $\log |\hat{u}_k| k$ as a function of $\log k$ is roughly periodic for several decades. This is the standard signature of scalings that has been found in many critical problems in dynamical systems. For example in [Shr84, dlLP02]. Some more details on scaling behaviors at the breakdown of some of these models will be reported later.

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

$$\mathcal{S}(\{x_n\}) = \sum_i \frac{1}{2}(x_i - x_{i+1} - a)^2 + \sum_{k\geq 2} \frac{A_k}{2} \sum_i (x_i - x_{i+k} - b_k)^2 + \sum_i V(x_i) \tag{33}$$

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

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

4.2.1. *The Frenkel-Kontorova model with first and second nearest neighbor interactions.* We consider first and second nearest neighbor interactions. We then the equilibrium equation becomes

$$2x_i - x_{i+1} - x_{i-1} + A(2x_i - x_{i+2} - x_{i-2}) + V'(x_i) = 0 \tag{34}$$

where the potential is given by the expression

$$V(\theta) = -\frac{\varepsilon}{4\pi^2}\cos(2\pi\theta) \tag{35}$$

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

$$\mathcal{P}[h] = \int_0^1 \frac{1}{2}(h(\theta) - h(\theta+\omega))^2 + \frac{A}{2}(h(\theta) - h(\theta+2\omega))^2 + V(h(\theta))d\theta \tag{36}$$

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

$$\begin{aligned} \mathcal{P}[u] = \int_0^1 \frac{1}{2}(u(\theta) - u(\theta+\omega))^2 + \frac{A}{2}(u(\theta) - u(\theta+2\omega))^2 d\theta \\ + \int_0^1 V(\theta + u(\theta))d\theta \end{aligned} \tag{37}$$

We are looking for a periodic function u that minimizes (37). Using Parseval's identity we can write the minimization problem in the following form

$$\min_{u\in\mathcal{A}_\rho}\left[\sum_{k\in\mathbb{Z}}\left[(1-\cos(2\pi k\omega))+A(1-\cos(2\pi k2\omega))\right]|\hat{u}_k|^2 + \int_0^1 V(\theta+u(\theta))d\theta\right]. \tag{38}$$

Problem (38) can be solved numerically by truncating the Fourier coefficients and minimizing the resulting functional. We implemented this method for ω equal to the golden mean. In figure 3, we plot the minimizers for $\varepsilon = 0.97$ since this value is close to the breakdown of analyticity computed by Greene [Gre79]. We notice that as we move A away from zero the solutions appear to be more regular for this particular value of ε. This behavior can be understood by observing the decay of the Fourier Series of the minimizers. In the section 5, we give a description of this phenomenon.

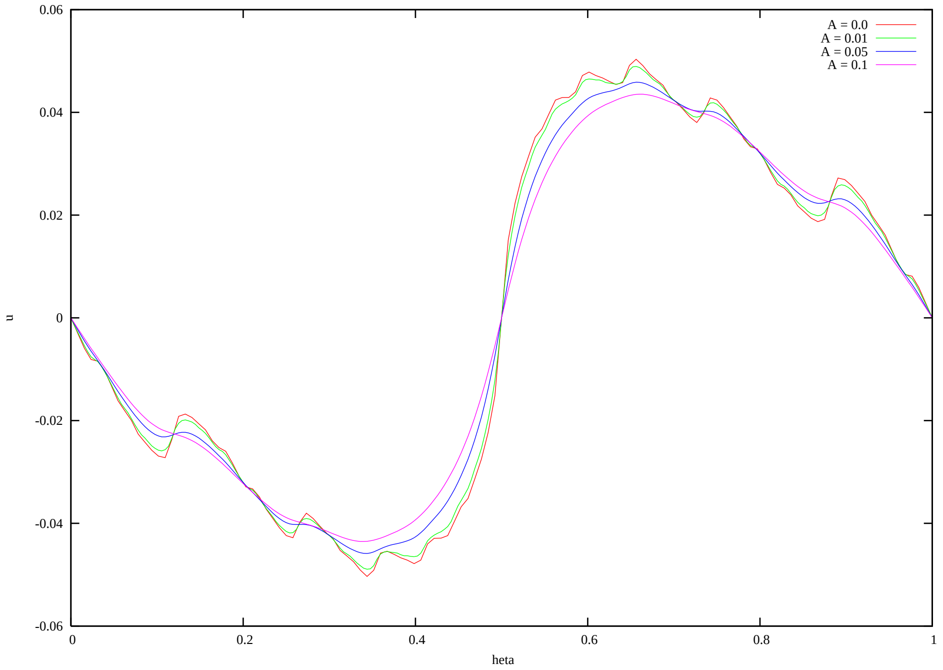

FIGURE 3. Minimizer $u(\theta)$ for $\varepsilon = 0.97$ and different values of A.

The quasi-Newton method. For the case of the extended F-K model in equation (16) the operators $\mathcal{C}$ and $\mathcal{G}$ simplify to

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

and

$$\mathcal{G}\eta(\theta) = -A\left(\Delta_1^{-1}\Delta_2\left[h'(\theta-2\omega)h'(\theta)\Delta_{-2}\Delta_{-1}^{-1}\eta(\theta)\right]\right). \tag{39}$$

We note also that as pointed out in [dlL08], the operators $\Delta_{-2}\Delta_{-1}^{-1}$ and $\Delta_1^{-1}\Delta_2$ are easy to compute since

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

and

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

These computations show that the operators $\mathcal{C}$ and $\mathcal{G}$ are readily computable numerically in this case. The inverse is then obtained computing a few terms of the Neumann series of $(\mathcal{C}+\mathcal{G})^{-1}$ and using the resulting function as a first guess for a Conjugate Gradient iterative method. We have used the CGNE algorithm (see [Saa03, p. 238-240]). This algorithm also allows us to minimize an H^r semi-norm with predetermined r as we iterate. The semi-norms we choose to minimize will be justified when we discuss the renormalization of the system in section 5.3.

4.2.2. *The Frenkel-Kontorova model with long-range interactions.* We consider the equilibrum equations for hull functions of the models. Hence, we consider

$$E[u] \equiv \sum_{k=1} A_k[u(\theta+k\omega)+u(\theta-k\omega)-2u(\theta)] + \lambda V'(\theta+u(\theta)) = 0 \tag{40}$$

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

$$E'[u]\eta(\theta) = \sum_{k=1} A_k[\eta(\theta+k\omega)+\eta(\theta-k\omega)-2\eta(\theta)] + V''(\theta+u(\theta))\eta(\theta) \tag{41}$$

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

$$M^d_{ii} = \sum_{k=1} 2A_k(\cos(\omega ik) - 1) \tag{42}$$

The matrix of the multiplication by a function U can be read off the Cauchy formula, (27),

$$M^m_{i,j} = \widehat{U}_{i-j} \tag{43}$$

Notice that M^d_{ii}, the coefficients of the difference operator are independent of the function u so that they can be precomputed once and for all for the algorithm. Indeed, in the case that $A_k = k^\alpha$, whith α integer, these coefficients can be computed explicitly (in the case α even, they agree with the Bernoulli polynomials introduced (29)). For example, in the case $\alpha = 2$, which is the one that we use to illustrate the results the small divisors in the diagonal part, are given by

$$\sum_{k=1}^{\infty} k^{-2}(\cos(2\pi k\theta) - 1) = \frac{\pi^2}{2}\left(\frac{1}{4} - (\theta - 0.5)^2\right) \tag{44}$$

The coefficients of the multiplication matrix are computed when we just compute the function $V''(\theta + u(\theta))$ following the approaches in Sections 3.3.2,3.3.3,3.3.4.

Remark 4.1. It is amusing to note that near $\theta = 0$, the function (44) is asymptotically linear. On the other hand, for the nearest neighbor interation the diagonal terms are $\cos(2\pi\theta) - 1$, which are quadratic. Hence, the small divisors are less severe for the problems with extended interactions than for the standard map.

Remark 4.2. The well known small divisor problems cause that the matrices have somewhat large condition numbers ($\approx 10^3$ in the examples. Hence, if one solves the equation with Gaussian elimination, it is extremely important to use pivoting. An alternative that we have found useful is to use the singular value decomposition [GVL96] which is much more numerically stable. The penalty in speed is not very severe (only a factor 2 or 3).

Remark 4.3. Since the most expensive step of the algorithm is to compute the inverse of the matrix, we note that it is possible to take several steps without the same inverse. The convergence will not be quadratic, only geometric, but since the steps are much faster, this can be faster.

Another alternative, which also leads to quadratic convergence but requires less updates is the algorithm of [Hal75]

$$\begin{aligned} u_{n+1} &= u_n - \mathcal{I}_n E(u_n), \\ \mathcal{I}_{n+1} &= \mathcal{I}_n - \mathcal{I}_n(\mathrm{Id} - E'(u_{n+1}))\mathcal{I}_n, \end{aligned} \tag{45}$$

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

Figure 4 illustrates several hull functions computed with this method.

In figure 5, we present the Fourier coefficients computed close to the breakdown ($\lambda = 2.3375$). For this computation we used $N = 2^{12}$ coefficients.

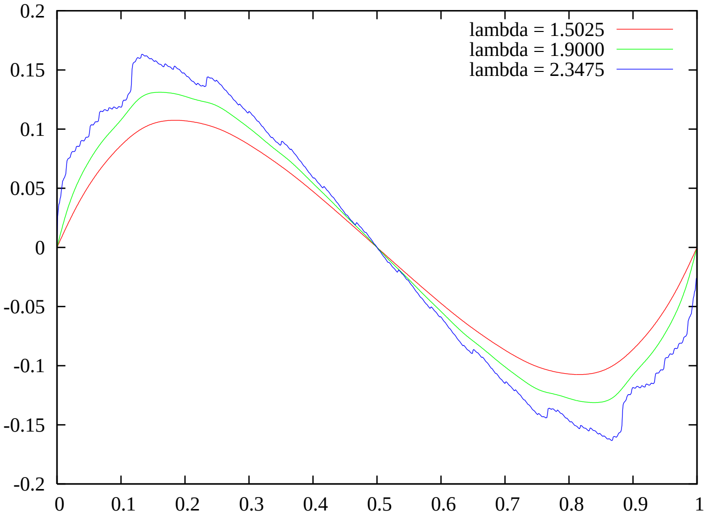

FIGURE 4. $u(\theta)$ for some values of λ.

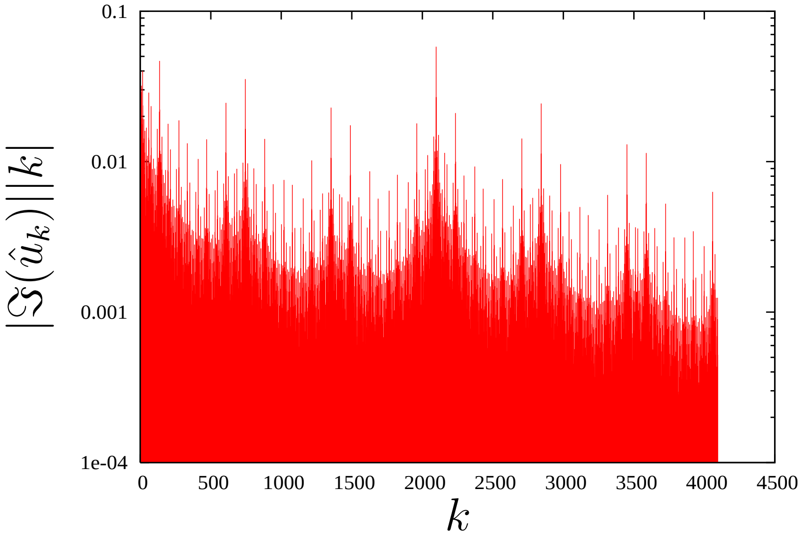

FIGURE 5. Natural logarithm of $\hat{u}_k$ versus the subindex k for $\lambda = 2.3375$ in model (40).

Even if this figure may look similar to figures 2,7, we call attention to the fact that in Figure 5, the horizontal scale is not logarithmic as in figures 2 and 7. In the standard map and in the short range models, the scaling keeps some of the features of the small divisors (the big spikes happen at the places where the small divisors are stronger). On the other hand, for the long range models, the spikes appear at places that are not determined by the small denominators.

5. Studies of the breakdown of analyticity

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

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

One important observation is that the theoretical results of [dlL08, CdlL08] give us a condition for the analyticity breakdown. Note that the methods described above in the paper will allow us to produce systematicaly a solution of the truncated equations. The rigorous results of [dlL08] show that if the approximate solution is well behaved, then, there are true solutions in a neighborhood.

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

Then, the algorithm to identify the boundary, is:

Algorithm 5.1. *Continue the solutions with respect to parameters, monitoring carefully the truncation error etc.*

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

Notice that, even for twist mappings, this method of computing the analyticity breakdown is different from the method in [Gre79]. Of course, the method above applies also to extended systems.

In Section 5.1, we will discover some implementation issues.

In Section 5.3 we present a renormalization argument from the theory of twist maps that leads to a quantitative prediction of the way that the Sobolev norms of the solutions blow up as we approach the boundary of analyticity breakdown. We conjecture that, the same scaling behavior happens for systems which are not nearest neighbors.

In Section 5.4 we present evidence that the numerical conjectures about scaling are true for several models.

If indeed the conjectures were true, they would allow a computation of the boundary of analyticity breakdown, which is more accurate than Algorithm 5.1

Algorithm 5.2. *Continue the solutions with respect to parameters, monitoring carefully the truncation error etc.*

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

Of course, Algorithm 5.2 can yield more accuracy in the computed transition point, but of course, it depends heavily on the scaling assumption.

We think that the regularities found indicate that there exists a renormalization group for extended models that generalizes the renormalization groups for twist mappings [Mac82, Mac83, Koc99].

We think that these regularities deserve a more detailed numerical exploration. Note that, since Algorithm 5.1 is independent of scaling, we can explore a wide class of models.

5.1. Some remarks about the numerical implementation.

Truncation of the solutions to a finite dimensions generates *spurious* solutions. These are solutions of the truncated problem that are not truncations of true solutions of the full problem. It is empirically found that, as the parameters become closer to breakdown, these spurious solutions become more abundant and become harder to distinguish from the true solutions. A Newton method may lock onto an spurious solution and be lead astray.

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

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

5.2. Some Preliminary explorations of the breakdown.

In figure 6, we present some of the values of the H^r semi-norms for the standard map we obtained using the algorithm using adaptive steps described above.

In figure 7, we present the Fourier coefficients computed close to the breakdown ($\varepsilon = 0.97$). For this computation we used $N = 2^{12}$ coefficients. The computation of each one step of the continuation method takes 0.0868 seconds in average in a modest desktop computer.

5.3. Some predictions from Renormalization theory.

As mentioned in Remark 2.1, the Frenkel-Kontorova model is equivalent to the standard map. The breakdown of analyticity of the standard map

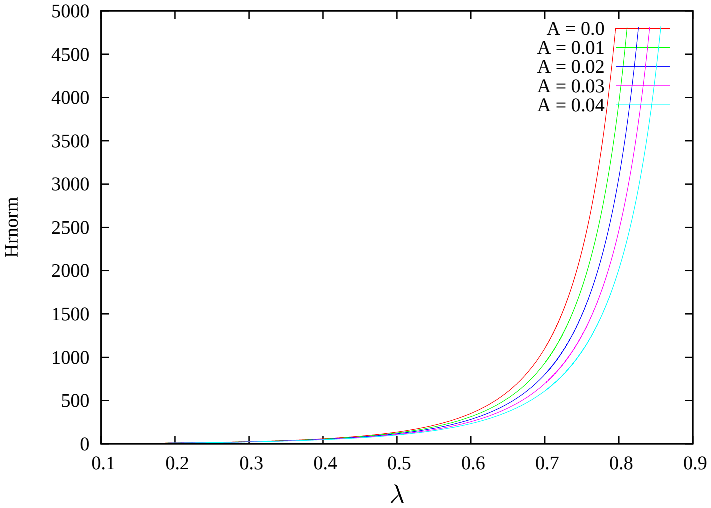

FIGURE 6. H^4 norm for fixed A

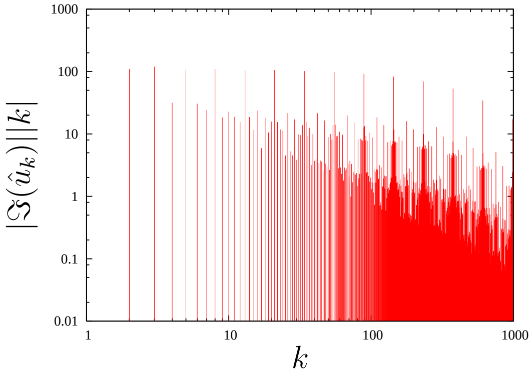

FIGURE 7. Natural logarithm of Fourier coefficients of $u(\theta)$ versus the natural logarithm of the subindex k for $\lambda = 0.97$ in the standard map.

has been extensively studied. In particular, it has been studied using Renormalization group [Mac82, Mac83, Koc04].

We want to adapt this renormalization group in such a way that it can be adapted to our problems. We follow [dlL92]. Consider a family of maps T_λ indexed by a parameter λ, with λ_{crit} being the critical parameter at which analyticity breakdown occurs. The main idea of renormalization is that taking an appropriate iterate of the map and rescaling $\lambda - \lambda_{\text{crit}}$, the problem remains unchanged. The appropriate iterate is given by the convergence of the continued fraction expansion of the rotation. To restore the rotation, we just need to scale the angles.

Hence, we conclude that the following scaling relation holds.

$$u_{\lambda_{\text{crit}}+\delta^{-1}(\lambda-\lambda_{\text{crit}})}(\gamma\theta) \approx u_\lambda(\theta) \tag{46}$$

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

In the particular case of ω the golden mean, there is a well known fixed point with $\delta \approx 1.6280$ See [Mac82, Mac83, AKW98, Koc04]. The exponential convergence of approximants to the golden mean is well known to be $(\sqrt{(5)}+1)/2 \approx 1.618034$.

The scaling relation leads to several predictions.

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

$$\sigma(\lambda) \approx A|\lambda_{\text{crit}} - \lambda|^{\log\gamma/\log\delta} \tag{47}$$

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

$$||D^r u_\lambda||_{L^2} \approx A_r|\lambda_{\text{crit}} - \lambda|^{(\log\delta/\log\gamma)(r-1/2)} \tag{48}$$

To deduce (47) from (46) just observe that reducing the critical parameter by a factor δ, decreases the analyticity radius by a factor γ.

To deduce (48) from (46), note that $\|D^r u_\lambda(\gamma\cdot)\|_{L^2} = \gamma^{r-\frac{1}{2}}\|D^r u_\varepsilon(\cdot)\|_{L^2}$ and that this is the change induced by scaling the parameter by a factor δ.

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

Remark 5.1. The predictions of the scaling relations can be broken up into two parts. A first one is the existence of the scaling relations such as (47) or (48) and the second one is that the exponents have the values that we are indicating.

If we consider the problem from the point of view of renormalization group and scaling relations, [Ami78, Kad00], it is natural to conjecture that the same scaling relations happen for models with short range (or decreasing fast enough) interactions. As we have remarked before, the breakdown of analyticity in models with long range interactions is very different.

5.4. **Numerical verification of the renormalization group predictions.** In this section, we present numerical evidence for prediction P2), since it is much easier for our methods. We note that prediction P1) was verified for the Standard map in [BCCF92] (as a matter of fact, the work of [BCCF92], preceded [dlL92] and motivated the scaling argument). In this paper, we will not be studying prediction P1) for the extended Frenkel-Kontorova model.

In Figure 8 we represent the critical value of analyticity breakdown determined fitting the blow up to several norms. As expected, the norm H^3 does not give very reliable results since the H^3 norm is marginal for the problem [Her86]. On the other hand, the norms that do blowup, indeed all give very compatible results.

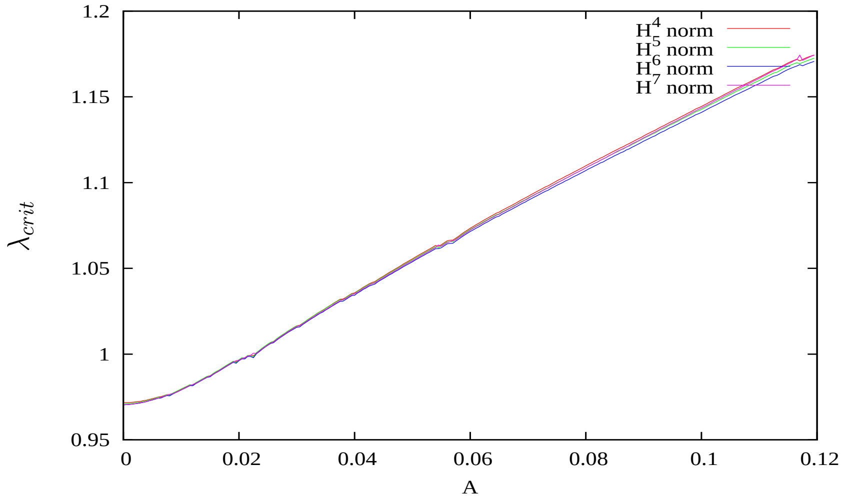

Figure 8. The critical value of model (38) as a function of the next-nearest coupling parameter

In Figure 5.4, we present the values of the blow-up exponent obtained by fitting the relation. Note that they remain almost constant.

In Figure 5.4 we present the difference between some of the scaling exponents presented in Figure 5.4. Note that they agree very well (more than 3 figures) with the value predicted theoretically.

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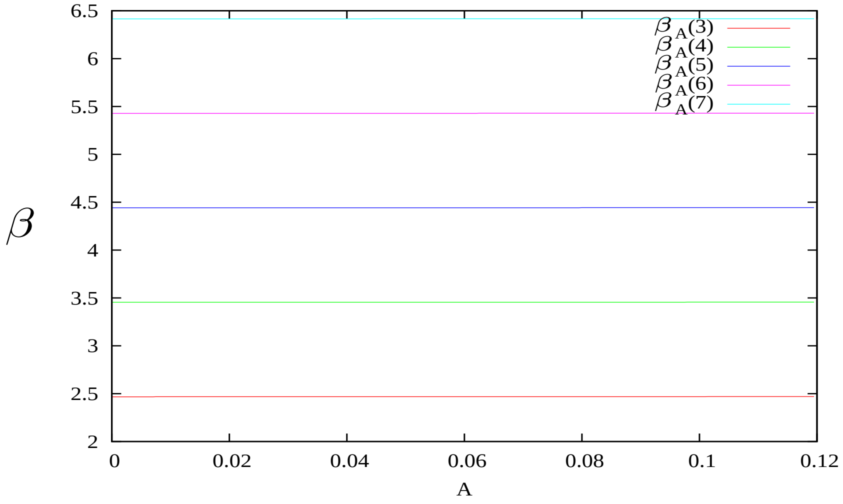

FIGURE 9. A vs. $\beta(r)$ for different values of r

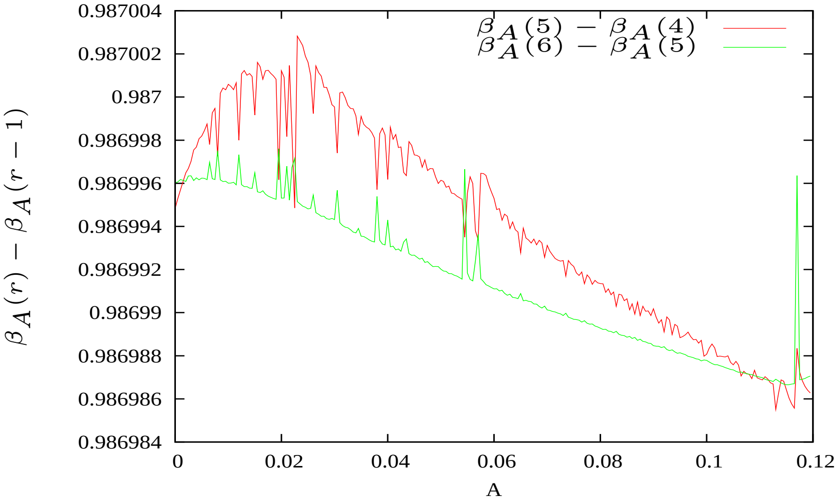

FIGURE 10. Differences between several exponents as a function of A

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