Computation of the breakdown of analyticity in statistical mechanics models

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Abstract

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

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

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

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I. INTRODUCTION

The phenomenon of *breakdown of analyticity*, appears in a multitude of physical contexts (See Section II) (dynamical systems, dynamics of fracture, deposition over a substrate, magnetism, quasi-periodic Schrödinger equations etc.) and has a variety of physical implications. It has, therefore been widely studied by a variety of methods from numerical exploration to rigorous mathematical results. See [1, 2, 3, 4, 5, 6, 7] among others.

In general, we are seeking configurations $\{x_n\}_{-\infty}^{\infty}$ which are equilibria of a variational problem (see section II) and which are determined by a hull function. That $x_n = h(n\omega)$ where $h(t+1) = h(t) + 1$. When the system depends on parameters, it is often observed that the function h is smooth for some values of the parameters and it is discontinuous for others. For the values when h is continuous, the system can easily move among equilibria, but when h is discontinuous, the system is pinned down [2].

The goals of this letter is to present an efficient algorithm to compute this transition and to present the results obtained by applying it to Frenkel-Kontorova models or to Heisenberg XY models of magnetism. These numerical calculations also indicate that in the neighborhood of these transitions, there are scaling relations similar to those of phase transition.

II. MODELS CONSIDERED

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

These models describe an array of atoms, indexed by an integer n. The state of the n atom is characterized by a number x_n. The configuration is, therefore, given by a sequence $\{x_n\}$. In the case of the Heisenberg XY model, the physical interpretation of x_n is the orientation of the spin of the n atom. In the original formulation of the FK model [8] x_n was the position of a planar dislocation in a crystal. In [2], the same model was used in the description of deposition over a substratum. Then, x_n is the position of the n deposited

atom. Given the above interpretations of the models, it is natural to include interactions that extend beyond nearest neighbors [9, 10, 11, 12].

The Physics of the model is determined by assigning an energy to each configuration. The energies we will consider are respectively:

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

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

$$E_{EFK} = \sum_n \sum_L \frac{1}{2} A_l |x_n - x_{n-l}|^2 + V(x_n) \tag{3}$$

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

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

A The equilibrium equations

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

The equilibrium equations are, respectively:

$$2x_n - x_{n-1} - x_{n+1} + V'(x_n) = 0 \tag{4}$$

$$\sin(2\pi(x_n - x_{n-1})) + \sin(2\pi(x_{n+1} - x_n)) \tag{5}$$

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

$$\sum_l A_l(2x_n - x_{n-l} - x_{n+l}) + V'(x_n) = 0 \tag{6}$$

Introducing the extra variable p_n, (4) can be considered as a dynamical system in two dimensions so that $p_{n+1} = p_n + V'(x_n), x_{n+1} = x_n + p_{n+1}$. Therefore, configurations which are critical for E_{FK} are orbits of celebrated standard map.

Note, however that the interpretation of (5),(6) as dynamical systems is rather difficult since there no general way to obtain x_n as function of $x_{n-1}, x_{n-2}, \ldots, x_{n-L}$.

B Configurations given by hull functions

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

$$x_n = h(n\omega) \qquad h(t+1) = h(t) + 1 \tag{7}$$

In FK, EFK models, ω is the inverse of the density. The equilibrium equations can be written in terms of the hull functions as:

$$2h(\theta) - h(\theta - \omega) - h(\theta + \omega) + V'(h(\theta)) = 0 \tag{8}$$

$$\sin(2\pi(h(\theta) - h(\theta - \omega)) + \sin(2\pi(h(\theta + \omega) - h(\theta))) \tag{9}$$

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

$$\sum_l A_l(2h(\theta) - h(\theta - l\omega) - h(\theta + l\omega)) + V'(h(\theta)) = 0 \tag{10}$$

It was shown in [2] that all ground states of FK models are given by hull functions. The argument was extended in [13] for EFK models.

The equations (8) were shown to have a variational structure [3, 4], but small modifications of the argument show that so do (9), (10). The paper [3, 4] showed that this variational principle is a very useful computational tool. The paper [14], developed a mathematically rigorous theory of minimizers of the variational principle of [3, 4] which was the beginning of the celebrated Aubry-Mather (AM) theory. See [15, 13], for a thorough treatment of (10).

The AM theory guarantees the solutions of equations (8), (10) for all choices of parameters and all ω. These solutions could be smooth or discontinuous. On the other hand, (9) does not satisfy the convexity conditions and there does not seem to be a theory of existence of solutions to (9).

C The phenomenon of analyticity breakdown

If h, the solution of (8),(9), (10), is continuous, there is a continuous family of critical points and the system can slide from one to other rather easily. Hence arbitrarily small forces can cause large effects. On the other hand, if h is discontinuous, there are gaps among the states the system is pinned down. The above alternative (pinned down or sliding) depends on the parameters of the system.

The problem we want to address is to compute the regions of parameters where the solution of (8),(9), (10) are smooth or discontinuous.

III. PERTURBATIVE RESULTS

When ω is sufficiently irrational

$$|\omega - p/q| \geq \kappa |q|^{-\tau} \forall p \in \mathbb{Z}, q \in \mathbb{Z} - \{0\} \tag{11}$$

there is a perturbative theory for smooth solutions, often known as the KAM (Kolmogorov-Arnold-Moser) theory (see [16] for a review). Extensions to variational problems were obtained in [17, 18] and, for systems with long range interaction in [19, 20]. In contrast with AM theory, the KAM theory requires that the frequencies are sufficiently irrational and that certain quantitative assumptions hold. On the other hand, KAM requires less convexity assumptions.

The core of [19, 20] is an iterative method that, given an approximate solution of (8),(9),(10), produces a significantly more approximate solution (the number of correct figures, roughly doubles).

Given the Fourier coefficients of h obtained by solving either (8),(9) or (10) up to an error e, there is a explicit correction Δ such that

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

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

Omitting some technical assumptions of a mathematical nature, the main result of [19, 20] is the following:

Theorem 1 *Consider (8),(9), (10) with V analytic. Assume also that ω satisfies the Diophantine condition (11).*

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

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

IV. ALGORITHM FOR THE COMPUTATION OF THE ANALYTICITY BREAKDOWN

Theorem 1 leads immediately to the following algorithm.

Algorithm 2

Choose a path in the parameter space

starting in the integrable case.

Initialize *the parameters at integrable, h_{ε_0}*

Repeat

Increase the parameters along the path

Run the iterative step

If *(Iterations do not converge)*

Decrease the increment in parameters

Else *(Iteration success)*

Record the values of the parameters

and the Sobolev norm of sol.

Until *Sobolev norm too large*

Note that Theorem 1 shows that there will be an analytic solution in a neighborhood unless the Sobolev norm blows up. After a calculation, one can check that the choice of threshold for blow up does not affect much the final result. More accurate results can be obtained by fitting some formula for the blow up.

In is interesting to compare the above criteria with other methods. The best known method [1] is based on the computation of periodic orbits which approximate the periodic solution. On the other hand, when V contains several harmonics, tracking periodic orbits becomes hard close to breakdown since they appear in complicated orders [21]. The formulation of the criterion in [1] does not seem clear in cases such as (10) where one cannot make sense of the residue. Another algorithm based on periodic orbits and their stable manifolds appear in [22]. Other algorithms based on variational methods for twist mappings are [23, 24, 25], but this do not generalize to (9), (10).

V. NUMERICAL RESULTS

We implemented the continuation method prescribed by Algorithm 2 using the methods introduced in [26]. In this section, we present some numerical results.

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

In the neighborhood of analyticity in figure 1 (a) we can find regions with a smooth

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

In figure 3, we present the neighborhood of existence of invariant tori for the model (3) with $A_l = 1/l^k$ and potential $V(x) = -\frac{\varepsilon_1}{2\pi}\cos(2\pi x) - \frac{\varepsilon_2}{4\pi}\cos(4\pi x) - \frac{0.3}{6\pi}\cos(6\pi x)$ and $\omega = \frac{\sqrt{5}-1}{2}$.

VI. CONCLUSIONS

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

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

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

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

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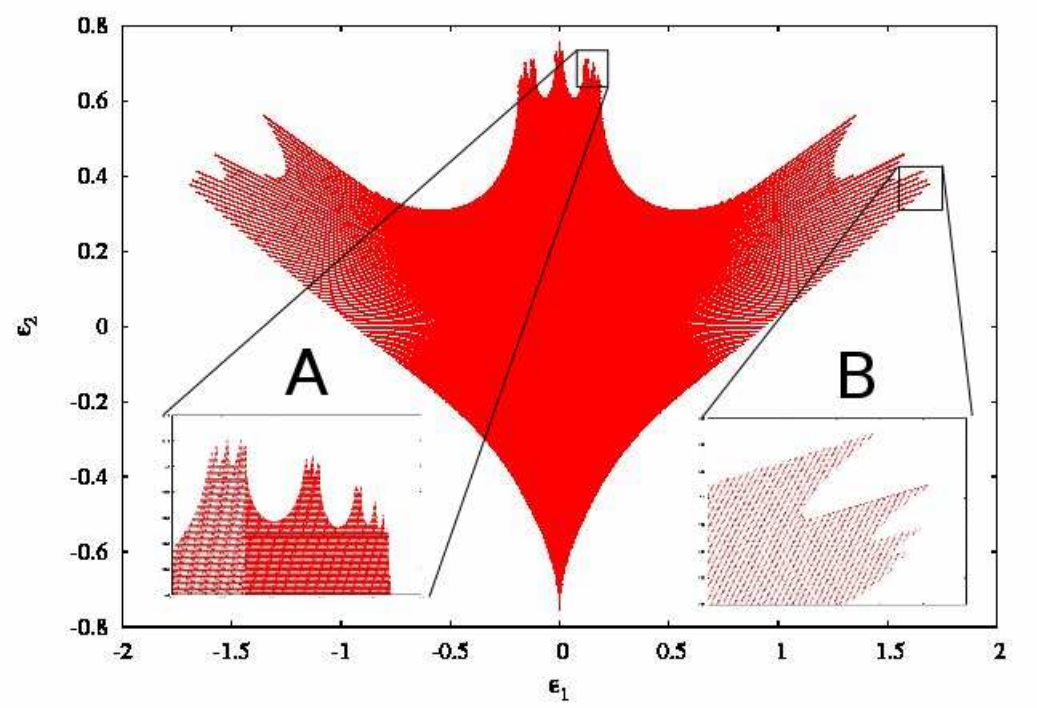
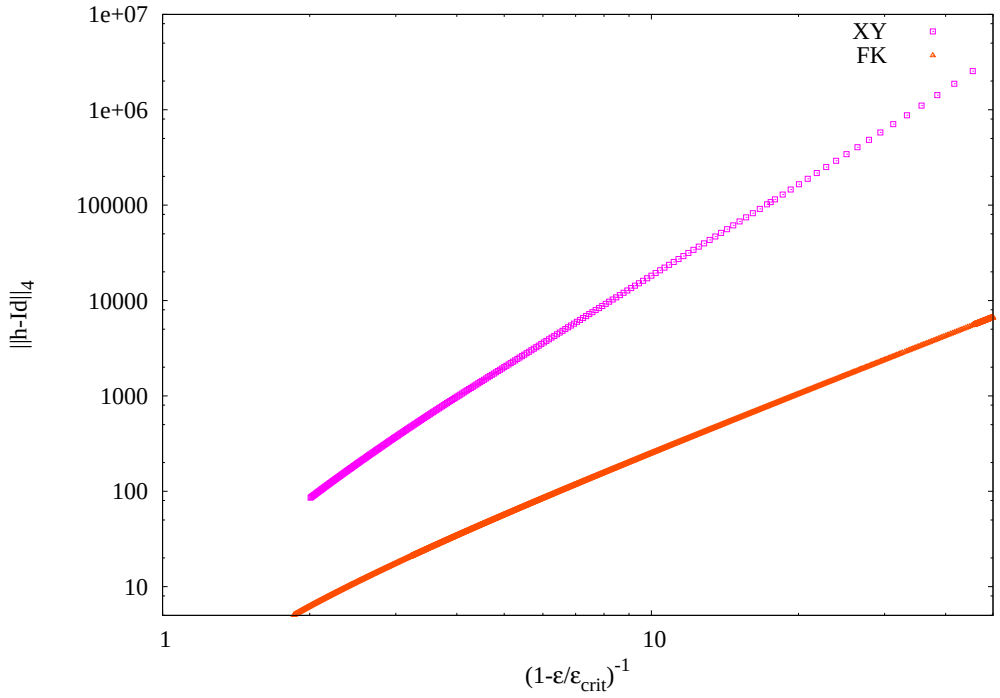


FIG. 1: Domain of $\varepsilon_1, \varepsilon_2$, for which the model (1) with potential $V(x) = -\frac{\varepsilon_1}{(2\pi)^2}\cos(2\pi x) - \frac{\varepsilon_2}{(4\pi)^2}\cos(4\pi x)$ has an invariant circle of rotation golden mean.

a)



b)

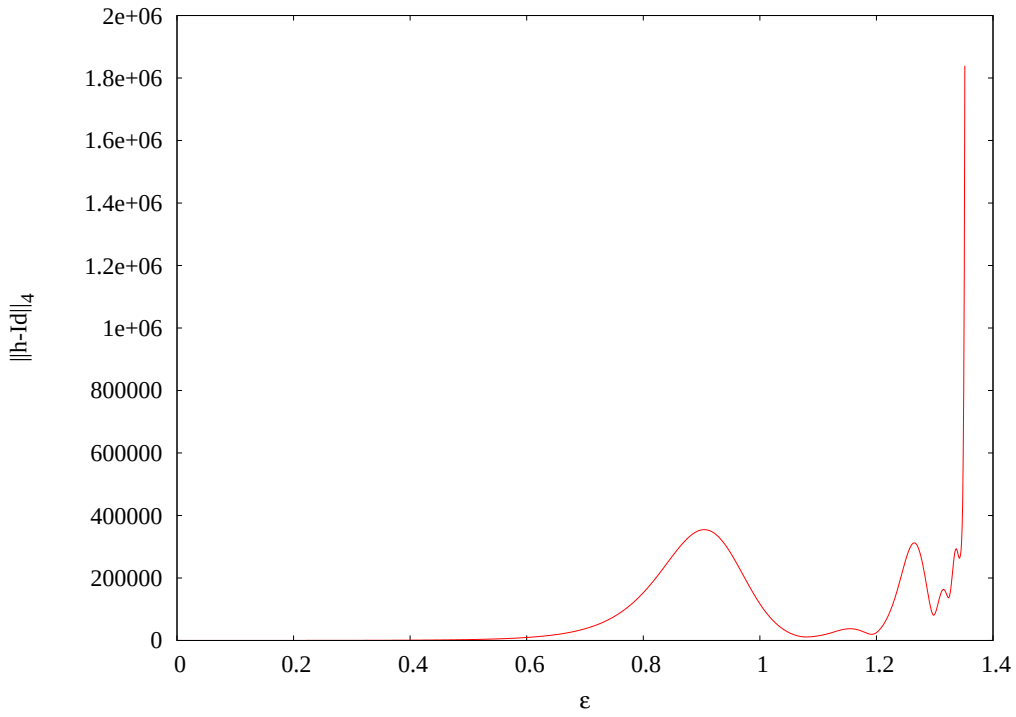


FIG. 2: a) Double logarithmic scale plot of $\|h_\varepsilon - Id\|_4$ with respect to $(1-\varepsilon/\varepsilon_{crit})^{-1}$ for models (1) with $V(x) = -\frac{\varepsilon}{(2\pi)^2}\cos(2\pi x)$. and (2) with $B = -\frac{\varepsilon}{(2\pi)^2}$. b) $\|h_\varepsilon - Id\|_4$ with respect to ε for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

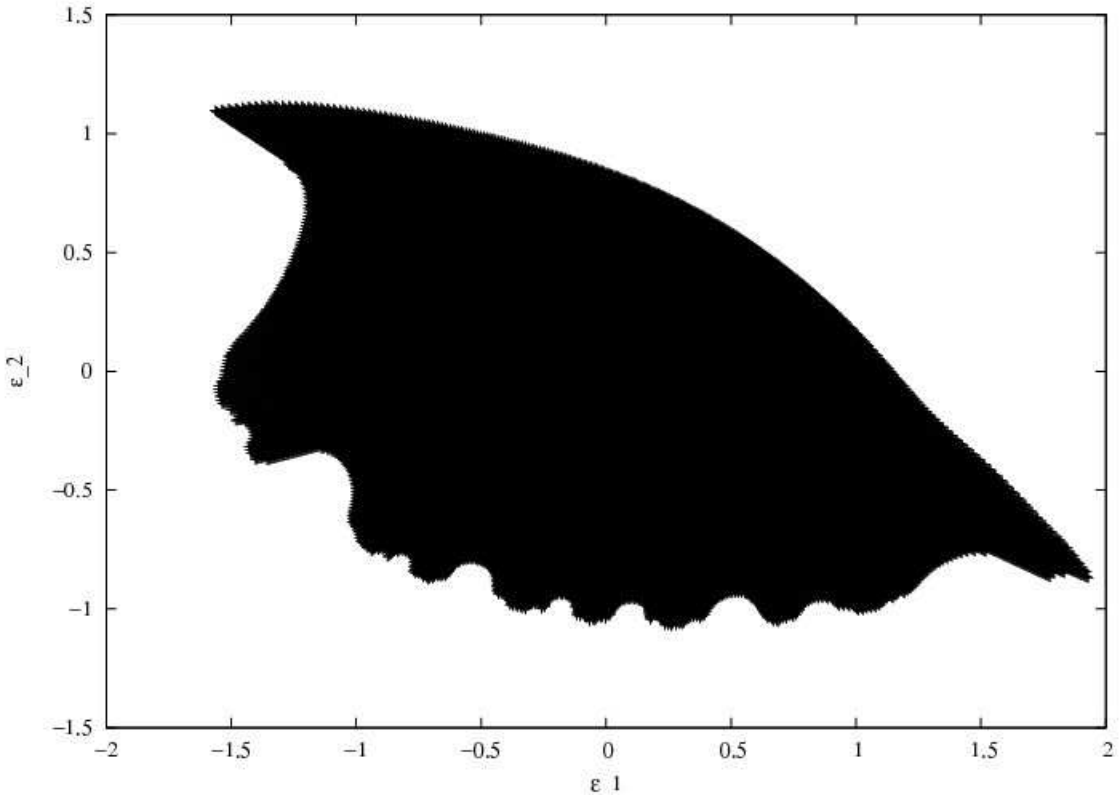


FIG. 3: Neighborhoods of existence of invariant circles for the model (1) with $A_l = \frac{1}{l^2}$, $\omega = \frac{\sqrt{5}-1}{2}$, and potential $V(x) = -\frac{\varepsilon_1}{2\pi}\cos(2\pi x) - \frac{\varepsilon_2}{4\pi}\cos(4\pi x) - \frac{0.3}{6\pi}\cos(6\pi x)$ in the parameter space $(\varepsilon_1, \varepsilon_2)$.