

**Computation of the breakdown of analyticity in statistical
mechanics models: numerical results and a renormalization group
explanation**

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Abstract

We consider one dimensional systems of particles interacting with each other through long range interactions that are translation invariance. We seek quasi-periodic equilibrium states.

Standard arguments show that if there are continuous families of quasi-periodic ground states, the system can have large scale motion, if the family of ground states is discontinuous, the system is pinned down. The transition between the two cases is called *breakdown of analyticity* and has been widely studied.

We use recently developed fast and efficient algorithms to compute all the continuous families of ground states even close to the boundary of analyticity. We show that the boundary of analyticity can be computed by monitoring some appropriate norm of the computed solutions.

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. We present a renormalization group explanation of these phenomena. This suggest that the renormalization group may have some complicated global behavior.

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INTRODUCTION

The phenomenon of *breakdown of analyticity*, appears in a multitude of physical contexts, see next section, (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 [1–7] and their references among others.

We will be considering one-dimensional discrete models, which appear naturally as models of dislocation planes in crystals in solid state Physics [8] and in other contexts.

We are seeking configurations $\{x_n\}_{n \in \mathbb{Z}}$ which are equilibria of a variational problem (see next section) and which are determined by a hull function. That is, $x_n = h(n\omega)$ where $h(t+1) = h(t) + 1$. In [2] it is shown that, under some convexity properties, all the ground states are of this form. The parameter ω has the physical interpretation of the inverse of a density and it is, therefore, natural considering it fixed.

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. It is shown in [2] that when h is continuous, the system can easily move among equilibria, but when h is discontinuous, the system is pinned down. In many examples, depending on the parameters, we can find both behaviors and the boundary between the two cases – the boundary of mobility or the boundary of transport – has been widely studied by physicists. In the mathematics literature, some particular models of the type considered here, appear as twist mappings and the breakdown of analyticity is precisely the breakdown of KAM tori.

The goals of this paper are to present an efficient algorithm to compute the breakdown of analyticity transition and to present the results obtained by applying it to Frenkel-Kontorova models (both with non-nearest neighbor interactions and long range interactions) or to Heisenberg XY models of magnetism. We also present a renormalization group explanation of the results. The numerical algorithms used in this paper have been justified mathematically in [9].

We note that the Frenkel-Kontorova model with nearest neighbor interactions is precisely the *standard map* in dynamical systems. Nevertheless, some of the models that we consider (e.g. the Frenkel-Kontorova model with long range interactions or the Heisenberg XY model) do not have interpretation as dynamical systems. So that the phenomenon of breakdown of

analyticity is somewhat more general than the phenomenon of breakdown of KAM tori in twist maps.

The paper [9] contains a short survey of the methods used to compute analyticity breakdown. Most of the methods used previously in the literature were designed for the case of dynamical systems. Notably, the Greene's method [1] or the obstruction criterion [10] which relied on the computation of periodic orbits. The method presented here allows to compute much more systematically and to explore a wider range of parameters than previously explored.

We find that, as predicted by the standard renormalization group picture, some regions of the boundary of analyticity are smooth and we find scaling relations. On the other hand, for other regions we find that the boundary has corners and that the scaling relations are not so straightforward. This suggests that the renormalization group has a complicated dynamical behavior. The possibility that the renormalization group could have an erratic behavior was suggested in [11]. The present paper gives evidence that this actually happens.

It is not surprising that this complicated behavior of the renormalization group had not been observed before because standard methods such as the Greene's method or the obstruction criterion rely on being able to guess the position of periodic orbits, which is, in turn related to the orderly behavior of the renormalization group [12]. (The complicated behavior of the renormalization group manifests itself in that the periodic orbits jump around dramatically and are hard to follow numerically [13, 14]).

MODELS CONSIDERED

In this paper, 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 real number x_n . The configuration is, therefore, given by a sequence $\{x_n\}_{n \in \mathbb{Z}}$. 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 [15–18].

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

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

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

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

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 substrate 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 EFK model we also consider harmonic interactions between non-nearest neighbors.

In the XY model the energy is the sum of 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.

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:

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

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

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

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

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, equilibrium configurations

for E_{FK} are orbits of celebrated standard map.

Note, however that the interpretation of (6) as dynamical systems is rather difficult since there is no general way to obtain x_n as function of $x_{n-1}, x_{n-2}, \dots, x_{n-k}$ if $A_l > 0$ for all l . Obtaining x_n in (5) involves computing $\sin^{-1}(\sin(2\pi x_n - x_{n-1}) + B \sin(2\pi x_n))$ which only makes sense if $|\sin(2\pi x_n - x_{n-1}) + B \sin(2\pi x_n)| \leq 1$, a non-trivial condition. Furthermore, if this condition is satisfied at one step, it may fail at the next.

We note that, even if the energy is a formal sum, the equilibrium equations are well defined mathematical objects. There are standard definitions to make sense of ground states – also called class-A minimizers in the mathematical literature – for variational principles given by formal sums [19].

Configurations given by hull functions

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

$$x_n = h(n\omega) \quad h(t+1) = h(t) + 1 \quad (7)$$

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

$$2h(\theta) - h(\theta - \omega) - h(\theta + \omega) + V'(h(\theta)) = 0 \quad (8)$$

$$\sin(2\pi(h(\theta + \omega) - h(\theta))) - \sin(2\pi(h(\theta) - h(\theta - \omega))) \quad (9)$$

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

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

It was shown in [2] that all ground states of FK models are given by hull functions. The argument was extended in [20] 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 [21], 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 [20, 22], for a thorough treatment of (10).

The AM theory guarantees the existence of 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 required by AM theory and we do not know of a theory of existence of solutions to (9) for general values of parameters even if there is a perturbative theory for small values of B [23, 24].

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 another rather easily. Hence arbitrarily small forces can cause large effects. On the other hand, if h is discontinuous, there are gaps among the ground states and the system is pinned down since jumping would require significant energy. The above alternative (pinned down or sliding) depends on the parameters of the system.

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

PERTURBATIVE RESULTS

When ω is sufficiently irrational, i.e., it satisfies the following Diophantine condition

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

there is a perturbative theory for smooth solutions, often known as the KAM (Kolmogorov-Arnold-Moser) theory (see [25] for a review). Extensions to variational problems were obtained in [26, 27] and, for systems with long range interaction in [9, 28]. 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 theory requires less convexity assumptions than AM theory.

The core of [9, 28] 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 at each step).

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

where N is the number of coefficients used to discretize h .

Omitting some technical assumptions of a mathematical nature, the main result of [9, 28] 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 r large enough, $\|e\|_r \equiv (\sum_n (1+k^2)^r |\hat{e}_k|^2)^{1/2}$ is sufficiently small compared to $\|h\|_r$.

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 (in a Sobolev norm as above).

Note that Theorem 1 can be used to justify the numerical computations. We can take as an approximate solution the function produced by the computer. If the error of the invariance equation is small enough with respect to $\|h\|_r$, we can be confident that we are producing something close to a true solution. This is invaluable when we are trying to approach values where the true solutions cease to exist. Then, one can take appropriate measures (e.g. increase the number of discretization points) or indicate that the computation has to stop.

Having some criterion that asserts the reliability of the computation is crucial when we are trying to compute reliably close to the boundary. It is found empirically that close to the boundary of existence there are many spurious solutions which can confuse sloppy methods. As it is well known by mathematicians, the smooth KAM tori, when they break down, leave Cantor tori, which may be confused with a KAM torus since they are rather dense.

ALGORITHM FOR THE COMPUTATION OF THE ANALYTICITY BREAK-DOWN

Theorem 1 leads immediately to the following algorithm.

Algorithm 2

Choose a path in the parameter space starting from 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 the solution

Until *Sobolev norm too large*

The ending point of the algorithm is the computed critical value.

To compute the domain of analyticity, one just needs to study several paths that scan different directions (take care of overhangs). Of course, if there are several processors or cores available, it is trivial to give the task of following different paths to different processors, so that the computation is very parallelizable.

Note that Algorithm 2 is at heart a very standard continuation method and that there are no bifurcations and only moderate condition numbers until the breakdown. Hence the continuation does not require any delicate tuning of choices of where to find auxiliary objects.

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.

It 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 [14]. 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 appears in [10]. Other algorithms based on variational methods for twist mappings are [29–31], but this do not generalize to (9), (10). A more systematic comparison between

algorithms appears in Appendix B of [9].

A RENORMALIZATION GROUP EXPLANATION

The standard scenario of breakdown

Since the 60's one of the most important technical tools to discuss phase transitions has been the renormalization group and the theory of scaling exponents [11, 32, 33]. It seems clear that the breakdown of analyticity transition shares several features with many of the standard phase transitions. In the dynamical systems context this has been documented in [34–38].

The easiest description of phase transitions is that there is a renormalization operator in the (infinite dimensional) space of interactions which describes one scale in terms of longer scales (in statistical mechanics one sometimes does the opposite). Hence, the asymptotic behavior of the renormalization group operator, gives information of the very short scale (i.e. the differentiability properties) of the functions considered.

For example, the standard picture of the breakdown of analyticity [36] is as follows:

In a neighborhood of the nontrivial fixed point, the maps on one side go to a trivial fixed point. Convergence of long iterations of renormalization to a trivial fixed point implies that the original map had an analytic invariant circle. Convergence to the non-trivial fixed point implies that there is an invariant circle but that it is not analytic. This part of the picture has been established rigorously in [37, 39–41].

On the other side of the stable manifold of the fixed point, there are very detailed conjectures on the behavior of renormalization group [12] which imply that there are no invariant circles, but rather uniformly hyperbolic Cantor sets. These conjectures have not been proved but [12] included supporting numerical evidence.

It should be emphasized that this standard picture is only meant to hold in a neighborhood of the non-trivial fixed point.

In the following, we will indicate how the computations presented above, fit into this standard picture and how they suggest that the renormalization group has some dynamically complicated behavior.

Scaling predictions of the standard scenario

First of all, we indicate that the standard renormalization picture predicts some behaviors which are consistent with some of the behaviors we found numerically.

The standard scenario predicts that in a neighborhood of the non-trivial fixed point:

- P1) For a generic family, the set of parameters experiencing analyticity breakdown, is a smooth codimension 1 surface.
- P2) There are scaling exponents for Sobolev (and C^r) norms of the hull function. The exponents are affine functions of the order of the Sobolev exponents.

The reason for P1) is clear: The set of models experiencing analyticity breakdown is a codimension 1 manifold, which will be intersected by a generic family in a codimension 1 set. Generically, the intersection will be a smooth set since it will be transversal.

The reason for P2) is more sophisticated and indeed, gives a very explicit expression for the linear coefficient of the blowup exponent in terms of the index of the Sobolev space.

We note that the renormalization consists in considering an iterate of the map and scaling in space. The application of renormalization close to breakdown implies that the parameters scale.

Therefore, denoting by $\tilde{\varepsilon} = \varepsilon_c - \varepsilon$, where ε_c is the critical value of the parameter we expect that

$$h_{\delta\tilde{\varepsilon}}(\theta) \approx \eta h_{\tilde{\varepsilon}}(\sigma\theta)$$

where δ is the unstable exponent of the renormalization fixed point, σ is a number theoretic number that indicates how fast the iterates considered in the renormalization are converging to the frequency (e.g. for golden mean frequency, when the convergents are Fibonacci numbers, we obtain $\sigma = \frac{1}{2}(\sqrt{5} + 1) \approx 1.6180339887\dots$

The value of δ is well known to be [36, 38] $\delta \approx 1.6280\dots$

If this scaling were true, the Sobolev semi-norms of h would satisfy

$$F_r^2(\delta\tilde{\varepsilon}) \equiv \int D^r h_{\delta(\tilde{\varepsilon})}(\theta)^2 d\theta \approx \int \eta^2 \sigma^{2r} D^r h_{\tilde{\varepsilon}}(\theta\sigma)^2 d\theta = \eta^2 \sigma^{2r-1} F_r^2(\tilde{\varepsilon})$$

This corresponds to

$$F_r(\tilde{\varepsilon}) \approx \tilde{\varepsilon}^{\frac{\log \sigma}{\log \delta} (r - \frac{1}{2} + \frac{\log \eta}{\log \sigma})} = \tilde{\varepsilon}^{0.98740\dots(r-E)} \quad (12)$$

NUMERICAL RESULTS

We implemented the continuation method prescribed by Algorithm 2 using the methods introduced in [24]. In this section, we present some numerical results.

In Figure 1, we present the set parameters $\varepsilon_1, \varepsilon_2$ for which there is a function, $h_{(\varepsilon_1, \varepsilon_2)}$ 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 Figure 2, 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 $\omega = \frac{\sqrt{5}-1}{2}$. Note that this model has infinite range and that the interactions decrease very slowly. This is the critical case of the hierarchical models [42, 43].

In Figure 3, we plot the critical values of ε obtained from a direct fit of (12) for different values of r and for different values of the coupling constant for non-nearest neighbor interactions in the EFK model. We see that the values obtained are very approximately constant and independent of the value of r .

Numerical evidence near the non-trivial fixed point

As for *P1*) we indicate that the regions in Figure 1 where the curve is smooth are apparent by visual inspection. More detailed magnifications – consistent with the precision of the calculations – also confirm that.

As for the more delicate and quantitative prediction *P2*), in Figure 4, we present a doubly logarithmic plot of $\|h_\varepsilon - \text{Id}\|_4$ for the XY and FK models. The linear behavior is apparent. We have found similar behavior in many other cases.

In Figure 5, we plot the Blow-up exponents of F_r as a function of r for the EFK model for different values of A_2 . We can see that the behavior fits very well the formula (12) and that the slope seem to be independent of A_2 .

Evidence of behavior beyond the standard scenario

Figure 1 presents obvious cusps in the ε_2 axis. This is just an artifact of the parameterization. The maps corresponding to ε_1 and $-\varepsilon_1$ are just the same map in different coordinates.

On the other hand, we have magnified regions A and B where there is genuinely complicated geometry of the domain of analyticity. There seems to be an accumulation of cusps. If one follows one of the paths in this region (see Figure 6) one can see that the norm has a very erratic behavior. It switches from growing to decreasing several times before blowing up.

In the renormalization group interpretation, the boundary of analyticity is the stable manifold of the non-trivial fixed point. Hence, the numerical evidence has to be interpreted as saying that the stable manifold has a complicated behavior. The computation in Figure 1 indicates that the stable manifold doubles back on itself. The computation performed on Figure 6 indicates that a smooth path approaches and then moves away from the boundary. Again, this can only happen if the stable manifold doubles back on itself. Therefore, we conclude that the stable manifold of the non-trivial fixed point contains several folds.

The standard dynamical systems mechanism to have manifolds doubling on themselves is the appearance of homoclinic intersections and indeed, the magnifications of Figure 1 are visually strikingly similar to the sections of homoclinic tangles.

Hence we think that the observations are consistent and indeed suggest that the renormalization group operator has a horseshoe. We note that [44] also has other evidence supporting the existence of horseshoes in the renormalization dynamics.

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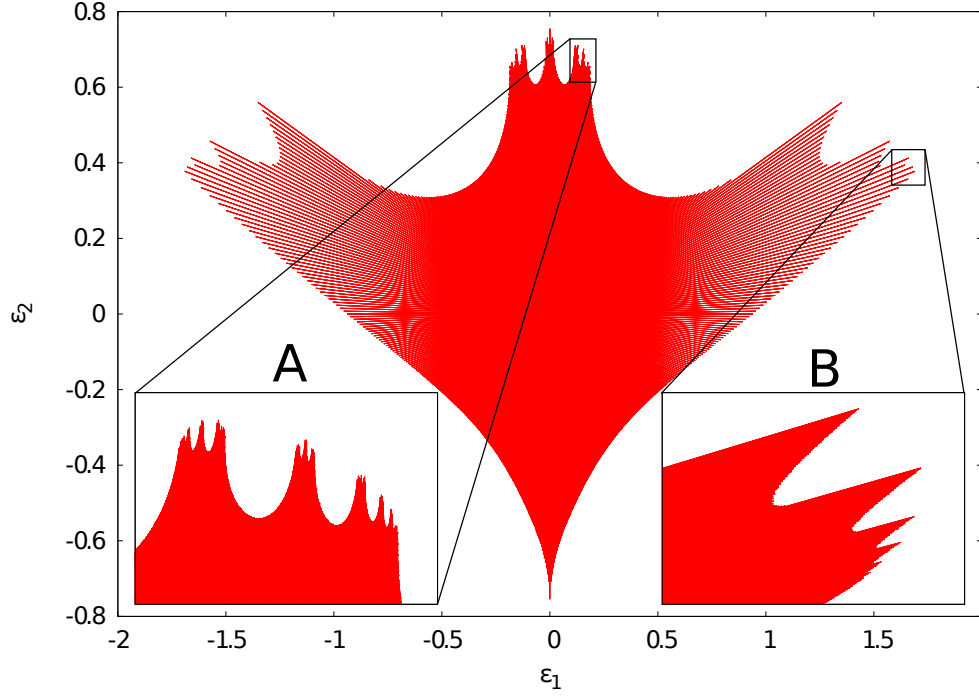


FIG. 1. Domain of $\varepsilon_1, \varepsilon_2$, for which the model (1) with potential $V(x) = -\frac{\varepsilon_1}{(2\pi)^2} \cos(2\pi x) - \frac{\varepsilon_2}{(4\pi)^2} \cos(4\pi x)$ has an invariant circle of rotation golden mean.

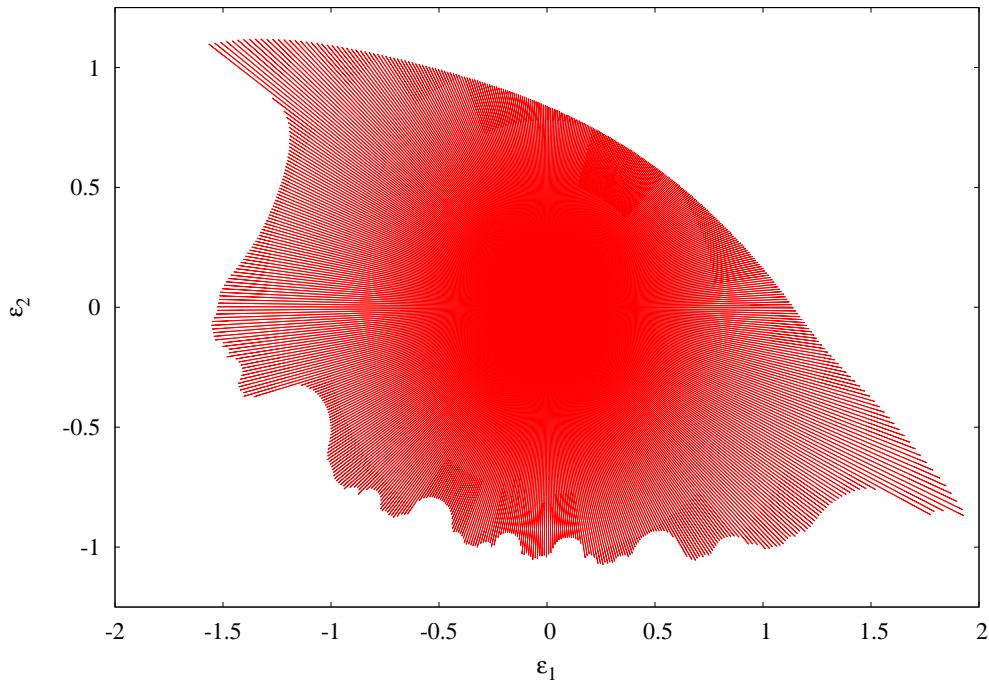


FIG. 2. Neighborhoods of existence of invariant circles for the model (1) with $A_l = \frac{1}{l^2}$, $\omega = \frac{\sqrt{5}-1}{2}$, and potential $V(x) = -\frac{\varepsilon_1}{2\pi} \cos(2\pi x) - \frac{\varepsilon_2}{4\pi} \cos(4\pi x) - \frac{0.3}{6\pi} \cos(6\pi x)$ in the parameter space $(\varepsilon_1,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

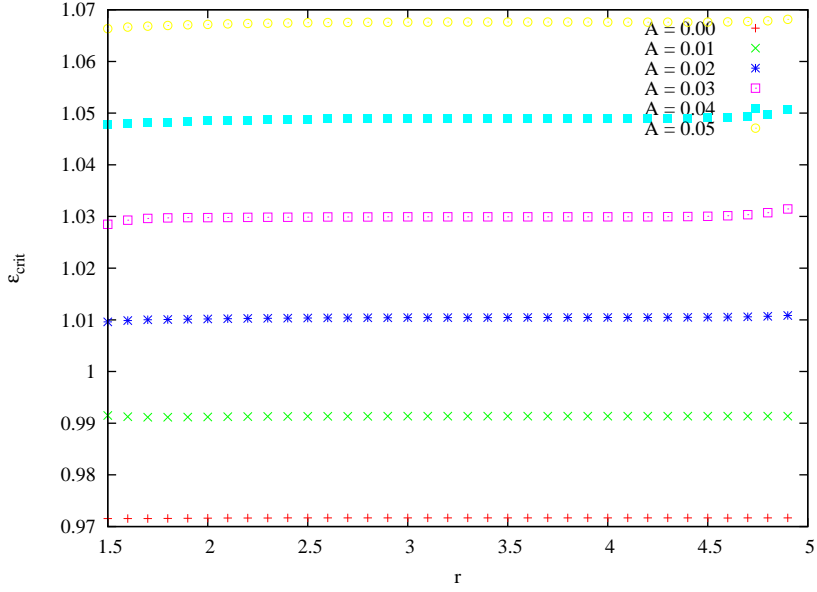


FIG. 3. Critical values computed monitoring the blow up of different Sobolev norms as a function of the order r .

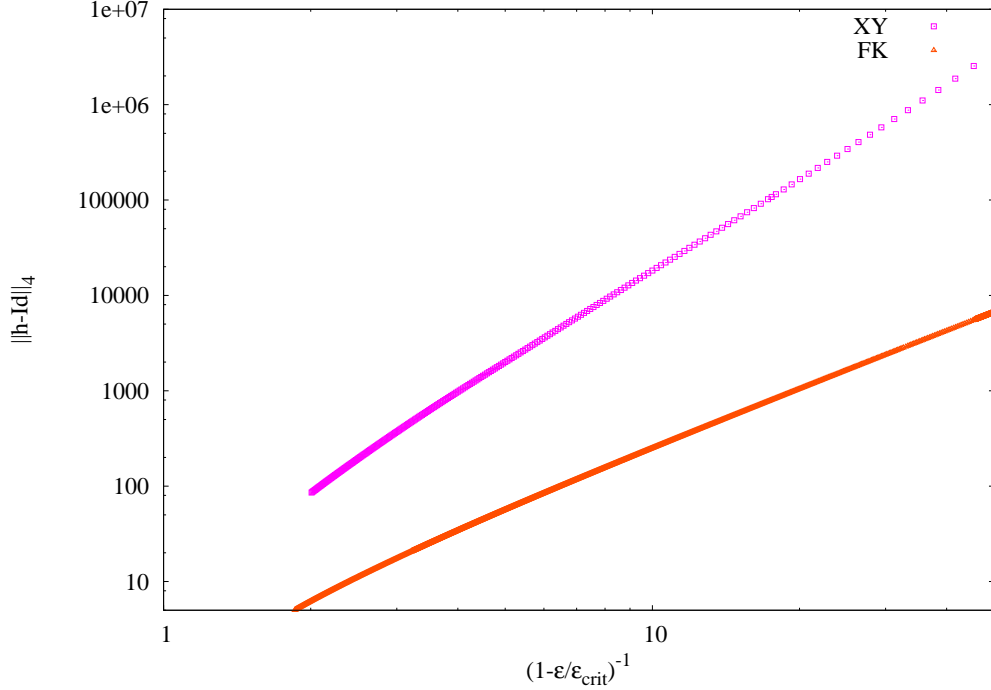


FIG. 4. Doubly logarithmic scale plot of $\|h_\varepsilon - Id\|_4$ with respect to $(1 - \varepsilon/\varepsilon_{crit})^{-1}$ for models (1) with $V(x) = -\frac{\varepsilon}{(2\pi)^2} \cos(2\pi x)$. and (2) with $B = -\frac{\varepsilon}{(2\pi)^2}$.

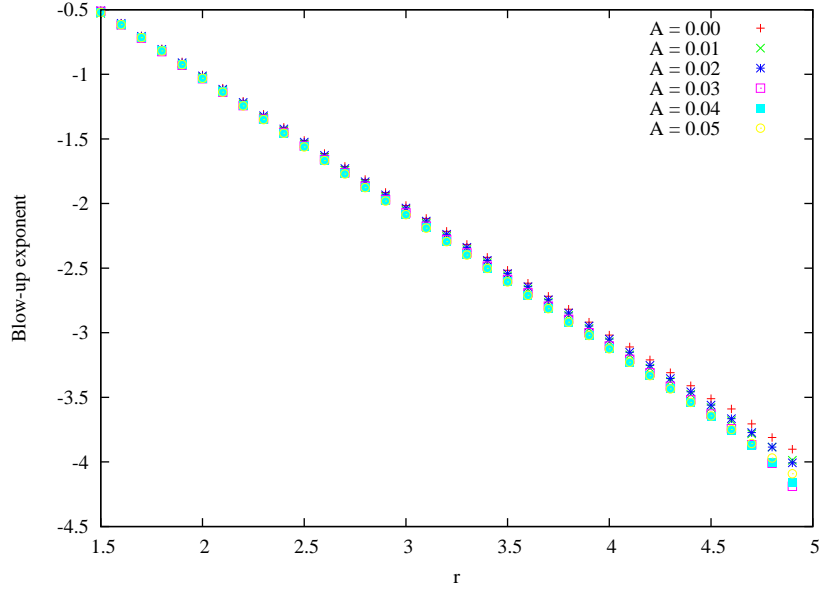


FIG. 5. Exponents of blow-up of Sobolev norms as a function of the regularity r for several values of the coefficient A_2 in the EFK model.

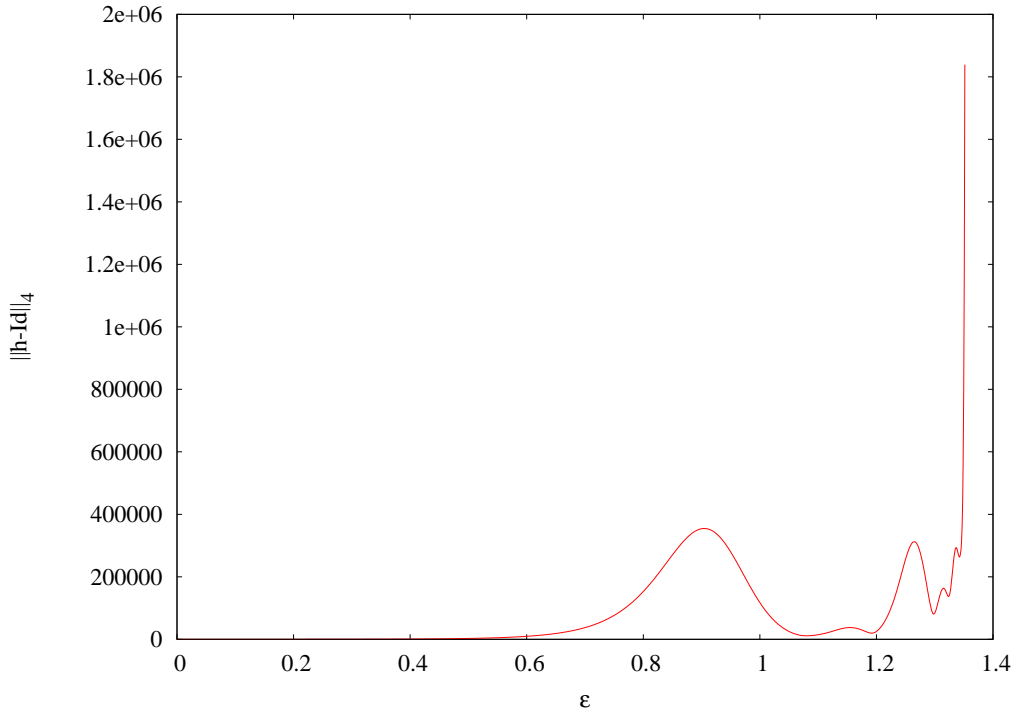


FIG. 6. $\|h_\varepsilon - Id\|_4$ with respect to ε for model (1) with $V(x) = -\frac{\varepsilon}{(2\pi)^2} \left(\cos(2\pi x) + \frac{\sqrt{2}-1}{4} \cos(4\pi x) \right)$.