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TITLE: THE TWIST MAP, THE EXTENDED FRENKEL-KONTOROVA MODEL AND THE DEVIL'S STAIRCASE

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The Twist Map, the Extended Frenkel-Kontorova

Model and the Devil's Staircase

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ABSTRACT

This paper reviews exact results which we obtained on the discrete Frenkel Kontorova (FK) model and its extensions, during the past few years. These models are associated with area preserving twist maps of the cylinder (or a part of it) onto itself. The theorems obtained for the FK model thus yields new theorems for the twist maps. We describe the exact structure of the ground-states which are either commensurate or incommensurate and assert the existence of elementary discommensurations under certain necessary and sufficient conditions. Necessary conditions for the trajectories to represent metastable configurations, which can be chaotic, are given. The existence of a finite Peierl Nabarro barrier for elementary discommensurations is connected with a property of non-integrability of the twist map. We next prove that the existence of KAM tori corresponds to undefectible incommensurate ground-states and give a theorem which asserts that when the phonon spectrum of an incommensurate ground-state exhibits a finite gap, then the corresponding trajectory is dense on a Cantor set with zero measure length. These theorems, when applied to the initial FK model, allows one to prove the existence of the transition by "breaking of analyticity" for the incommensurate structures when the parameter which describes the discrepancy of the model to the integrable limit varies. These theorems also allows one to obtain a series of rigorous upper bounds for the stochasticity threshold of the standard map which for the order 5, already approaches at 25% the value which is numerically known. Finally, we describe a theorem proving the existence of a devil's staircase for the variation curve of the atomic mean distance versus a chemical potential, for certain properties of the twist map which are generally satisfied.

I. Introduction. Models description

Up to now, applications of the properties of nonintegrable maps and particularly the possibility that they have to exhibit a chaotic behavior, have been mostly devoted to physical systems which are really dynamical. However, they also have interesting applications for understanding static structural properties of condensed matter. The aim of this paper is to describe some of these applications. Instead to give a detailed report of our talk (which would be too long), we mostly focus on the rigorous results which we obtained. The reader can refer to[16] where the physical applications of this work have been focused at the expenses of a precise mathematical description which as a counterpart is given here.

We initially studied the Frenkel Kontorova model[2] (noted hereafter FK model). However, due to difficulties in the publication of these early works, these results have only been published in parts and with incomplete proofs in journals of limited audience. We take the opportunity of this paper to recall, to clarify and to emphasize some particular important points which apparently have been ignored or misunderstood in the literature, but which already gave answers to certain presently controversed questions (for example on the existence of chaotic ground states in the FK model). The exact results which we obtained on its ground-states and on its metastable states, also turned out to have important applications for the standard map. We recently improved and extended these results to a larger class of models corresponding to twist maps and for which we obtained interesting new theorems. In this paper, we describe them in the most recently improved form, but we do not include their proofs which are generally long and complicated.

However, we detail some corollaries which have immediate applications with their pro s when they are simple. The first parts of the most important proofs are submitted to publication (Ref. 6 and 7). The second part (Ref. 8) is still in preparation.

This study is essentially analytical and yields only qualitative results of topological nature. However, explicit rigorous calculations can be carried out on a particular but pathological model with the form (1) where V(x) is replaced by a piecewise parabola periodic potential[2,3,7]. We also performed few numerical calculations mostly for the illustration of the theory (Fig. 1 and 4). Some recent numerical calculations[14] have also been performed on the transition by breaking of analyticity in order to explicit critical quantities and critical exponents.

Let us describe now, the Frenkel Kontorova[1] model, in its original version. It corresponds to a chain of elastically coupled atoms submitted to a periodic potential

$$\phi(\{u_i\}) = \sum_i [\lambda\ V(u_i)+W(u_{i+1}-u_i) - \mu\cdot(u_{i+1}-u_i)] \tag{1.a}$$

the atom i is at abscissa u_i. The coupling potential W is harmonic

$$W(u_{i+1}-u_i) = \frac{1}{2}(u_{i+1}-u_i)^2 \tag{1.b}$$

(The energy unit is chosen such that the coupling constant in (1.b) be one). The periodic potential V with period 2a is sinusoidal.

$$V(u_i) = \frac{1}{2}(1-\cos \frac{\pi u_i}{a}) \tag{1.c}$$

λ the amplitude of this potential is an adjustable parameter. The chain is submitted to a tensile force μ (or a chemical potential) which allows one to change the distance between neighboring atoms in the absence of periodic potential ($\lambda=0$). The configurations $\{u_i\}$ of model (1) which have the most physical interest are those which corresponds to the ground-states for various boundary conditions or with free ends and those which corresponds to metastable configurations. All these configurations are solutions of the equation

$$\frac{\partial \phi}{\partial u_i} = (-u_{i+1}-u_{i-1}+2u_i) + \frac{\lambda\pi}{2a} \sin \frac{\pi u_i}{a} = 0 \tag{2}$$

but this equation also exhibits many other unphysical solutions (in our physical context) which correspond to unstable configurations. (Note that the parameter μ disappears when writing equation(2)).

This equation can be recursively solved[2] by iterating the area preserving two dimensional map $\tilde{T}_s$ which maps the point $\tilde{P}_i$ with coordinates (u_i,u_{i-1}) onto the point $\tilde{P}_{i+1}$ with coordinates (u_{i+1},u_i). From equation (2), we get

$$\tilde{P}_{i+1} = \tilde{T}_s(\tilde{P}_i) = (2u_i + \frac{\lambda\pi}{2a} \sin \frac{\pi u_i}{a} - u_{i-1} , u_i) \tag{3}$$

This map can be fold up onto a torus $[0,2a[\times[0,2a[$ by defining

$$\theta_i = u_i \quad \text{modulo } 2a \tag{4}$$

It is now well-known that such a map exhibits many kinds of trajectories which are either chaotic or not. Figures 1 shows some trajectories for $\lambda = 0.15$ (Fig. 1-a), $\lambda = 0.20$ (Fig. 1-b) and $\lambda = 0.25$ (Fig. 1-c). About 1000 iterated points have been plotted from each initial point. These figures exhibit trajectories which are either rotating on one or several smooth closed curves or are chaotic. The behavior of two dimensional area-preserving maps has been intensively studied particularly during the past few years and we refer for example to the important work of Greene[9] on this subject.

By the change of variables

$$p_i = u_{i+1} - u_i \tag{5}$$

this map becomes the well-known standard map which have been studied as a model for certain dynamical systems (for example the motion of an ion in a plasma)

$$(p_{i+1},\theta_{i+1}) = \tilde{T}_s(p_i,\theta_i) = (p_i + \frac{\lambda\pi}{2a}\sin\frac{\pi\theta_i}{a}\ ,\ p_{i+1}+\theta_i) \tag{6}$$

This standard map, which maps the cylinder [0,2a[onto itself, is a prototype for the twist maps of the annulus onto itself (see Ref. 5) A twist map is a map $\tilde{P}_{i+1} = \tilde{T}(\tilde{P}_i)$ of the annulus onto itself (An annulus is defined as the part of the cylinder (p,θ) which is limited by two circular sections $p = \rho_o$ and $p = \rho_1$) which satisfies

$$\begin{pmatrix} p_{i+1} \\ \theta_{i+1} \end{pmatrix} = \tilde{T} \begin{pmatrix} p_i \\ \theta_i \end{pmatrix} = \begin{pmatrix} T_1(p_i,\theta_i) \\ T_2(p_i,\theta_i) \end{pmatrix} \tag{7}$$

where

1) T_1 and T_2 are differentiable in p and θ with continuous derivatives. $\tilde{T}$ is area preserving and invertible,

2) T_1 and T_2 have period 2π with respect to the variable θ,

3) For any fixed value of θ, $T_2(p,\theta)$ is a strictly monotonous function of p,

4) The two boundaries of the annulus are invariant by $\tilde{T}$ which also preserves their orientation.

This standard map $\tilde{T}_s$ in (6) allows one to represent any stationary configuration of model (1) modulo 2a (which can be either physically stable or unstable) by a trajectory in the dynamical system with the discrete time i and the evolution operator $\tilde{T}_s$. But let us emphasize again, that our specific problem is not to find the properties of arbitrary trajectories, but to find those which corresponds to physically stable configuration. Let us also emphasize that the physical stability of a configuration must not be confused with the stability in the map of the associated trajectory.

Although our theory was initially developed for a slightly generalized form of model (1), we recently found that the method which we used, can be extended with few changes to a wider class of one dimensional models with first neighbor interactions. The map associated with these models by extremalizing their energy, turns out to include the class of twist maps above defined in (7) but our map $\tilde{T}$ is not necessarily restricted to an annulus. The energy of this class of model (or variational form) which contains model (1) as a particular case is

$$\phi(\{u_i\}) = \sum_i L(u_{i+1},u_i) \tag{8.a}$$

where L(x,y) is an arbitrary function of the two variables x and y which have the following properties:

1) L(x,y) is continuous with a lower bound;

2) L(x,y) is diagonally periodic with period 2a that is for any x and y

$$L(x+2a, y+2a) = L(x,y) \tag{8.b}$$

3) the crossed second derivative of L(x,y) is strictly negative that is there exists a positive constant C such that for any x and y

$$-\frac{\partial^2 L}{\partial x \partial y}(x,y) > C > 0 \tag{8.c}$$

By setting $p_i = \partial L(u_i, u_{i-1})/\partial u_i$, the conjugate variable of u_i, the equation $\partial\phi/\partial u_i = 0$ generates an area preserving map $(p_{i+1}, \theta_{i+1}) = \tilde{T}(p_i, \theta_i)$ with the same properties as the twist map (7) except that it maps the cylinder (or a part of it) onto itself and not necessarily an annulus onto itself.

Our theory[6] introduces a distinction between the concept of minimum energy configuration (m.e. configuration) and the concept of ground-states. The reason for this distinction is that under certain boundary conditions, for example the constraint

$$\lim_{N-N'\to\infty} u_N - u_{N'} = 2a \tag{10}$$

the configuration of model (1) which satisfies this condition and which have the minimum energy is in fact a defect (a soliton in the continuous limit) and is not usually considered as a ground-state. The set of minimum energy configurations is defined as the set of all possible limits of ground-states of finite systems with arbitrary boundary condition at u_N and $u_{N'}$ when N goes to $+\infty$ and N′ goes to $-\infty$. This set of m.e. configurations is called $\mathcal{Q}$. We keep the name ground-state for m.e. configurations which are represented by recurent trajectories in the associated map. (A recurent trajectory returns into any neighborhood of any point of the trajectory). This definition turns out to correspond to the usual intuition of a ground-state (see Ref. 6 for more details). This set is called $\mathcal{G}$ and is included in $\mathcal{Q}$.

We found the topological structure of the sets $\mathcal{Q}$ and $\mathcal{G}$ without any explicit calculation of m.e. configuration. These results are described in the following section 2. Before the description of these results let us briefly explain the general ideas which allows one to find a method which works when some topological and symmetry properties are satisfied.

1) We note that the set $\mathcal{Q}$ is closed for the weak topology that is, the limit of a convergent sequences of m.e. configurations is a m.e. configuration. This property is only a consequence of the fact that the energy of the model depends continuously on the atomic positions.

2) We note the existence of a group of transformation G' which transforms a configuration into other configurations with the same energy. Particularly $\mathcal{Q}$ and $\mathcal{G}$ are invariant by G'. This group G' is defined by the transformations $g_{n,p}$ which transforms a configuration $\{u_i\}$ into:

$$g_{n,p}(\{u_i\}) = \{u_{i+n}-2pa\} \tag{12}$$

n and p are two arbitrary integers. This property is a consequence of the homogeneity of the model (all the atoms play an identical role) and of the periodicity condition (10.b).

3) Condition (10.c) allows to prove the fundamental lemma which is:

Fundamental lemma Let $\{u_i\}$ and $\{v_i\}$ be two m.e. configurations. then the sequence (u_i-v_i) has at most one node for $-\infty< i < \infty$ (i.e. one change of sign). If the two configurations $\{u_i\}$ and $\{v_i\}$ are asymptotic for $i \to \pm\infty$, the point at infinity must be considered as a node.

Considering a m.e. configuration $\{u_n\}$, the group G' allows one to construct an infinite number of m.e. configurations from which the limits are also m.e. configuration. These m.e. configurations can be compared one with each other with the above fundamental lemma which yields inequalities. By combining these methods in a sequence of proofs which is quite long and complicated,[6] one finds the exact topological structure of the set $\mathcal{Q}$ and $\mathcal{G}$ now described.

2. Topological Structure of the set of m.e. configurations and of ground-state in the extended FK model (proofs in Ref. 6.b).

We first found

Theorem 1. For any m.e. configuration in $\mathcal{Q}$, the limit (11) is defined and does not depend on the way by which $(N-N')$ goes to infinity.

Conversely, for any value of ℓ, there exists a m.e. configuration $\{u_i\}$ in $\mathcal{Q}$ such that the limit (11) be ℓ.

The corresponding trajectory in the twist map have the winding number $\frac{\ell}{2a}$ which is its mean number of revolutions around the cylinder per iteration of the map. Because of this theorem, we can split the set $\mathcal{Q}$ (and $\mathcal{G}$) into subsets $\mathcal{Q}_\ell$ (and $\mathcal{G}_\ell$) which are defined as the configurations in $\mathcal{Q}$ (and $\mathcal{G}$) with winding number $\frac{\ell}{2a}$ and such that:

$$\mathcal{Q} = \bigcup_\ell \mathcal{Q}_\ell \quad \text{and} \quad \mathcal{G} = \bigcup_\ell \mathcal{G}_\ell \tag{13}$$

with for any $\ell \neq \ell'$

$$\mathcal{Q}_\ell \cap \mathcal{Q}_{\ell'} = \emptyset \quad \text{and} \quad \mathcal{G}_\ell \cap \mathcal{G}_{\ell'} = \emptyset \tag{14}$$

The two following theorems describe the structure of $\mathcal{Q}_\ell$ and $\mathcal{G}_\ell$, first for $\frac{\ell}{2a}$ an irrational number and next for $\frac{\ell}{2a}$ a rational number.

<u>Theorem 2</u>. Let $\frac{\ell}{2a}$ be an irrational number then:

1) The set $\mathcal{Q}_\ell$ of m.e. configurations of the above defined extended FK models, is non-void and is totally ordered that is if $\{u_i\} \neq \{v_i\}$ both belongs to $\mathcal{Q}_\ell$ then for all n either

$$u_n < v_n \tag{15.a}$$

or

$$u_n > v_n \tag{15.b}$$

2) The whole set $\mathcal{G}_\ell$ of ground-states configurations of model (8) ($\mathcal{G}_\ell \subset \mathcal{Q}_\ell$) is nonvoid and can be parametrized with one or two hull functions f(x) which are strictly increasing. a) When f(x) is continuous, a unique function allows one to parametrize the full set $\mathcal{G}_\ell$. b) When f(x) is discontinuous, two determinations $f^+(x)$ and $f^-(x)$ are necessary to parametrize $\mathcal{G}_\ell$. $f^+(x)$ and $f^-(x)$ correspond the right continuous and the left continuous determination of the same discontinuous, strictly increasing function. In other words, we have:

$$\lim_{\substack{\delta\to 0\\ \delta>0}} f^-(x+\delta) = f^+(x) \tag{16.a}$$

and

$$\lim_{\substack{\delta\to 0\\ \delta<0}} f^+(x+\delta) = f^-(x) \tag{16.b}$$

c) When $f^\pm(x)$ is discontinuous at x_o, it is also discontinuous at the points $x_o+h\ell+2ka$ where h and k are arbitrary integers. As a result, the set of discontinuity points of $f^\pm(x)$ is dense on the real axis.

d) Functions $g^{\pm}(x) = f^{\pm}(x)-x$ are periodic with the period 2a of $L(x,y)$.

e) Finally, for any ground-state which belongs to $\mathcal{G}_\ell$, there exists a phase α and a determination of f: f^+ or f^- when f is discontinuous (the determination is unique when f is continuous) such that

$$u_n = f^{\pm}(n\ell+\alpha) = n\ell+\alpha+g^{\pm}(n\ell+\alpha) \tag{17}$$

Conversely, any configuration $\{u_n\}$ defined by (17) for an arbitrary phase and one of the two determinations f^+ or f^- when f is discontinuous, is a ground state in $\mathcal{G}_\ell$.

This hull function f(x) obviously depends on $\frac{\ell}{2a}$. A configuration $\{u_n\}$ as defined by (17) is called incommensurate. It describes a crystal structure of atoms at distance ℓ which is modulated by the function g with the period 2a incommensurate with ℓ. Let us now describe the structure of $\mathcal{Q}_\ell$ and $\mathcal{G}_\ell$ for $\frac{\ell}{2a}$ rational.

<u>Theorem 3</u>. Let $\frac{\ell}{2a} = \frac{r}{s}$ be a rational number. (r and s are two irreducible integers). Then

1) The set $\mathcal{G}_\ell$ is nonvoid and is totally ordered. (i.e. for $\{u_i\} \neq \{v_i\}$ in $\mathcal{G}_\ell$ then for all n we have either (15.a) or (15.b).)

2) For any $\{u_i\}$ in $\mathcal{G}_\ell$, we have for all n

$$u_{n+s} = u_n + 2ra \tag{20}$$

(This ground-state is called commensurate. It has a unit cell of s atoms with length 2ra.)

3) When the set $\mathcal{G}_\ell$ is continuous, which means that it can be parametrized by continuous functions $\{u_n(\alpha)\}$ where α is a continuous parameter which varies from $-\infty$ to $+\infty$ (for example u_o), then $u_n(\alpha)$ is a

continuous strictly increasing function of α and we have

$$\mathcal{Q}_\ell = \mathcal{G}_\ell \tag{21}$$

4) When $\mathcal{G}_\ell$ is a discontinuous set, it is closed and there exists for each discontinuity a couple of ground-states $\{v_n^-\}$ and $\{v_n^+\}$ in $\mathcal{G}_\ell$ such that there exists no ground-states in $\mathcal{G}_\ell$, $\{v_n\}$ which satisfies for all n

$$v_n^- < v_n < v_n^+ \tag{22}$$

Then, there exists a m.e. configuration $\{u_n\}$ in $\mathcal{Q}_\ell$ such that for all n

$$v_n^- < u_n < v_n^+ \tag{23.a}$$

and

$$\lim_{n\to+\infty} (v_n^+ - u_n) = 0 \tag{23.b}$$

$$\lim_{n\to-\infty} (u_n - v_n^-) = 0 \tag{23.c}$$

Such a configuration $\{u_n\}$ is called an "advanced elementary discommensuration". There also exists m.e. configurations $\{u_n\}$ in $\mathcal{Q}_\ell$ called "delayed elementary discommensuration" such that for all n

$$v_n^- < u_n < v_n^+ \tag{24.a}$$

and

$$\lim_{n\to-\infty} (v_n^+ - u_n) = 0 \tag{24.b}$$

$$\lim_{n\to\infty} (u_n - v_n^-) = 0 \tag{24.c}$$

5) The union of $\mathcal{G}_\ell$ and of the set of advanced elementary discommensurations in Q_ℓ is called Q_ℓ^+. Identically, the union of $\mathcal{G}_\ell$ with the set of delayed elementary discommensurations is called Q_ℓ^-. Then Q_ℓ^+ and Q_ℓ^- are totally ordered sets (with the definition given in (15)) and we have

$$Q_\ell = Q_\ell^+ \cup Q_\ell^- \tag{25.a}$$

$$\mathcal{G}_\ell = \mathcal{G}_\ell^+ \cup \mathcal{G}_\ell^- \tag{25.b}$$

This theorem proves that when the boundary condition (11) is satisfied with $\frac{\ell}{2a}$ a rational number, then the ground-state is indeed commensurate and satisfies (20). It can be obtained by finding the absolute minimum of the energy per unit cell with this condition (20). There generally exists s minima (modula 2a) (r and s are irreducible integers) because of the invariance of the energy per unit cell under the s cyclic permutations $\{u_n\} \to \{u_{n+p}\}$ $p = 1, 2, \ldots s$. It may also exist ks minima (for example k = 2 is possible if the model has a symmetry by reflexion) or also a continuum of minima but these two situations are exceptional.

In this theorem, we distinguish two different situations. The situation where $\mathcal{G}_\ell$ is a continuous set is found for example in the case of integrable maps. It corresponds to the absence of locking of the commensurate configurations by the lattice and can be considered as exceptional. The situation, where $\mathcal{G}_\ell$ is discontinuous turns out to be the most general case. Then, the lattice locking does not vanish. This is a necessary and sufficient condition to have discommensurations (see Fig. 2). These ones are called elementary because they correspond to the minimum energy of the system for certain boundary conditions similar to (10). They were already known as solitons in continuous models for incommensurate structures.[10] Thus, we also prove there existence (under certain conditions) in a discrete model for any commensurability ratio r/s.

Since any twist map (7) corresponds to a variational form (8) for some choice of L(x,y), these theorems predicts the existence of certain trajectories in the twist map with particular properties as a corollary of theorems 1, 2 and 3:

Let ω_o be the winding number of $\tilde{T}$ (defined by (7)) on the invariant circle $p = \rho_o$ and ω_1, its winding number on the invariant circle $p = \rho_1$. In order to fix the ideas, we assume that $\omega_o < \omega_1$. Then for any $\omega_o \leq \omega \leq \omega_1$, there exists a trajectory with winding number ω. If ω is an irrational number, this trajectory is quasi-periodic (in an extended sense because function f in (17) is not necessarily continuous) and is dense either on a continuous closed loop or on a Cantor set which is parametrized by the function $f^{\pm}$ in (17). (This result has also been recently proved by Mather.[24]) If ω is rational number r/s, it is a periodic cycle $\{F_i\}$ i = 1, ... s with period s ($\tilde{T}^s(F_i) = F_i$). When the set of periodic cycles with period s of $\tilde{T}$ does not form a closed continuous loop around the cylinder, (unlike certain integrable twist maps) there exists initial points h which by applying the transformations T^{sn} are asymptotic to one of the points F_i of the periodic cycle for $n \to -\infty$ and to another point F_j of the same periodic cycle for $n \to +\infty$. (These points F_i and F_j are in consecutive order with the order relation given in (23)) Such points are called in mathematics, heteroclinic points. This point h belongs to the intersection of two curves (see Fig. 3): the dilating sheet W_i^+ of F_i which is the set of points which converge to F_i by iterating the transformation $\tilde{T}^s$ and the contracting sheet W_j^- of F_j which is the set of points which converge to F_j by $\tilde{T}^s$. Let us note that the point F_i must be linearly unstable with respect to $\tilde{T}^s$ (that is the Jacobian matrix of $\tilde{T}^s$ at F_i has a real eigenvalue with modulus larger than one) in order to be allowed to apply a theorem which predicts the existence of a dilating sheet W_i^+ (Ref. 11). It may happen, although F_i is unstable with respect to the operator $\tilde{T}_s$, that its Jacobian matrix has an eigenvalue with modulus one. Then, a proof for the existence of a continuous dilating or contracting sheet is necessary. (We have not yet performed this proof).

3. Metastable configurations and their corresponding trajectories in the twist map

Theorems 1, 2 and 3 definitely prove that although the equations $\partial\phi/\partial u_i = 0$ exhibits many chaotic solutions, the ground-state of model (8) is never chaotic, whatever is the boundary condition (11), and particularly it has no entropy. Nevertheless, as we already pointed several years ago in Ref. 2 (for the simpler model (1)) model (8) may exhibit for certain boundary conditions (11) metastable configurations which are chaotic but have more energy per atom than the real ground-states. The ground-state which is obtained for the same boundary conditions is called defectible, while if it is the unique metastable configuration, it is called undefectible.

In this section, we investigate some of the necessary properties of the trajectories in the twist map which correspond to metastable configurations. We also investigate the linear stability of the trajectories in the map and shows that this concept of stability is not connected to the physical stability of the corresponding configuration although these two concepts have sometimes been confused in the literature. Let $\{p_i, u_i\}$ be a trajectory of the twist map $\tilde{T}$. The corresponding configuration $\{u_i\}$ is a solution of the equation $\partial\phi/\partial u_n = 0$

$$\frac{\partial L}{\partial u_n}(u_{n+1}, u_n) + \frac{\partial L}{\partial u_n}(u_n, u_{n-1}) = 0 \tag{26}$$

By definition, the physical stability (called metastability) of this configuration $\{u_n\}$ means that the second order expansion of the energy (8) with respect to small atomic displacements $\{\delta_n\}$

$$\delta\phi = \frac{1}{2}\sum_n \left[\left(\frac{\partial^2 L(u_{n+1}, u_n)}{\partial u_n^2} + \frac{\partial^2 L(u_n, u_{n-1})}{\partial u_n^2}\right)\delta_n^2 + 2\,\frac{\partial^2 L(u_{n+1}, u_n)}{\partial u_{n+1}\partial u_n}\,\delta_{n+1}\,\delta_n\right] \tag{27}$$

is a positive quadratic form in $\{\delta_n\}$. This condition is equivalent to the positivity of the phonon frequencies squares obtained from the time Fourier transform of the small motion equations:

$$\omega^2\delta_n = -\frac{\partial\delta\phi}{\partial\delta_n} = \frac{\partial^2 L(u_{n+1}, u_n)}{\partial u_{n+1}\partial u_n}\,\delta_{n+1} + \frac{\partial^2 L(u_n, u_{n-1})}{\partial u_n\partial u_{n-1}}\,\delta_{n-1} + \left(\frac{\partial^2 L(u_{n+1}, u_n)}{\partial u_n^2} + \frac{\partial^2 L(u_n, u_{n-1})}{\partial u_n^2}\right)\delta_n \tag{28}$$

(the atoms have a unit mass and δ_n also denotes the time Fourier transform of $\delta_n(t)$).

For each value of ω, this equation can be recursively solved from the knowledge of δ_o and δ_1. Then the vector (δ_{n+1},δ_n) is a linear function of the vector (δ_n,δ_{n-1}). It is convenient to set the new variables.

$$\pi_n = \frac{\partial^2 L(u_n,u_{n-1})}{\partial u_n^2}\,\delta_n + \frac{\partial^2 L(u_n,u_{n-1})}{\partial u_n \partial u_{n-1}}\,\delta_{n-1} \tag{29}$$

in order to find a linear relation

$$\begin{pmatrix} \pi_{n+1} \\ \delta_{n+1} \end{pmatrix} = (\bar{J}(p_a,u_n) - \omega^2\,\bar{R}(p_n,u_n)) \begin{pmatrix} \pi_n \\ \delta_n \end{pmatrix} \tag{30.a}$$

where $\bar{J}(p_n,u_n)$ is the Jacobian matrix of the twist map $\tilde{T}$ at (p_n,u_n) and

$$\bar{R}(p_n,u_n) = \frac{-1}{\partial^2 L(u_{n+1},u_n)/\partial u_{n+1}\partial u_n} \begin{pmatrix} \frac{\partial^2 L(u_{n+1},u_n)}{\partial u_n^2} & 0 \\ 0 & 1 \end{pmatrix} \tag{30.b}$$

When $\omega = 0$, Eq. (28) to be solved, only needs to perform the product of Jacobian matrices:

$$\bar{M}_n(p_o,u_o) = J(p_n,u_n)\,J(p_{n-1},u_{n-1}) \cdots J(p_o,u_o) \tag{31}$$

Otherwise, the behavior of $\bar{M}_n$ for n going to infinity just determines the Lyapounov exponent γ of this trajectory by the definition

$$\gamma = \lim_{n\to+\infty} \frac{1}{2n} \ln ||\bar{M}_n^t \cdot \bar{M}_n|| \tag{32}$$

When γ is zero, the trajectory $\{p_n, u_n\}$ is called linearly stable. Because this matrix product does not diverge (or slowly diverges) we can prove[8] that the zero frequency belongs to the phonon spectrum given by Eq. (28).

When γ is not zero, the trajectory $\{p_n, u_n\}$ is unstable with respect to the initial conditions. Then, the zero frequency may not belong to the phonon spectrum, but if it does belong, the corresponding eigenstates in the neighborhood of the zero frequency are necessarily exponentially localized.

As a result, one sees that the linear stability of the trajectory $\{p_n, u_n\}$ only gives informations on the spectrum of the small motion equation at the frequency zero, but no informations on the physical stability of the corresponding configurations. Indeed, our previous papers exhibit examples of trajectories which are either linearly stable or unstable in the twist map and for which the corresponding configurations are either stable or unstable or vice-versa (see for example Ref. 21). However, one can use the recursive relation (30) in order to find a necessary condition for the physical stability of the stationary configurations satisfying (26). Because of the condition (8.c) the off diagonal terms of the Jacobi matrix (A Jacobi matrix is a symmetric tridiagonal matrix) defined by the Eq. (28) or by the quadratic form (27), are all negative. Then, it can be proved[8] that

Theorem 4. A trajectory in a two-dimensional map (associated to a one-dimensional model with first neighbour interactions) corresponds to a metastable configuration if and only if, any sequence δ_n $(-\infty < n < +\infty)$

generated from any arbitrary initial condition (π_o,δ_o) by the product along this trajectory of the Jacobian matrices (3)), has at most one change of sign.

Note that this theorem also applies to model (8) when the periodicity condition (8.b) is dropped. The map is then on the two dimensional plane and not on the cylinder. The proof of this theorem is an application of the theory of Jacobi matrices. (See for example Ref. 13). (A well-known corollary of this theory, asserts that the eigenenergies of a one dimensional Schröedinger equation are in the same order than the number of nodes of the corresponding eigenstates.) This theorem have straightforward applications for predicting the physical unstability of the configurations corresponding to certain trajectories. We have with the same hypothesis as in theorem 4.

Corollary of theorem 4. The configurations corresponding

1) To a periodic cycle which is elliptic;
2) To a periodic cycle which is hyperbolic (or parabolic) with reflexion; and
3) To trajectories dense on one or several differentiable tori (KAM tori) which are homotopic to zero are physically unstable.

(A more complicated proof of this corollary was already given in Ref. 21, appendix A and B. This result was also given in Ref. 2.) For its proof, we first examine the case of a periodic cycle of the twist map with period s. We consider the sequence of matrices $\bar{M}_{ks}$ in (31) which is equal to $\bar{M}_s^k(p_o,u_o)$. When the periodic cycle is elliptic, the matrix $\bar{M}_s$ is by definition equivalent to a rotation (in nonorthogonal axis), then the vector (π_{ks},δ_{ks}) is rotating on an ellipse around the origin. Therefore, the sequence δ_{ks} (and also δ_n) have infinitely many changes of sign which by theorem 4 proves the first assertion of the corollary. When the periodic cycle is hyperbolic with reflexion, by definition, the matrix $\bar{\bar{M}}_s$ has two real negative eigenvalues with product 1. If (π_o,δ_o) is chosen to be an eigenvector of $\bar{\bar{M}}_s$, the signs of δ_{ks} change for each consecutive k, because the corresponding eigenvalue is negative. The sequence δ_{ks} has then infinitely many changes of sign which proves the second assertion of the corollary.

When the trajectory $\{p_n,u_n\}$ is rotating and dense on a set of s differentiable tori (KAM tori) which are homotopic to zero (which means that they can be shrunk continuously on the manifold of the map), the configuration $\{u_n\}$ can be parametrized with s periodic differentiable functions g_1, g_2 .. g_s with period 2π

$$u_{ks+p} = g_p(k\theta+\alpha) \tag{33}$$

where α is arbitrary phase and θ is the average of the angle of rotation of $\tilde{T}^s$ on each torus which is incommensurate with 2π. By inserting (33) in (26) and by differentiating with respect to the phase α, it comes out that

$$\delta_{ks+p} = g_p'(k\theta+\alpha)$$

is a solution of Eq. (28) for $\omega = 0$ (This sequence (34) is also generated from δ_o and δ_1 by a product of Jacobian matrices). Since the derivative of any periodic function has at most two changes of sign per period, and because $\frac{\theta}{2\pi}$ is irrational, the sequence generated by (34) has infinitely many changes of sign. The third assertion of the corollary is thus proved by theorem 4.

There often exists KAM tori of the twist map which are not homotopic to zero (they go around the cylinder), then the parametrization of the trajectory on this torus takes a form different from (34), which is (as in (17))

$$u_n = n\ell + \alpha + g(n\ell+\alpha) \tag{35}$$

where g is a differentiable function with period 2a. The corresponding configuration i[illegible]ally stable when

$$\delta_n = 1 + g'(n\ell+\alpha) \tag{36}$$

is always positive. We will see in the following section that this condition is always satisfied for such a KAM torus.

As a result, the metastable configurations of model (8) are represented by trajectories which does not satisfy the condition of the corollary of theory 4 and thus can be either

1) Hyperbolic or parabolic periodic cycles without reflexion, or

2) Dense on a KAM torus which <u>not</u> homotopic to zero, or

3) Imbedded in the chaotic region (however, this condition does not imply that they are chaotic).

We have examples for these three cases. However, these conditions are not sufficient to have metastable configurations. Using theorem 4, it is particularly easy to check numerically the physical stability of the configuration corresponding to a trajectory. It suffices to perform the Jacobian matrix product (31) along a trajectory which is obtained by iterating the map $\tilde{T}$. Then we check the changes of sign of an arbitrary sequence δ_n. All our numerical experiments[14] for a chaotic trajectory have shown that any sequence δ_n exhibit a great density of change of sign. As a result all the observed trajectories which are chaotic in the map correspond to physically unstable configurations. This results confirms the early observation of Shilling and Thomas.[15] But this numerical experiment does not prove that chaotic configuration which are physically stable, does not exist. (In fact, we can prove rigorously their existence in model (1) for λ large enough.) It only suggests that the chaotic metastable configurations are represented by a set of trajectories which have zero measure in the map, and thus are numerically unaccessible because of the limited accuracy of the computer. By contrast, the KAM tori which are nonhomotopic to zero, (when they exist) have a finite measure and are shown to correspond to undefectible ground-states (see the following section 4). We did not prove this conjecture but Ref. 16 gives some other physical arguments which support this assumption.

Consequently, the numerical calculations of the chaotic metastable configurations, are not reliable when they are simply generated by map iterations. In order to avoid these map problems in the chaotic region, we obtained the metastable configurations by a variational method.[14]

Integrating the set of equations

$$\frac{du_i}{ds} = - \frac{\partial \phi}{\partial u_i} \tag{37}$$

with respect to the variable s, yields a solution $\{u_i(s)\}$ which, for any initial configuration $\{u_i(0)\}$, converges to a limit $\{u_i^\infty\}$ which is necessarily a metastable configuration. A special choice of the initial conditions which is given by theorem 1 in Ref. 6-a or 4, or theorem 2 in Ref. 6-b (but a symmetry hypothesis is also required to have this theorem) yields a limit which is a ground-state. (The solutions shown in Fig. 1 of Ref. 4 were calculated by this way). It seems that the problem of studying the physical stability of the configurations generated by map iterations, has not been carefully considered in some of the recent publications on this subject (see for example Ref. 18 and 19). In the second reference[19] it is particularly obvious, in virtue of the corollary of theorem 4 that the configurations which are represented by KAM tori homotopic to zero, cannot be ground-states because they are physically unstable. (See also Ref. 16 and 20 for a more detailed comment of these references).

4. General theorems on the transition by breaking of analyticity and the Peierls Nabarro barrier

We turn back to the study of the ground-states which have been done in section 2. Theorem 2 considered two situations for the incommensurate ground-states of model (8). In the first situation, the hull function is continuous (and generally analytical in analytical models because of the KAM theorem). In the second situation, the hull function becomes discontinuous on a dense set of points. In model (1), the variation of the parameter λ allows one to get a transition from the first situation to the second one. We called this transition: transition by breaking of analyticity.[2] We noted that this transition corresponds to the occurrence of a lattice locking on the incommensurate ground-states that is in other words the occurrence of a finite Peierls Nabarro barrier (noted hereafter PN barrier) which must be passed through for translating continuously the incommensurate ground-state. In this section, we describe some of the exact results which we obtained on the PN barrier and the transition by breaking of analyticity. The application of these results to the standard map allows one to easily obtain bounds for the stochasticity threshold.

Let us first examine the case for which $\frac{\ell}{2a}$ is a rational number and $\mathcal{G}_\ell$ is a discontinuous set (theorem 3).

It is proven that it is impossible to continuously slide the corresponding commensurate ground-states without passing energy barriers. We also recently proved[(8)] that there necessarily exists another stationary commensurate configuration $\{v_n\}$ which just corresponds to the top in energy of the continuous paths corresponding to the translation of the commensurate ground-state (by keeping it commensurate) which pass the lowest possible barrier for the energy per unit cell. The periodic cycles of the twist map corresponding to the commensurate ground-state $\{u_n\}$ (which are hyperbolic or exceptionally parabolic without reflexion) and the periodic cycle corresponding to this commensurate configuration $\{v_n\}$ (which are either elliptic, or hyperbolic or parabolic with reflexion in both cases) are those which have been considered by Greene[(9)] for studying the stochasticity threshold of the KAM tori in the standard map. When $\mathcal{G}_\ell$ is discontinuous, we know that there exists elementary advanced and delayed discommensurations. Let $\{u_n\}$ be for example an advanced discommensuration and $\{v_n^+\}$ and $\{v_n^-\}$ the two commensurate ground-states with the properties described in (23). The configuration $\{v_{n+s}-2ra\}$ is also an advanced discommensuration which satisfies the same conditions (23). It corresponds to the discommensuration $\{v_n\}$ translated by $-s$ lattice spacings or equivalently by a unit cell of the commensurate ground-state. To defined the Peierls Nabarro barrier of this discommensuration, we consider a continuous path $\mathcal{C}(t) = \{w_n(t)\}$ such that

$$\mathcal{C}(0) = \{w_n(0)\} = \{u_n\} \tag{38.a}$$

and

$$\mathcal{C}(1) = \{w_n(1)\} = \{u_{ns}-2ra\} \tag{38.b}$$

It joins the two translated configurations the energy difference (which is proved to be finite)

$$E(\mathcal{C}(t)) = \underset{t}{\mathrm{Sup}}\ \phi(\{w_n(t)\} - \phi(\{u_n\}) \tag{39}$$

is the energy barrier which is passed through for the translation of this discommensuration along the path $\mathcal{C}(t)$. The PN barrier of the discommensuration $\{v_n\}$ is defined as

$$E_{PN}(\{v_n\}) = \underset{\mathcal{C}(t)}{\mathrm{Inf}}\ E(\mathcal{C}(t)) \tag{40}$$

which is the lowest energy barrier which must be passed for a continuous translation of the discommensuration.

We pointed in section 2 that an advanced discommensuration is represented by the trajectory of an heteroclinic point h which belong to the intersection of the dilating sheet W^+ of the point F_i^-, (which is the initial point of the trajectory corresponding to $\{v_n^-\}$) and to the contracting sheet W^- of the point F_j^+ corresponding to $\{v_n^+\}$ (F_i^- and F_j^+ are fixed points for the twist map). Then we prove

Theorem 5 The Peierls Nabarro barrier of an elementary discommensuration vanishes if and only if the dilating sheet W^+ of F_i^- and the contracting sheet W^- of F_j^+ merge into a unique continuous curve which joins F_i^- to F_j^+. (The merged curve which correspond both to W^+ and W^-, is called a separatrix.)

It is the situation which occurs in integrable maps. Thus this theorem proves that if the PN barrier does not vanish, the map cannot be integrable. However, we have not yet completely elucidated the nature of the intersection of W^+ and W^- when this PN barrier does not vanish. We expect that the intersection of W^+ and W^- is always transverse or in other words that the curve W^+ and W^- are not tangen. at their intersection.

Now, we turn back to the case of the incommensurate ground-states. We can prove several theorems. The two first ones deal with the case for which there exists in the twist map an invariant continuous and closed curve Γ_ℓ which is nonhomotopic to zero and on which the twist map is conjugate to a rotation with winding number $\frac{\ell}{2a}$. In other words, a trajectory $\{p_n, u_n\}$ on this curve Γ_ℓ can be parametrized by a continuous hull function $f_k(x)$ such that for all n

$$u_n = f_k(n\ell+\alpha) \tag{41}$$

with $f_k(x)$-x periodic with period 2a (α is some arbitrary phase) then we proved the following theorem[4,8]

Theorem 6 Let us assume the existence of an invariant continuous curve Γ_ℓ on which the twist map is conjugate to a rotation with winding number $\frac{\ell}{2a}$, then this set Γ_ℓ is identical to the set of trajectories representing the ground-state of $\mathcal{G}_\ell$. (This theorem also applies when $\frac{\ell}{2a}$ is rational).

Particularly, this cure Γ_ℓ can be a KAM torus with an irrational winding number $\frac{\ell}{2a}$. When this KAM torus exists, it necessarily represents the set of ground-state $\mathcal{G}_\ell$. Since we know that when KAM tori exists, they have a finite measure on the cylinder, most of them (that is with probability 1 can be approached by sequences of KAM tori with winding numbers $\ell_i/2a$ such that ℓ_i goes to ℓ either with $\ell_i > \ell$ or $\ell_i < \ell$. Let us call these tori "true" KAM tori. Most KAM tori are "true". Then, we have the theorem.

Theorem 7 When the set of incommensurate ground-state $\mathcal{G}_\ell$ is represented by a "true" KAM torus Γ_ℓ, then the incommensurate ground-states of $\mathcal{G}_\ell$ are undefectible (by definition a ground-state is called undefectible, when, apart a phase shift, it is the only metastable configuration of the system with the same boundary conditions (11)).

In the situations, considered by theorem 6 and 7, the PN barrier which corresponds to the translation of the incommensurate structure is zero. Then the gap in the phonon spectrum of the incommensurate ground-state $\{u_n\}$ given by Eq. (28) is proven to vanish. (The gap is the smallest phonon frequency given by 28). Conversely a finite PN barrier does not imply a finite gap although generally they are both finite (or both zero). However when the gap is finite, we obtained the following theorem which have a quite complicated proof.[8]

Theorem 8 Let $\{u_n\}$ be an incommensurate ground-state of model (8). Let us assume that the gap in frequency of the small motion Eq. (28) be strictly positive. Then, the hull function f describing the incommensurate ground-state is discrete (see theorem 2). In other words, $f^{\pm}(x)$ can be written as a sum of step functions.

$$f^{\pm}(x) = \sum_i f_i \; Y^{\pm}(x-x_i) \tag{42}$$

where f_i is the amplitude of the step function located at x: (By definition $Y^{\pm}(x) = 0$ for $x < 0$, $Y^{\pm}(x) = 1$ for $x > 0$ and $Y^{+}(0) = 1$

$Y^{-}(0) = 0)$. Then, the Lyapounov exponent γ given by (32) for this incommensurate ground-state is strictly positive.

For reasonably differentiable models 8, we conjectured in Ref. (6-a) that the hull function f of an incommensurate ground-state should be either

1) absolutely continuous that is f(x) is differentiable almost everywhere

$$f(x_1) - f(x_o) = \int_{x_o}^{x_1} f'(\zeta)d\zeta \qquad (43)$$

or 2) singular continuous (f(x) is continuous with a zero derivative almost everywhere) or 3) discrete (f(x) is discontinuous and can be written with the form (42)).

We have not rigorously proven this conjecture but we have shown in Ref. 4 that model (1) exhibits situations for which the hull function f is either analytical or discrete. The following section 5 reports these proofs with more detaiis which yields incidently a series of exact upper bounds for the transition by breaking of analyticity or equivalently for the stochasticity threshold of the standard map.

5. Existence proof and Exact bounds for the transition by breaking of analyticity in the standard map

In the standard map (6) associated with model (1), the Kolmogorov Arnold Moser theorem[5,23] predicts that for almost any irrational $\frac{\ell}{2a}$, there exists $\lambda_2(\ell)$ such that for $|\lambda| < \lambda_2(\ell)$, there exists an invariant torus on which the map is conjugate to a rotation with winding number $\frac{\ell}{2a}$. Then applying theorem 6 yields that the trajectories of this KAM torus represent the ground-states of $\mathcal{G}_\ell$ and that their hull function is differentiable. Conversely, when λ becomes large enough the intuitive image of the problem, suggests that the atoms locate in the bottoms of the periodic potential and thus that the function f becomes discrete.

This hull function satisfies the functional equation

$$F(x) = f(x+\ell) + f(x-\ell) - 2f(x) = \frac{\lambda\pi}{2a} \sin(\frac{\pi}{a} f(x)) \tag{44}$$

which is obtained by inserting (17) in (21). Because of the periodicity property of this model we can restrict our study to the case $0 < \ell < 2a$. Since f(x) is monotonous increasing it comes out that for any x

$$f(x+\ell-2a) < f(x) < f(x+\ell) \tag{45.a}$$

These inequalities (45) in (44) yields

$$|F(x)| < 2a \tag{45.b}$$

As a result, when

$$\lambda > \frac{4a^2}{\pi} > \lambda_c \tag{46}$$

Eq. (44) and inequality (45.b) shows that the hull function $x+g(x) = f(x)$ cannot take any value $(2n+1)/a$ where n is an integer. Consequently f(x) must be discontinuous and because of theorem 6 there exist no invariant continuous curves which are nonhomotopic to zero on which the standard map is conjugate to a rotation. As a result, there exists no KAM tori for any winding number. Then inequality (46) gives a rigorous upper bound for the stochasticity threshold $\hat{\lambda}_c$ for the standard map which have been calculated by Greene[9] and which is in our units

$$\hat{\lambda}_c \# 0.9716 \times \frac{2a^2}{\pi^2} = \operatorname*{Sup}_{\ell} \lambda_c(\ell) \tag{47}$$

In fact this bound can be improved by only considering the positivity of the quadratic form (27)

$$\delta\phi = \frac{1}{2} \sum_n \left[\left(2 + \frac{\lambda\pi^2}{2a^2} \cos \frac{\pi}{a} u_n)\right) \delta_n^2 - 2\delta_{n+1}\delta_n \right] \tag{48}$$

for any ground state $\{u_n\}$. Assuming that the hull function $f(x)$ be continuous, it is possible to choose the phase α such that

$$u_o = f(\alpha) = a \tag{49}$$

(where we expect that the discontinuity of f should first appear) be on the top of the periodic potential. Next, we prove that in certain range of λ, all stationary configuration $\{u_n\}$ with $u_o = a$, are such that their quadratic form (48) is not positive. No ground-state can exist with a continuous hull function whatever is the atomic mean distance and consequently no KAM torus nonhomotopic to zero can exist. For this proof we set

$$u_1 = x \tag{50.a}$$

The stationary Eq. (2) yields

$$u_{-1} = 2a-u \ , \ u_2 = 2x-a + \frac{\lambda\pi}{2a} \sin\left(\frac{\pi}{a} x\right) \ , \ u_{-2} = 2a - u_2 \ , \tag{50}$$

For convenience, we also set

$$\Lambda = 2 - \frac{\lambda\pi^2}{2a^2} \tag{51.a}$$

$$X = 2 + \frac{\lambda\pi^2}{2a^2} \cos \frac{\pi}{a} x \tag{51.b}$$

$$Y = 2 - \frac{\lambda\pi^2}{2a} \cos \frac{\pi}{a} (2x + \frac{\lambda\pi}{2a} \sin \frac{\pi}{a} x) \tag{51.c}$$

First, we consider the minor of order 1, $\Delta_1 = A$. When it is negative, the quadratic form (48) cannot be positive. For

$$\lambda > \frac{4a^2}{\pi^2} > \hat{\lambda}_c \tag{52}$$

A is negative and there exist no KAM tori. Second, when $\lambda < 4a^2/\pi^2$ we consider the minor of order 2

$$\Delta_2 = \begin{vmatrix} A & -1 \\ -1 & X \end{vmatrix} = A\,X - 1 \tag{53.a}$$

when $\lambda < 4a^2/\pi^2$. It is smaller for any x than

$$\left(2 - \frac{\lambda\pi^2}{2a^2}\right)\left(2 + \frac{\lambda\pi^2}{2a^2}\right) - 1 = 3 - \left(\frac{\lambda\pi^2}{2a^2}\right)^2$$

Consequently Δ_2 is always negative when

$$\frac{4a^2}{\pi^2} > \lambda > \sqrt{3}\,\frac{2a^2}{\pi^2} > \hat{\lambda}_c \tag{53.b}$$

When this condition is satisfied, there also exists no KAM tori which are nonhomotopic to zero. A third order bound is obtained by considering the minor of order 3

$$\Delta_3 = \begin{vmatrix} X & -1 & 0 \\ -1 & A & -1 \\ 0 & -1 & X \end{vmatrix} = X(AX-2) \tag{54.a}$$

which is negative for any x when

$$\frac{4a^2}{\pi^2} > \lambda > \sqrt{2}\,\frac{2a^2}{\pi^2} > \hat{\lambda}_c \tag{54.b}$$

This inequality improves the upper bounds (46), (52) and (53.a) for the stochasticity threshold $\hat{\lambda}_c$. By considering higher order minors of the quadratic form, we obtain better bounds for λ_c. For example, we considered the order five:

$$\Delta_5 = \begin{vmatrix} Y & -1 & 0 & 0 & 0 \\ -1 & X & -1 & 0 & 0 \\ 0 & -1 & A & -1 & 0 \\ 0 & 0 & -1 & X & -1 \\ 0 & 0 & 0 & -1 & Y \end{vmatrix} = (XY-1)(AXY-2Y-A) \tag{55.a}$$

In order to avoid cumbersome calculations, which in principle are possible, we only checked numerically the sign of (AXY-2Y-A) for $0 < x < 2\pi$ with A, X, Y given by (51). Then, we found that for

$$\sqrt{2} \geq \frac{\lambda\pi^2}{2a^2} > 1.230 \pm 0.005 > \hat{\lambda}_c \tag{55.b}$$

(AXY-2Y-A) is negative for any x. As a result, either Δ_5 or (XY-1) (which also is a minor of the quadratic form (48) is negative. Consequently when (55.b) is satisfied, there exists no KAM tori nonhomotopic to zero which still improves the upper bound of λ_c. Note that this bound 1.230 ± 0.005 is now only 25% above the value (47) calculated by Greene and that this result is a strict bound obtained with a very short numerical calculation. (Note that J. Mather also obtained the bound 4/3 with a method which is apparently different.[24]) We conjecture that the sequence of bounds obtained by writing the positivity for $u_o = a$ of the sequence of minors Δ_n which follows Δ_1, Δ_2, Δ_3, (Δ_4) and Δ_5 converge to the exact value of λ_c but we have not checked numerically this assertion.

Let us turn back to the study of the functional Eq. (44). We reproduce here, for the model (1) the proof of Ref. 4 (which we hope more clear) which shows that for λ large enough the hull function f becomes discrete. When (46) is satisfied, we have

$$\left|\sin \frac{\pi}{a} f(x)\right| \leq \frac{4a^2}{\lambda\pi} \tag{56}$$

which implies that for any x there exists an integer n such that

$$- f_o + na \leq f(x) \leq f_o + na \tag{57.a}$$

with

$$f_o = \frac{a}{\pi} \text{Arcsin} \frac{4a^2}{\lambda\pi} \tag{57.b}$$

We now write that the diagonal terms of the quadratic form (48) is positive which yields another inequality for all x

$$- \frac{4a^2}{\lambda\pi^2} < \cos \frac{\pi}{a} f(x) \tag{58}$$

Otherwise, inequality (57.a) for n odd implies by using (57.b)

$$\cos \frac{\pi}{a} f(x) < \cos \frac{\pi}{a} (f_o+na) = - \left(1 - \left(\frac{4a^2}{\lambda\pi}\right)^2\right) \tag{59.a}$$

When

$$\lambda > \frac{4a^2}{\pi^2} \sqrt{\pi^2+1} \tag{59.b}$$

Inequalities (58) and (57.a) are incompatible for n odd, thus the integer n which appears in (57.a) must be even. As a result, when (59.b) is satisfied, we obtain for all x

$$\cos \frac{\pi}{a} f(x) > \cos \frac{\pi}{a} f_o = \quad 1 - \left(\frac{4a^2}{\lambda\pi} \right)^2 > 0 \tag{59.c}$$

Now, we can apply theorem (8) for proving that function f is discrete by checking that (59.c) implies that the gap of the phonon spectrum is larger or equal to $\sqrt{1 - (4a^2/\lambda)^2}$ and thus strictly positive. But, a direct proof is also quite simple. For that, we prove that the continuous part $F_c(x)$ of $F(x)$ in (44) is a constant by proving that it is both periodic and monotonous increasing.

$F_c(x)$ is periodic because it is the variation $h_c(x+\ell) - h_c(x)$ from x to $(x+\ell)$ of the continuous part of the periodic function $h(x) = f(x) - f(x-\ell) = \ell + g(x) - g(x-\ell)$. (Note however that the continuous part of a periodic function is not necessarily periodic).

$F_c(x)$ is monotonous increasing because in the last member of (44), 1) $f(x)$ is monotonous increasing 2) $\sin(\pi/a\ f(x))$ is strictly increasing in the vicinity of each value taken by $f(x)$ because of the inequality (59.c). As a result, $f(x)$ obtained from $F(x)$ by (44) is also discrete.

The results described in this section rigorously prove the existence of a breaking of analyticity in the standard map although we have not proved that it exactly occurs at a well defined λ_c. Anyway we obtained explicit bounds of λ_c. This transition is numerically found well defined on the Figs. 4 which show the trajectories corresponding to the ground states for $\ell/2a = 441/997$ (which is practically an irrational number) and for $\lambda = 0.167$, $\lambda = 0.20$ and $\lambda = 0.212$. (These ground-states have not been calculated by iterating the standard map because, as we know, it is an unstable process for $\lambda > \lambda_c(\ell)$ but by using the gradient method described by Eq. (37)).

6. Final Remarks on the devil's staircase and the order without periodicity

The above theorems have an application for the theory of the devil's staircase which we briefly describe now.

Let us consider model (8) to which we add a tensile force μ (or chemical potential)

$$\phi_\mu(\{u_i\}) = \sum_i [L(u_{i+1},u_i) - \mu\cdot(u_{i+1}-u_i)] \tag{60}$$

(As for model (1), the addition of this tensile force does not change the twist map associated to this model). The ends of the chain are let free for finding the ground-state of this model, we first consider the average energy per atom (for μ=0)

$$\psi(\ell) = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} L(u_{i+1},u_i) \tag{61}$$

for the ground-state(s) with atomic mean distance ℓ (which we proved to be a well defined function) and we minimize the energy per atom $\psi(\ell)-\mu\ell$. Then, we prove that the atomic mean distance ℓ varies as a devil's staircase versus μ. We have

Theorem 9 The variation curve $\ell(\mu)$ of the atomic mean distance ℓ of the ground-state of model (60) with free ends versus the tensile force μ has the following properties.

1) the curve $\ell(\mu)$ is monotonous increasing and is continuous.

2) for each rational $\frac{\ell}{2a} = \frac{r}{s}$, $\ell(\mu)$ is constant on a finite interval δ if and only if the corresponding set $\mathcal{G}_\ell$ (described in theorem 3) is discontinuous.

In general, when the twist map is not integrable, $\mathcal{G}_\ell$ is not continuous for all rationals ℓ. As a result $\ell(\mu)$ has a constant step at each rational $\frac{\ell}{2a}$.

This curve is called a devil's staircase.[25] In this book, B. Mandelbrot also shows other physical examples which involves such pathological curves. On the basis of solid physical arguments, we conjectured[2,3] that this curve $\ell(\mu)$ is a complete devil's staircase for $\ell_1 < \ell < \ell_2$ when for all irrational $\frac{\ell}{2a}$ in this interval, the set $\mathcal{G}_\ell$ are discontinuous. (By definition, a devil's staircase is called complete[2] when it is entirely composed of steps, or equivalently when $\ell(\mu)$ has a zero derivative almost everywhere, or equivalently when the Stieltjes measure $\ell(\mu)$ has no absolutely continuous part). We also conjectured that it becomes incomplete (that is its derivative becomes finite on a finite measure set) when for some $\frac{\ell}{2a}$ irrational (which have finite measure) the sets $\mathcal{G}_\ell$ are represented by KAM tori. (Let us mention that our theory would become rigorous, if a uniform bound of the exponential interactions between the discommensurations could be obtained). Anyway, we can exhibit exact models (which however have some pathologies) in which a complete devil's staircase[7] can be proved to exist and also explicitly calculated. As we explained in Ref. 2, 3 and 16 a complete devil's staircase physically corresponds to an irreversible but continuous transformation which is a quite unusual behavior. But, indeed similar features been observed in certain experiments.

It has also been experimentally observed structures which are neither periodic or quasi-periodic (incommensurate). Are they chaotic? We generalized some aspects of this theory on the twist maps, to all structures in any dimensions which are obtained from the minimization of an energy (i.e. a variational form). We introduced an abstract dynamical system in which the usual time group is replaced by the translation group of the space in which the structure is imbedded. Using this representation, we proved that there always exists a "minimal invariant closed set" (by definition, it does not contain any smaller closed set invariant under the action of the group) which correspond to a ground-state. Translated in physical terms, this property implies the existence of ground states with a new kind of long range order which could be neither periodic nor incommensurate. We called this new kind of long range order "weak periodicity". It also correspond physically to a "local order at all scales". In Ref. (16), we briefly describe this theory but with some more details than here. Particularly, surprising examples of "undecidable structures" obtained by tiling the plane are given, prove that such strange structures does exist in theoretical models. Moreover they have no entropy. Let us emphasize that our assertions are not in contradiction with those of Ruelle[27] on the existence of "turbulent ground-state" although they seem to disagree. Indeed for D. Ruelle, "turbulent" means nonperiodic and "non-quasi-periodic". With this definition, we agree with his assertion on the existence of turbulent ground-state. However our definition of turbulent is more restrictive because we require that the structure has a finite entropy.

Although, we have no proof, we believe that except in exceptional models with accidental degeneracy, the ground-state of most models obtained by minimizing a free energy has no entropy although it can be neither periodic nor quasi-periodic. It is necessarily "weakly periodic" (but this property is still quite physically imprecise). Of course, we do not exclude defectible ground-states for which there may exist many other metastable configurations. Although they have more energy than the ground-state these configurations should play an important role for the thermodynamical properties of the structure.[16]

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Figure Captions

Fig. 1. Map of the transformation $\tilde{T}_s$ in (6) showing the trajectories of the initial points M_i plotted on the figures for $\lambda = 0.15$ Fig. 1.a, $\lambda = 0.2$ Fig. 1.b and $\lambda = 0.25$ Fig. 1.c. For each initial M_i, about 1000 points of the trajectory $\tilde{T}_s^n(M_i)$ $0 \leq n \leq 1000$ have been plotted. For $\lambda = 0.15$, most trajectories lie on smooth closed curves (KAM tori) except the trajectory generated by M_i which maps a chaotic cloud of points in a narrow area. For $\lambda = 0.2$ this chaotic area becomes much wider while for $\lambda = 0.25$ this chaotic area fills most of the map except in some isolated islands.

Fig. 2. Scheme of an advanced elementary discommensuration $\{u_i\}$ for $\ell/2a = 1/5$. u_i is plotted as a function of i. The phase shift, 2a/5, occurs in the region $14 < i < 15$. Far from this region the configuration is commensurate.

Fig. 3. Scheme showing the initial points of the trajectories in the twist map which represent the commensurate ground-states for $\ell/2a = 2/3$: $F_1 = \tilde{T}(F_3)$, $F_2 = \tilde{T}(F_1)$, $F_3 = T(F_2)$. (These points form a periodic cycle with period 3). The beginning of the dilating sheet of F_1, F_2 and F_3 are also represented with only one intersection point one with each other. The arrow indicates the direction of the motion of a point of the sheet by the twist map. Thus it indicates if the sheet is dilating or contracting. The trajectories generated by the points $h_a^{(1)}$, $h_a^{(2)}$ and $h_a^{(3)}$ correspond to advanced elementary discommensurations. Those generated by $h_d^{(1)}$, $h_d^{(2)}$, and $h_d^{(3)}$ corresponds to delayed elementary discommensurations.

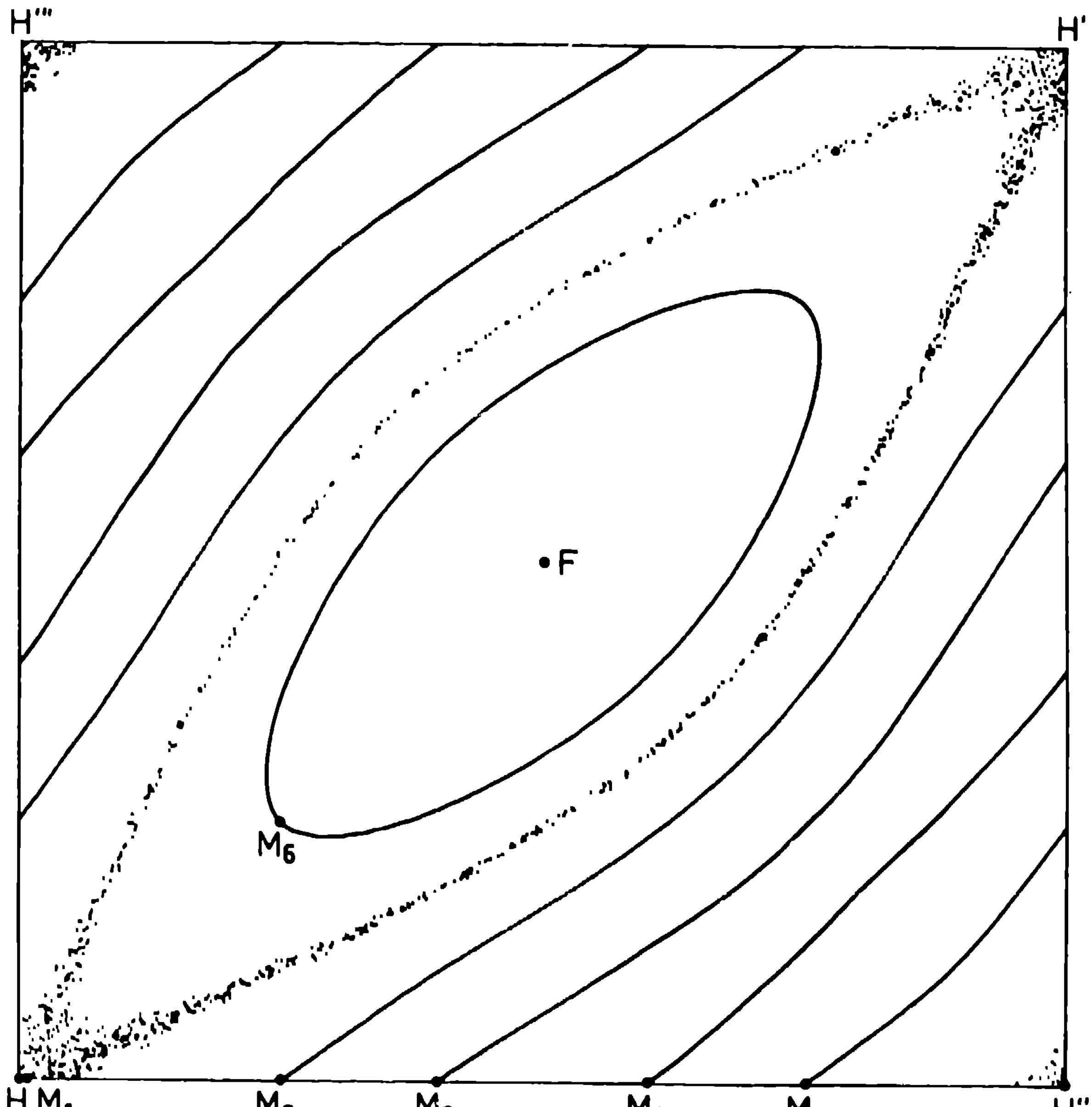
Fig. 4. From Aubry, André (1980) Ref. 4. Trajectories of the map (6) representing the ground-state of the FK model for $\ell/2a = 441/997$ (which is practically an irrational number)

on Fig. 4.a for $\lambda = 0.167$

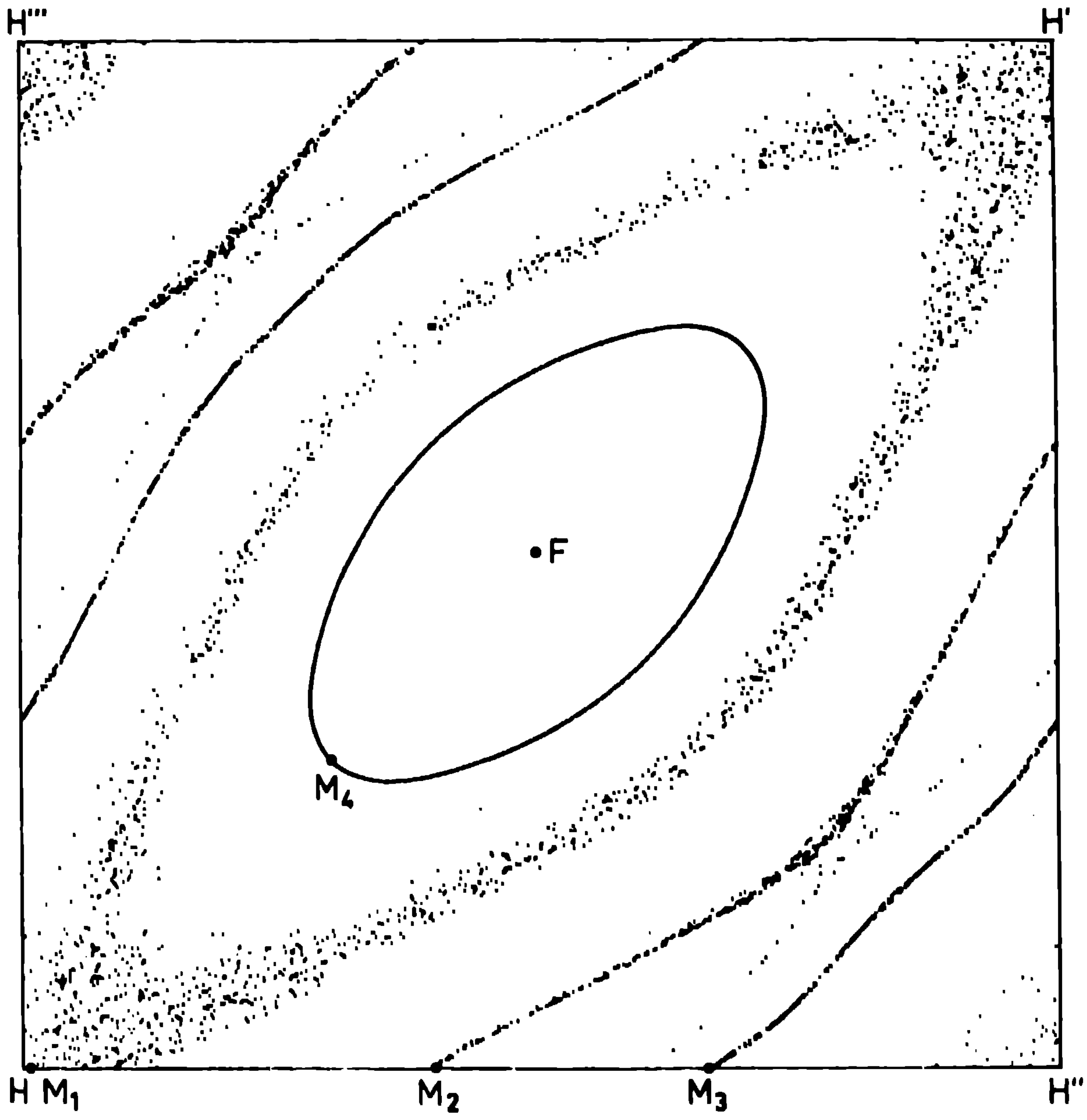
on Fig. 4.b for $\lambda = 0.2$

on Fig. 4.c for $\lambda = 0.212$

Note the sharp change in the aspect of the trajectory which signals the transition by breaking of analyticity at $\lambda_c \# 0.2$. For $\lambda < \lambda_c$ (Fig. 4.a) the trajectory is dense on a KAM torus. At $\lambda \sim \lambda_c$ (Fig. 4.b) the density of a point on the torus exhibits critical fluctuation; while for $\lambda > \lambda_c$ (Fig. 4.c) the trajectory is dense and quasi-periodic on a Cantor set which survives to the KAM torus. Compare with Figs. 1 which exhibits arbitrary trajectories. In fact, all of them corresponds to unstable configurations except those generated by the points M, M, M and M of Fig. 1.a the trajectory of which generate



H'''
H'
F
M6
H M1
M2
M3
M4
M5
H''


H'''
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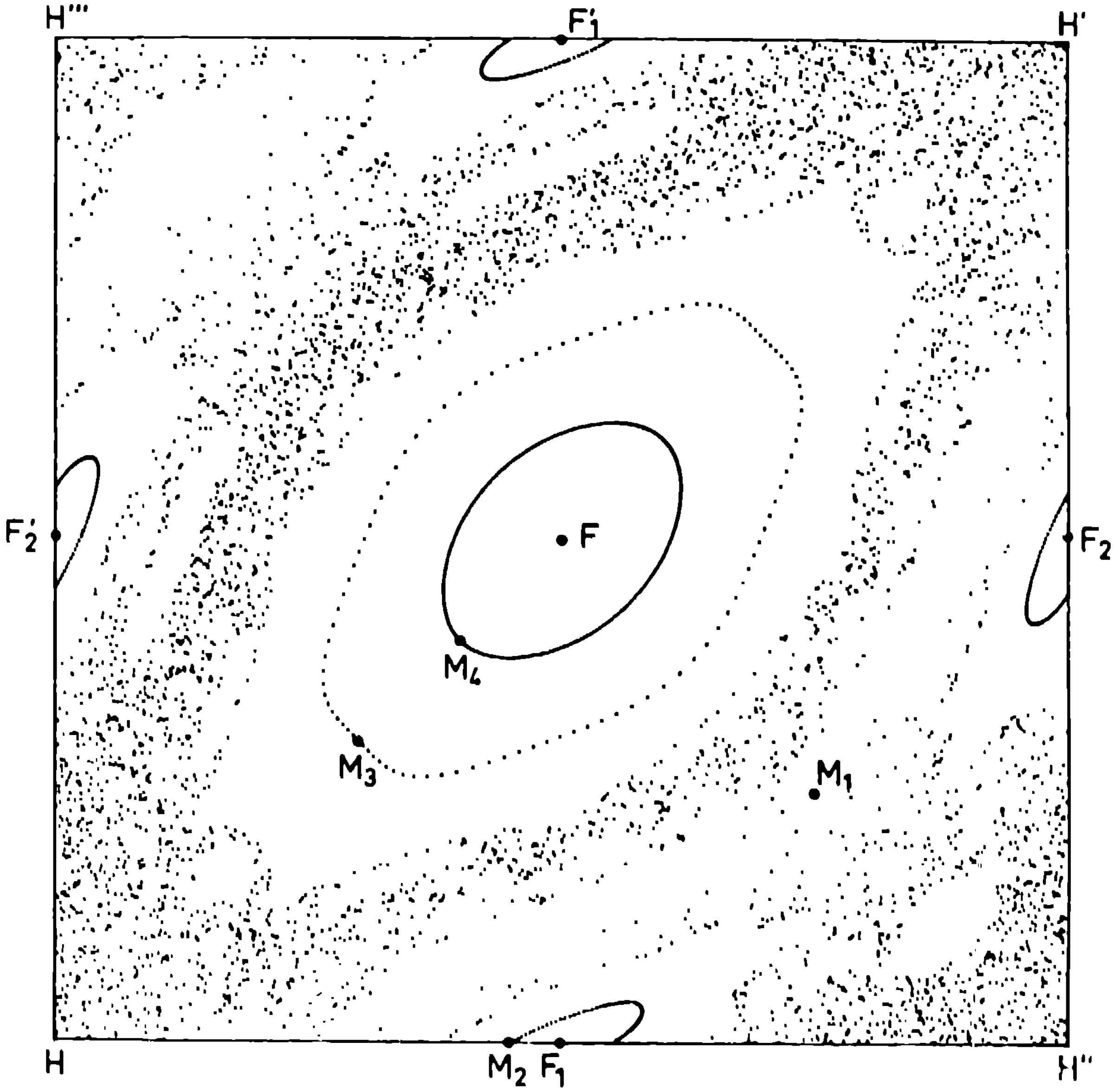
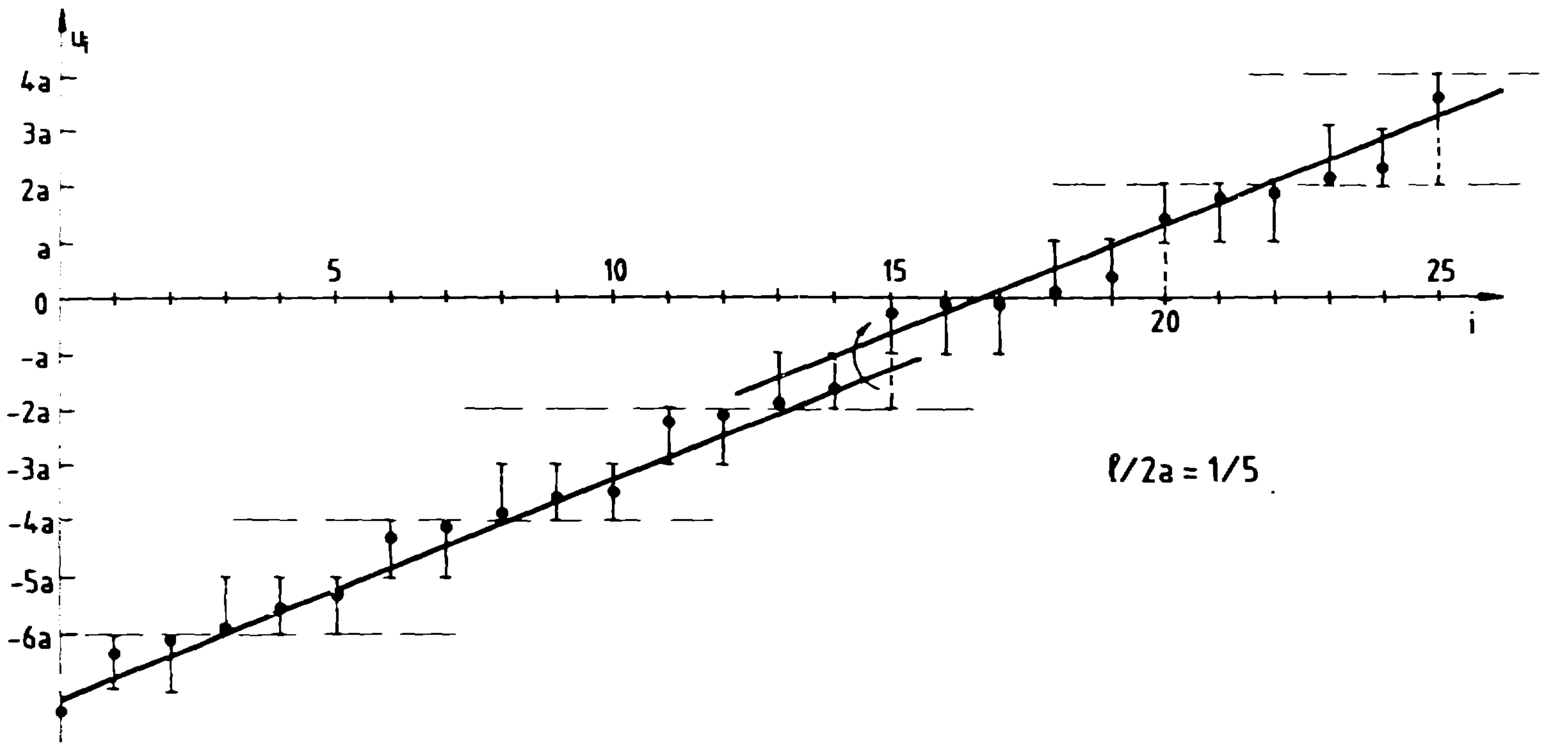
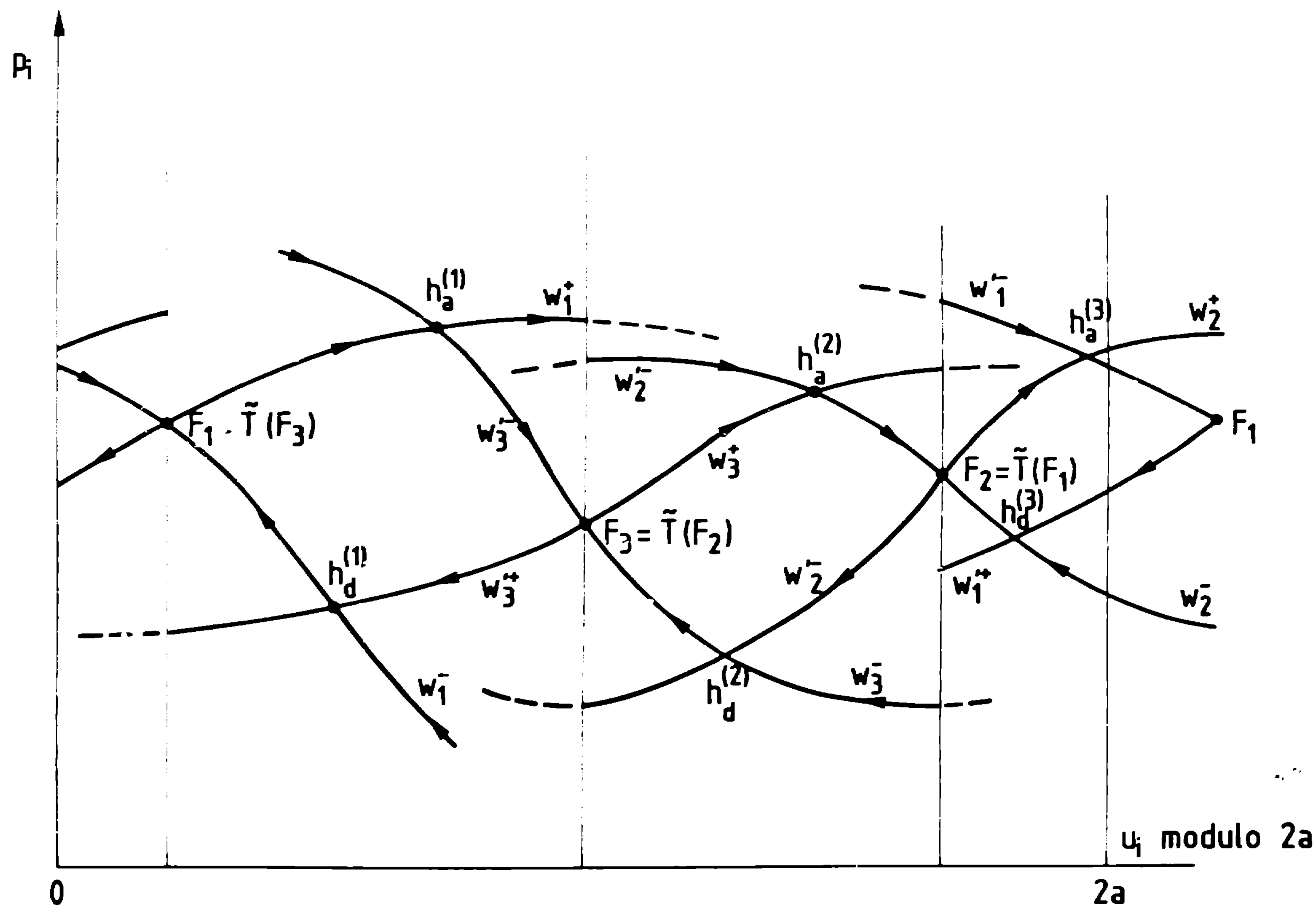


H'''
F'1
H'
F'2
F
F2
M4
M3
M1
H
M2
F1
H''



u_i
4a
3a
2a
a
0
-a
-2a
-3a
-4a
-5a
-6a
5
10
15
20
25
i
ℓ/2a = 1/5



p_i
$h_a^{(1)}$
w_1^+
$w_1^{\prime -}$
$h_a^{(3)}$
w_2^+
$h_a^{(2)}$
$w_2^{\prime -}$
$F_1 \cdot \tilde{T}(F_3)$
$w_3^{\prime -}$
w_3^+
F_1
$F_2 = \tilde{T}(F_1)$
$h_d^{(3)}$
$F_3 = \tilde{T}(F_2)$
$h_d^{(1)}$
$w_3^{\prime +}$
$w_2^{\prime -}$
$w_1^{\prime +}$
w_2^-
w_1^-
$h_d^{(2)}$
w_3^-
u_i modulo 2a
0
2a