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Devil's Staircase and Order
Without Periodicity in Classical Condensed Matter

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ABSTRACT

The existence of incommensurate structures proves that crystal ordering is not always the most stable one for nonquantum matter. Some properties of structures which are obtained by minimizing a free energy are investigated in the Frenkel Kontorova and related models. It is shown that an incommensurate structure can be either quasi-sinusoidal with a phason mode or built out of a sequence of equidistant defects (discommensurations) which are locked to the lattice by the Peierls force. In that situation the variation of the commensurability ratio with physical parameters forms a "complete devil's staircase" with interesting physical consequences. Some general results for all structures which minimize a free energy are given. In addition to the known crystal and incommensurate structures, the existence of a new class of structures which have local order at all scale is predicted. Properties of the new class are described in physical terms and possible applications to certain amorphous or nonstoichiometric compounds are discussed.

L'existence de structures incommensurables prouve que contrairement à une idée très répandue, l'ordre cristallin n'est pas toujours l'ordre le plus stable dans la matière solide non quantique. De nombreuses autres déviations à l'ordre parfait cristallin sont également connues : antiphases dans les alliages, composés non-stoechiométriques, amorphes. Cette grande diversité suggère au premier abord une certaine similitude avec les nombreux comportements d'un système dynamique : mouvements périodiques, quasi-périodiques, chaotiques, intermittents... Cependant, une différence importante tient au fait que la structure de la matière solide tend à la minimisation de son énergie libre, ce qui favorise toujours un certain ordre (à moins que des dégénérescences accidentelles ne conduisent à une structure chaotique avec entropie de configuration).

Des résultats sur un modèle pour les structures incommensurables, que nous pouvons maintenant étendre à une plus large classe montrent que lorsque deux forces tendant à produire des structures de période différente, entrent en compétition, la structure résultante peut être de deux types différents. C'est : 1) soit une structure incommensurable modulée quasi-sinusoidalement avec un mode de glissement de la modulation (phason). 2) soit une structure incommensurable formée par une succession équidistante de défauts (par exemple les discommensurations). Dans ce deuxième cas les défauts sont accrochés au réseau par la force de Peierls (ce qui permet éventuellement des configurations de défauts désordonnées mais en équilibre métastable). En variant, la température ou la pression, le rapport de commensurabilité δ des deux périodes varie. La courbe de variation de δ qui possède une partie constante à chaque valeur rationnelle tout en restant continue, est appelée escalier du diable. Cependant, cette courbe ne se manifeste par des caractères physiques observables différents de ceux d'une transformation réversible et continue que lorsque les configurations rencontrées sont formées de défauts (escalier du diable complet). Des accrochages aux commensurabilités rationnelles deviennent observables et simultanément la transformation physique est irréversible bien que restant continue.

Certaines extensions de cette théorie permettent de prouver en toute généralité, qu'il existe toujours une structure minimisant une énergie libre donnée et présentant au moins un ordre local. Le cas physiquement le plus courant correspond aux structures cristallines et incommensurables (avec phason) qui sont invariants par rapport à un certain groupe de translation (agissant éventuellement dans un hyperespace dans lequel est immergé la structure) cf. de Wolf. Dans le cadre du même formalisme mathématique, on démontre qu'il existe aussi des structures sans période, sans entropie et possédant un certain ordre à grande distance induit par l'ordre local à toutes les échelles. Ces structures de défauts "hyperdiaboliques" qui ont des propriétés très différentes des structures habituelles (irréversibilité, centre tunnel....) pourraient aider à l'interprétation de certaines structures observées dans des amorphes et des composés non stoechiométriques.

I. Introduction. Experimental evidence and questions?

In certain range of temperature, pressure etc... it is experimentally observed that certain crystals spontaneously exhibit a periodic modulation⁽¹⁾ which has a period which is not a rational combination of the three natural periods of the crystal. Strictly speaking, these structures which are called incommensurate, have lost their periodicity. A great number of such compounds have been discovered in the past ten years. In a first approach we can distinguish two main classes; 1) the conducting compounds are the first one. The origin of the force which creates their lattice modulation is known to be an electronic instability. Many of them are one-dimensional conductors such as TTF-TCNQ⁽²⁾ but there exists also two-dimensional conductors⁽³⁾ which becomes periodically modulated at low temperature. In these compounds, the simultaneous occurrence of a static periodic lattice distortion (PLD) and of a static charge density wave (CDW) with the same period, is associated with a metal insulator transition. In one-dimensional conductors, the wave vector of the PLD-CDW is the double of the wave-vector of the electron wave function at the Fermi surface and consequently it can only vary when the number of electrons in the conduction band also varies; 2) the second class is those of insulating compounds such as K_2SeO_4 , $S = C(NH_2)_2$, $(N-(CH_3)_4)_2 ZnCl_4$ ⁽⁴⁾ etc.... In these compounds the origin of the force which creates the periodic modulation is not precisely known but is certainly due to conflicting interactions between the atoms or molecules and may involve in many cases, dipolar interactions. Conversely to one-dimensional conductors, the wave vector of the modulation in insulating compounds is not fixed and it generally varies versus temperature or pressure.

However, many other compounds which are known for a longer time, also exhibit periodic modulations but instead to involve the atomic displacements, it is the local magnetization⁽⁵⁾ or the concentration of two different kinds of atoms (alloys) which is periodically modulated.⁽⁶⁾

Now, we believe that it is important to point out in parallel with the above examples, certain non-stoichiometric compounds which can be produced by chemistry in solid state. Although they have a well defined chemical formula, these ones, instead to be described by integer numbers as usually, contains irrational numbers. One of the more curious example is $\text{Hg}_{3-\delta}\text{AsF}_6$ where the number δ is shown to vary continuously versus the temperature.⁽⁷⁾ At low temperature, its structure exhibits the two incommensurate periods of the mercury chains superimposed to the crystal structure of AsF_6 . Among many examples, we also mention KCP and platinum oxalate⁽⁸⁾ which are also one dimensional conductors. In these compounds, there still exists an underlying crystal structure but the concentration per unit cell of the ions Cl^- or Br^- is apparently an irrational number. This concentration just determine the number of free electrons in the conduction band. However, it is not yet known whether the ions Cl^- or Br^- are randomly distributed or ordered in the host crystal.

The above structures are spontaneous deviations from a perfect crystal order and their existence proves that perfect crystal ordering is not always the most stable one for non-quantum matter. The problem of glasses also is still controverted. Is it always a metastable state? Is it a liquid with a very high viscosity or does it exist a glass transition T_g below which the glass is different from a liquid? And if this one exists, what is the change of structure from a liquid to a

glass? Nevertheless, it has been observed that many glasses have a local order which can extend quite far. Recent attempts⁽⁹⁾ have been done to understand glass structures from a deterministic point of view instead of assuming random distributions of atoms.

We are lead to set the question: how the structure of a material can break the translational symmetry* of the three dimensional space? A crystal keeps a discrete three dimensional translation group under which it is invariant. But intuitively, an incommensurate structure have more translational symmetry than an amorphous despite a priori both structures have none. However, a theory have been recently developed for describing the symmetries of incommensurate structures by considering them as a skew three-dimensional section of periodic structures in larger dimensional space.⁽¹⁰⁾ (called superspace).

In this paper, first through an example and next with some general results, we try to give some lights on the ways by which the translational symmetry of the space could be broken (for sake of simplicity in this first approach, we do not consider any rotational symmetry but only the translation group. In further studies, the full group of symmetry should be considered).

Our approach is done in principle for infinite structures which minimize a free energy $\phi(\{\tilde{u}_i^A\}, \{\tilde{u}_i^B\}, \dots)$ where $\tilde{u}_i^A$ represents the time average coordinates of the atom i of type A, $\tilde{u}_j^B$ the time average coordinates of the atom j of type B, This free energy determines the interacting forces between the atoms which we assume not to be long range (the concentration of each kind of atoms is determined by the

*By contrast to compact groups, which are usually considered in solid-state physics, much less is known about non compact groups. In fact, many useful properties of compact groups are lost for non-compact groups.

minimization of the free energy). In this large class of models, the atoms are not labelled by their coordinates on an underlying lattice but of course the same results can be obtained with slight change if we do it (our initial theory was done on a lattice).⁽¹⁴⁾ We can also include other variables such as classical spins or we can consider molecules instead of atoms and introduce their angular coordinates. The essential property of the model which is required, is that its free energy be invariant by some group of translation which acts globally on the structure. For example changing $\{\tilde{u}_i^A\}$, $\{\tilde{u}_j^B\}$ -- into $\{\tilde{u}_i^A + \tilde{R}\}$, $\{\tilde{u}_j^B + \tilde{R}\}$ -- where $\tilde{R}$ is an arbitrary vector of $\mathbb{R}^3$ does not change the free energy of the systems. Instead to be $\mathbb{R}^3$, this translation group could be $\mathbb{Z}^3$ the translation group of invariance of an underlying lattice (or more generally any non-compact abelian group). At the first stage of our approach the dimensionality of the space in which the structure is studied does not matter. In the particular following Frenkel Kontorova model⁽¹¹⁾ (noted hereafter FK model) the free energy of the model is only invariant by a one-dimensional discrete abelian group $\mathbb{Z}$. This theory neglects the thermodynamical and quantum fluctuations. For this reason, we believe that the frozen structures (fluctuationless), that we expect, cannot exist in 1 and 2 dimensions space but could exist in 3d-space when the thermal and quantum fluctuations are small enough.

We only give few mathematical details in this paper. They are described in other papers which are already published or in preparation.⁽¹⁴⁻¹⁵⁾ We primarily focus on physical ideas in connection with experimental observations. In the second section of this paper, we recall results that we obtained on the Frenkel Kontorova model.* We

*Note that we did not calculate the ground-state (except in the model described in appendix A) but that we found rigorously its properties by topological methods.

describe our early results in terms of defect properties. [Here the defects are discommensurations and can exist intrinsically in the ground-state. Thus, their existence does not cost any extra energy but in fact decreases the configuration energy. This is a typical situation in systems which are both defectible and frustrated].⁽¹³⁾ This paper tries to clarify our early papers and to give additional details but nevertheless the reader must refer to them for a better understanding and for finding the figures which are not reproduced here.

In this next section we describe separately two situations in the FK model. In the first one, the concentration of discommensurations is fixed by boundary conditions. It is a similar situation to 1d conductors in which the number of electrons in the conduction band is fixed. In the second situation, the concentration of discommensurations is not fixed and is determined by a chemical potential; this situation is similar to insulating incommensurate structures in which the wave-vector of the modulation generally varies. We describe properties of the variation of the commensurability ratio of the FK model with respect to the model parameters. (The variation curve is a devil's staircase).⁽²³⁾ We next discuss some experimental consequences of the existence of a devil's staircase.⁽¹³⁾⁽¹⁵⁾

The third section of this paper generalizes in part, some of the results obtained on the FK model, to all structures which minimize a classical free energy. The basic idea is that the equation, which extremize a free energy can also be interpreted as the evolution equations of a dynamical system the action of which is just this free energy. Thus, the usual time (group $\mathbb{R}$) of dynamical systems is formally replaced by the space (group $\mathbb{R}^3$) but this one can have any other

dimensionality. The essential property of this space is to be an abelian and non-compact group. Then, the ground-states of the system is embedded as a trajectory in the phase space of this dynamical system. With only topological arguments, we can prove that there always exist ground-states with some kind of long range order which we call "weakly periodic" or "with local order at all scale". Particularly such kind of structure can be either a crystal or an incommensurate structure (with phason). The ground-state is then represented by a "trajectory" which is rotating and dense on a manifold which has the topology of a $(n+d)$ dimensional torus. (n is the number of incommensurate modulations of the crystal and d the dimension of the space). But we also prove by the existence of counter examples, that the ground-state structure may be neither a crystal nor an incommensurate structure with phason. The FK model already provides example of incommensurate structures without phason. There exists more striking example in tiling the 2-d plane for which the ground-state is not periodic neither incommensurate but nevertheless has zero entropy. We still know very few about the properties of this new kind of order. We make some speculations on its physical properties which distinguish it from those of a chaotic structure and on its possible relevance to explain the properties of certain non-stoichiometric or amorphous structures that we have quoted at the beginning of this introduction.

2. The discrete Frenkel Kontorova model and its extension

The energy of this model⁽¹¹⁾ is

$$\begin{aligned} \phi(\{u_i\}) = \sum_i \left[\frac{1}{2} (u_{i+1} - u_i)^2 + \frac{\lambda}{2} \left(1 - \cos \frac{\pi u_i}{a} \right) \right. \\ \left. - \mu x(u_{i+1} - u_i) \right] \end{aligned} \quad (1)$$

It is a one-dimensional chain of atoms, which are elastically coupled. This chain is submitted to a periodic potential with amplitude λ and with period $2a$. The energy of a configuration $\{u_i\}$ is invariant by global translations which are multiple of $2a$, $\{u_i\} \rightarrow \{u_i + 2ka\}$ with k any integer. This set of translation form a discrete group $\mathbb{Z}$. The ground-state of this model depends either on the boundary conditions or on the tensile force μ when the end of the chain are let free. It can break this translation symmetry group $\mathbb{Z}$ in several ways which we are going to describe.

When the boundary conditions are fixed, the atomic mean distance is determined as

$$\ell = \lim_{N-N' \rightarrow \infty} \frac{u_N - u_{N'}}{N - N'} \quad (2)$$

N and N' are the indices of the two ends of the chain. In the absence of periodic potential ($\lambda=0$), the distance between neighboring atoms is constant and is ℓ . When $\lambda \neq 0$, the period $2a$ of the periodic potential conflicts with this period ℓ . When the ratio of the two periods $\frac{\ell}{2a}$ is an irrational number, the ground-state undergoes a continuous transition with respect to the amplitude λ of the potential between two phases which are both incommensurate. However, it is possible to construct a compact symmetry group G which let invariant the set of ground-states and such that at the transition, this symmetry group reduces to a non-compact subgroup G' (see Ref. 16). This transition which was called transition by breaking of analyticity in our earlier papers corresponds to the breaking of the compacity of this group G . (G' is dense in G but is not closed and is not identical to G).

This transition can be related with the threshold toward stochasticity which is observed in the standard map.⁽¹⁷⁾ Indeed, the ground-states and the metastable configurations of this model satisfies

$$\frac{\partial \phi}{\partial u_i} = \frac{\lambda \pi}{2a} \sin \frac{\pi u_i}{a} + 2u_i - u_{i-1} - u_{i+1} = 0 \quad (3)$$

(note that these equations are independent of μ).

By writing (3) as a recurrence equation

$$u_{i+1} = \frac{\lambda \pi}{2a} \sin \frac{\pi u_i}{a} + u_i + p_i \quad (4a)$$

$$p_{i+1} = u_{i+1} - u_i \quad (4b)$$

we find that the knowledge of u_1 and $u_0 = u_1 - p_1$ determines recursively u_i for all positive i (the inverse of the transformation (4) determines u_i for all negative i). The map $\tilde{T}$ which applies the point $P_i = (p_i, \theta_i)$ with $\theta_i = u_i$ modulo $2a$ onto the point $\tilde{P}_{i+1} = \tilde{T}(\tilde{P}_i) = (p_{i+1}, \theta_{i+1})$ is a diffeomorphism of the cylinder (p, θ) onto itself. The determinant of the jacobian matrix of $\tilde{T}$ is one and thus $\tilde{T}$ is area preserving. This map is usually called the standard map and has been studied by many authors as a model for the onset of intrinsic stochasticity in plasmas.⁽¹⁷⁾

We can now extend our theory on the FK model to all structural models in one-dimension, the stationary equations of which can be transformed into those of a twist area preserving map⁽¹⁸⁾ of the cylinder onto the cylinder. More precisely, the free energy of this class of one-dimensional model (that we call the FK class) can be written:

$$\phi(\{u_i\}) = \sum_i L(u_{i+1}, u_i) \quad (5a)$$

where the interacting energy $L(x, y)$ 1) has a lower bound (which is obviously necessary to have ground-states) 2) has a diagonal period $2a$ that is for any x and y

$$L(x+2a, y+2a) = L(x, y) \quad (5b)$$

3) and such that the crossed second order derivative $\frac{\partial^2 L}{\partial x \partial y}$ be strictly negative for all x and y .

(Model (1) is readily shown to be of this form.) Particularly, we can include in this class a model which have been studied by B. Huberman and E. Fradkin. For that, we do a transformation which in fact is equivalent to a Poincaré section⁽²⁰⁾ on the trajectories corresponding to its equation of stationarity. We mention here the definition of this model, which could be useful to understand the properties of certain smectic crystals with two incommensurate periodic modulations, because it shows that the devil's staircase phenomena is the consequence of two conflicting periods, one of them being eventually the period of an underlying lattice, but this is not necessary. Its free energy is

$$\begin{aligned} \phi(\{u(x)\}) = \int dx \left[\frac{1}{2} \left(\frac{du}{dx} \right)^2 \right. \\ \left. + A \cos(u(x) - q_1 x - \alpha_1) + B \cos(u(x) - q_2 x - \alpha_2) \right. \\ \left. - \mu \times \frac{du}{dx} \right] \end{aligned}$$

where μ , A , B , q_1 , q_2 are given parameters; α_1 and α_2 are two arbitrary phases; $u(x)$ is the phase field of the modulation of the smectic. If

$A = 0$ (or $B = 0$) this problem readily reduces to a time independent sine-Gordon equation (the pendulum equation) and its ground state $u(x)$ is periodically modulated. But when A and B are both nonzero, two modulating periods appear and generally conflict as in the FK model. When they are incommensurate one with each other, a transition by breaking of analyticity with respect to the relative phase shifts of the two modulations occurs versus the parameters A or B . The physical interpretation is the same as in the FK model although it takes a different analytical form because of the continuity of the field $u(x)$. However, in this limited paper, we will not describe it and we essentially focus on the FK model where the same phenomena more clearly occurs since one of the two periods (the period of the lattice) is fixed.

Turning back to the standard map, it is now well admitted that iterating $\tilde{T}$ yields trajectories which, depending on the initial conditions, can be either a periodic cycle (after that a finite number of iterations one reaches the initial point) either rotating on a smooth closed curve with an irrational winding number or more strangely, for a deterministic equation, a chaotic trajectory onto the cylinder (let us note that our study brings the rigorous proof of the existence of these chaotic trajectories). We refer the reader to a review paper in which this chaotic behavior is described.⁽⁴⁶⁾

We have to pick up among the full set of trajectories generated by $\tilde{T}$, those which corresponds either to the ground-state or at least to physically metastable states.* Fixing the atomic mean distance ℓ by (2) is equivalent to fix the winding number $\frac{\ell}{2a}$ of the trajectory which is its average number of revolution around the cylinder. The simplest case is obtained for $\frac{\ell}{2a}$ rational.

→ next page

2.1 Commensurate ground-states, discommensurations, Peierls-Nabarro barrier⁽²¹⁾

Let $\ell = 2a \frac{r}{s}$ be the atomic mean distance between neighbouring atoms with r and s two irreducible integers. We prove that the ground-state with the boundary conditions (2) is indeed a commensurate ground-state: it satisfies for all n

$$u_{n+s} = u_n + 2ra \quad (6)$$

The chain has a unit cell of s atoms with a length $2\pi a$. The corresponding trajectory in the $\tilde{T}$ map representation is a periodic cycle with period s . Although simple, this result requires a quite non trivial proof since a priori, it would have been possible with the boundary conditions (2), that the chain shared into two phases with different atomic mean distances ℓ_1 and ℓ_2 . This situation would happen if a first order transition from ℓ_1 to ℓ_2 existed. In fact, as a consequence of (6), there is no first order transition in the FK model which is in contradistinction with the early results of several authors.⁽²²⁾

Condition (6) in (1) allows to find the ground-state by minimizing the energy per unit cell

$$\Phi_s = \sum_{i=0}^{s-1} \left[\frac{1}{2} (u_{i+1} - u_i)^2 + \frac{\lambda}{2} \left(1 - \cos \frac{\pi u_i}{a} \right) \right] - 2\mu r a \quad (7)$$

with respect to the s variables $u_0, u_1, u_2 \dots u_{s-1}, u_s = u_0 + 2ra$.

This minimization can be done in two steps. First, we minimize (7)

*Let us point that our rigorous proof does not use the map representation although the results appear more explicit in this representation.

when fixing the phase

$$\alpha = \left(\frac{1}{s} \sum_{i=0}^{s-1} u_i \right) - ra \quad (8)$$

of the commensurate configuration. (It is the average position of the atoms in the first unit cell refer to its half length). The minimum $V_s(\alpha)$ of (7) is a periodic function of the phase α with two periods. The first one is $2a$ since configurations $\{u_i\}$ and $\{u_i+2a\}$ have the same energy (7). The second period is $2a \frac{r}{s}$ since the configurations $\{u_0, u_1, \dots, u_{s-1}, u_s = u_0 + 2ra\}$ and $\{u_1, u_2, \dots, u_s, u_{s+1} = u_0 + 2ra\}$ also have the same energy (7), therefore the prime period of $V_s(\alpha)$ is readily found to be $\frac{2a}{s}$. Next, we have to minimize $V_s(\alpha)$ versus α , to find the commensurate ground-state. In general, for a periodic function, there is only one absolute minimum in each period. For sake of simplicity, we assume that this is the case for $V_s(\alpha)$. Thus the phase α locks on one of the values generated by the discrete sequence $\alpha_k = \alpha_0 + \frac{2ka}{s}$ (k integer) which corresponds to the absolute minima of $V_s(\alpha)$.

We now consider configurations $\{u_i\}$ which are asymptotic at both infinity to commensurate ground-states but with a different phase α , for example α_0 for $i = -\infty$ and α_k for $i = +\infty$, there exists an intermediate region of the infinite chain which is stretched of the length $\frac{2a}{s} \times k$. In fact, we prove that such kind of configurations also exist as a minimum energy configuration of model (1) for certain boundary conditions but only for $k = \pm 1$. This configuration is called an advanced discommensuration and for $k = -1$, it is a delayed discommensuration (these ones are also elementary or topological defects). In standard theories, discommensurations are explicitly found by using after some approximations,

the continuous sine-Gordon equation. In our approach which considers exactly the discreteness of the model, we prove the existence of these defects without calculating them. We also prove that for $|k| \neq 1$ there exists no minimum energy configuration which corresponds to a phase shift of $k \times \frac{2a}{s}$. In fact the energy of such a configuration can be lowered by splitting this defect into k discommensurations which tend to separate at infinite distance. (However, such k -discommensuration could exist as metastable states).

Assuming now that the location of an advanced (or delayed) discommensuration can be fixed at an arbitrary abscissa x , $v(x)$ is the energy to create a discommensuration at this abscissa x on the commensurate ground-state with atomic mean distance $\ell = 2a \frac{r}{s}$. The new configuration is $\{u_i\}$. The shifted configuration $\{u_{i+s} - 2ra\}$ is also a discommensuration on the same commensurate ground-state but which is located at $x - 2ra$. It has the same energy than $\{u_i\}$. As a result, $v(x)$ is periodic with period $2ra$ but is generally not a constant. In each period, the absolute minimum of $v(x)$ at $x_{\min}$ is generally unique and corresponds to the spontaneous location of the discommensuration when x is not fixed. To move this discommensuration by one lattice spacing $2ra$, it is necessary to pass an energy barrier $E_B = v(x_{\max}) - v(x_{\min})$ (Peierls Nabarro barrier note: from hereafter PN barrier) where $x_{\max}$ corresponds to the abscissa of the absolute maximum of v . Let us note that for $x = x_{\max}$, the energy of the discommensuration being a maximum of $v(x)$, the corresponding configuration $\{u_i\}$ is also a solution of equation (3) but is obviously unstable under small perturbations. (We call these configurations unstable discommensurations). Because of this PN barrier, it is possible to construct random distributions of advanced

and delayed discommensurations providing that they are sufficiently far one from each other in order that the interacting forces be dominated by this lattice locking force. Since these configurations are built randomly, they must appear in the map representation as chaotic trajectories. We have here a simple physical proof for the existence of stochastic trajectories.

Remark. More precisely, in the map representation a discommensuration is represented by the trajectory of an heteroclinic point but the corresponding unstable discommensuration is also represented by the trajectory of an heteroclinic point which belongs to the intersection of the same dilating and contracting manifold (see Ref. 24 for details) (we mean here the stability of the physical configuration, not the stability of the trajectory in the $\tilde{T}$ map). As a result, these two heteroclinic points belongs to the same chaotic region. In fact, each chaotic trajectory of this region corresponds physically to a random distribution of discommensurations which are either stable or unstable with equal probability and thus the whole configuration is unstable with probability one. This remark shows that the numerical calculation in the map representation of a chaotic trajectory which corresponds to a physically stable configuration is practically impossible. (See Appendix B). (It is also rigorously proven that a non-zero PN barrier implies the existence of chaotic trajectories. If by chance this PN barrier vanishes, the chaotic region associated with these random distributions of discommensurations vanishes while the dilating and contracting manifold merges into a unique curve called separatrix).

2.2 Incommensurate configurations

We now assume that the atomic mean distance ℓ is such that $\frac{\ell}{2a}$ (the winding number) be an irrational number. This irrational number can be approached by a sequence of rational numbers. (The more appropriate sequence $\ell_i/2a = r_i/s_i$ which converges to $\frac{\ell}{2a}$ is obtained by truncation at order i of the continuous fraction expansion of $\frac{\ell}{2a}$

$$\frac{\ell}{2a} = \eta_0 + \frac{1}{n_1 + \frac{1}{n_2 + \dots + \frac{1}{n_i + \dots}}} \quad (9)$$

If the chain of N atoms (N large) has a length $N\ell$, it can be obtained by stretching the commensurate chain of length $N\ell_i$ by $N(\ell - \ell_i)$. (We assume for example $\ell > \ell_i$). Stretching the chain by $2a/s_i$ is equivalent to create an advanced discommensuration onto the commensurate chain. Thus the incommensurate chain can be viewed as a commensurate chain

with $\frac{N(\ell - \ell_i)}{2a/s_i}$ discommensurations that is a density $\rho = s_i(\ell - \ell_i)/2a$ of

discommensurations per atom. In the ground-state of the chain with $\ell/2a$ an irrational number, these discommensurations must be equidistant since we proved that the structure is incommensurate. More precisely, it is proved that there exists a hull function $f(x)$ such that

$$u_i = f(i\ell + \alpha) = i\ell + \alpha + g(i\ell + \alpha) \quad (10)$$

be a ground-state for any phase α .

f is monotonous increasing and g is a periodic function with the period $2a$ of the underlying potential of the chain (for a zero potential $g(x) = 0$). This function $f(x)$ undergoes with respect to the amplitude λ of this potential, a transition which corresponds to the loss of its analyticity. There exists for most irrational $\frac{\ell}{2a}$, a non zero $\lambda_c(\ell)$ such that for $\lambda < \lambda_c(\ell)$, $f(x)$ is an analytical function while for $\lambda > \lambda_c(\ell)$ f is discontinuous with an infinite number of discontinuities and no continuous part. In the map representation, the trajectory which represents the ground state is rotating with winding number $\frac{\ell}{2a}$ on a closed smooth curve for $\lambda < \lambda_c(\ell)$ (a Kolmogorov Arnold Moser torus) while for $\lambda > \lambda_c(\ell)$ it is still a rotation with the same winding number but on a Cantor set (see Fig. 1-a in Ref. 14 or 16). In the second situation and because of (10), the trajectory which corresponds to the ground-state is never chaotic despite it is imbedded in the chaotic region of the standard map (see Fig. 1-c in Ref. 14 or 16) (*).

This transition is physically equivalent to the occurrence of a finite PN barrier. The discommensurations which forms the incommensurate structure are at the distance $2a/(s_i(\ell - \ell_i))$ one from each other. When λ is small, their thickness becomes very large so that they strongly overlap. Although, not trivial, the PN barrier then rigorously vanishes because of this overlapping. (This is a consequence of the famous Kolmogorov Arnold Moser theorem). The chain can then freely slide on the periodic potential. It has a phason mode and moreover it is indeformable which means that it cannot accept any defect: this ground-state is the only solution of $\partial\Phi/\partial u_i = 0$ with the atomic mean distance ℓ .

*In the chaotic region, most trajectories in probability are chaotic, but the ground state just belong to the set of measure zero which is non chaotic.

When λ increases, the thickness of the discommensurations decreases, their overlap also diminishes so that for $\lambda > \lambda_c(l)$, the PN barrier appears again for each discommensuration. The whole chain becomes locked on the periodic potential. Any small translation of the chain which corresponds to a slight change of the phase α in (10) requires to jump the PN barrier for some discommensurations. This process is discontinuous and the resulting position of the atoms depends discontinuously on the phase α . Consequently, the hull function f has discontinuities in any interval of variation of the phase α . Moreover, this configuration is defectible which means that because of this PN barrier, it is possible to lock the discommensurations on the lattice at location which are different from those they would occupy in the real ground-state. Random distributions of stable discommensurations with the same density form chaotic configurations which always have more energy than the real ground-state and thus are metastable.*

The same arguments can be developed by changing the rational number $l_1/2a = r_1/s_1$ which approximates $l/2a$ and with respect to which the discommensurations are considered. When $\lambda < \lambda_c(l)$ and when s_1 becomes large, the distance between neighbouring discommensurations also becomes large** but their thickness becomes larger so that the discommensurations necessarily strongly overlap. Conversely, for $\lambda > \lambda_c(l)$ the thickness of the discommensurations remains finite and they do not overlap for large s_1 .

*For most irrational numbers, this distance diverges as s_1 . For the other ones (Liouville numbers) it diverges faster.

**The phonon gap of this incommensurate configuration is finite because of a Peierls force but conversely the gap in the energy creation of defects is zero. In spite of the existence of metastable states with an energy very close from the ground-state energy, the entropy of the model goes to zero when the temperature goes to zero. However, the specific heat can exhibit an anomalous behavior at low temperature and in 1 dimension because of this fact as shown in Ref. 47 in a model equivalent to (1) in the limit $\lambda = \infty$.

When the winding number $\ell/2a$ goes to a rational number $\ell_i/2a$, the density of discommensurations on this commensurate configuration with atomic mean distance ℓ_i , goes to zero. Consequently $f' \cdot \ell$ close enough to ℓ_i , the discommensurations does not overlap so that the PN barrier remains finite which implies that $\lambda_c(\ell)$ must go to zero for $\frac{\ell}{2a}$ going to any rational number. Since $\lambda_c(\ell)$ is not zero, for most irrational $\frac{\ell}{2a}$, this function of ℓ cannot be continuous at the irrational values of $\frac{\ell}{2a}$ although it is continuous at the rational values. In fact this strange property is not physically observable, because when $\frac{\ell}{2a}$ is a rational number with a large denominator s , the PN barrier strictly vanishes only for $\lambda = 0$ and thus $\lambda_c(\ell) = 0$, but there exists a sharp cross-over at a finite $\lambda_{c,o}(\ell)$ below which the PN barrier becomes very small. This commensurate ground-state practically undergoes at $\lambda_{c,o}(\ell)$ the same transition than a true incommensurate one at $\lambda_c(\ell)$. The determination of the order s at which the cross-over at $\lambda_{c,o}$ can be viewed as a transition obviously depends on the accuracy of the observation, larger is s , sharper is the cross-over. Our numerical calculation on incommensurate structures were done in fact for commensurate structures with $s \sim 1000$ but the accuracy is already good for $s \sim 100$. (Note that $\lim \lambda_{c,o}(\ell_i) = \lambda_c(\ell)$ where ℓ_i is defined by the successive truncation of (9)). In some sense, s plays the role of the finite size of system which undergoes a transition at the infinite size limit. (When the size of the system is finite, it only exhibits a cross-over.)

Like most transitions, the transition by breaking of analyticity exhibit critical quantities. For example, for $\lambda \rightarrow \lambda_c(\ell)$, the rate of decay of the harmonics of the hull function $f(x)$ is going to zero,* and for $\lambda \rightarrow \lambda_c(\ell)$ with $\lambda > \lambda_c(\ell)$ the coherence length ξ (i.e., the size of

the defects of the ground-state)** is diverging while the gap (i.e., the smallest phonon frequency) goes to zero. Recent renormalization approaches⁽²⁶⁾⁽²⁷⁾ which are essentially focused on the study of the stochasticity threshold in the standard map, should be adaptable for the calculation of critical exponents in the particular cases for which $\frac{\ell}{2a}$ has a periodic continuous fraction expansion.

The more commonly used number is the golden mean where $n_i = 1$ for all i in (9). (When $\frac{\ell}{2a}$ is an arbitrary irrational number, it is not clear whether the critical exponents are well defined or not.)⁽⁴⁸⁾

2.3 Application to certain metal-insulator transition

We suggested to explain certain metal insulator transitions in one-dimensional deformable lattices by a transition by breaking of analyticity on the phase shift on both the lattice and the electrons.^{(28)***} (For the electrons, this transition is not described in this paper but is shown to be equivalent to the localization of the eigen functions (see Refs. 14 and 16). Then the parameter $\frac{\ell}{2a}$ is the density of electrons in the conduction band which is assumed to be an irrational number and λ is a parameter which corresponds to an effective electron-phonon coupling. In a phenomenological approach it can be linearly related to the

³Conversely to what we claimed in Ref. (16), the phason velocity is not critical and does not vanish for $\lambda \rightarrow \lambda_c(\ell)$.

**The coherence length ξ is the inverse of the Lyapounov exponent $\gamma = 1/\xi$ associated with the trajectory corresponding to this ground-state in the T map.

***The electrons are considered spinless. Note also that this transition is essentially a consequence of the conflict of the lattice period and the Fermi period, and thus is different from those of other models also describing metal insulator transition in 1d models. We predict in fact the same qualitative properties in this model as ok than in the FK model (9). Particularly, if the chemical potential μ of the electron can be varied, we expect that the Fermi wave vector varies as a devil's staircase which is incomplete in the Frohlich superconductor regions and complete in the insulating regions.

temperature. When decreasing the temperature from the Peierls temperature, the amplitude λ of the potential which creates the periodic modulation increases from zero. Then, the value of λ_c corresponds to the transition temperature between the conducting state at high temperature which is in fact a Fröhlich superconductor (the PN barrier on the periodic lattice distortion is zero), and the insulating state at low temperature that we interpreted by a periodic structure of equidistant localized polarons locked on the lattice by the PN barrier. Let us emphasize that our model predicts that Fröhlich conductivity is incompatible with localized electrons. The arguments which are developed to predict the existence of this transition were in fact symmetry arguments and should not be very sensitive to the details of the model. Particularly we expect the same features in the SSH model.⁽⁴⁹⁾

In a more recent paper,⁽²⁹⁾ the same kind of arguments have been partially developed (the critical behavior of the electronic wave function was not considered at the transition) for explaining the metal-insulator transition in polyacetylene versus the concentration of doping ions. The model which is considered is different from the FK model, but the phenomenology is exactly the same. Instead to be λ , the parameter is the concentration of doping ions which corresponds to the winding number $\frac{\ell}{2a}$. (λ is assumed much smaller than $\sup \lambda_c(\ell)$). The critical values of this concentrations should be given in principle by the equation $\lambda_c(\ell_c) = \lambda$ which yields an infinite number of metal-insulator transitions. Indeed, around each rational ion concentration there is a small interval of concentration for which the PN barrier locks the

charged "solitons"*, but for small λ (thick solitons) and for high order rational concentration, this PN barrier is negligible since, in fact, $\lambda < \lambda_{c,0}(\ell)$. As a result for small λ and for a small variation of the doping ion concentration in the neighbourhood of $\frac{1}{2}$, only one transition by breaking of analyticity is physically observable from an insulating state to a conducting state (the other rationals which are close to $\frac{1}{2}$ are necessarily of high order).

2.4 Variation of the atomic mean distance versus λ or μ (free ends) the devil's staircase⁽¹⁵⁾⁽³⁰⁾

When the ends of the chain in the FK model are let free, the atomic mean distance ℓ varies versus the model parameters λ or μ . We use in the next, the parameter μ but the same kind of behavior hold with respect to λ . Function $\ell(\mu)$ is continuous** (no first order transition can exist in the FK model and its extension) but for each rational value $\frac{\ell(\mu)}{2a} = \frac{r}{s}$ there exists a finite interval in $\mu, [\mu_-(\ell_r), \mu_+(\ell_r)]$ in which the function $\ell(\mu)$ is constant and equal to ℓ_r . The width of each step is given by

$$\mu^+(\ell_r) - \mu^-(\ell_r) = \frac{s}{2a} [e^+(\ell_r) - e^-(\ell_r)] \quad (11)$$

*Instead of the word soliton, our terminology use the word discommensuration (in our early papers phase defects), since a soliton is in principle a solitary wave in an integrable model. Here, the solution is locked and the model is not integrable

**Note that $\ell(\mu)$ is monotonous increasing, but that $\ell(\lambda)$ is not necessarily monotonous (this property depends on μ). (See Appendix A).

where $e^+(\ell_r)$ is the energy to create an advanced discommensuration on a commensurate ground-state and $e^-(\ell_r)$ is the energy to annihilate a delayed discommensuration on the same commensurate ground-state. (15)(30)

The existence of a constant step at each rational $\frac{\ell}{2a} = \frac{r}{s}$ on the curve $\ell(\mu)$ can be simply explained. For each commensurate ground state, the locking of the phase which is obtained by minimizing $V_s(\alpha)$ (see 2.1) allows an energy gain which increases its domain of stability since the phase locking of incommensurate ground-state does not gain any energy while for higher order commensurate ground-state, this energy gain goes to zero. (If by chance $V_s(\alpha)$ was a constant, there is no energy gain in locking the phase. The advanced and delayed discommensurations then have infinite thickness and zero energy so that the width of the step given by (11) is zero. This situation occurs for example in the FK model for $\lambda = 0$ and for all commensurate ground-states but then the model is trivially integrable).

This continuous curve $\ell(\mu)$ which have an infinite number of constant steps, is called a devil's staircase. (23) We call this devil's staircase complete in a given interval $[\mu_1, \mu_2]$ (with $\mu_1 < \mu_2$) when the sum of the length of the steps $[\mu^-(\ell_r), \mu^+(\ell_r)]$

$$S(\mu_1, \mu_2) = \sum_{\ell_r} (\mu^+(\ell_r) - \mu^-(\ell_r)) \quad (12)$$

for all rational numbers $\ell_r/2a = r/s$ which belongs to the interval of variation of $\frac{\ell}{2a}$, is equal to the length of the whole interval $(\mu_2 - \mu_1)$. (We can say equivalently that the derivative of $\ell(\mu)$ is zero almost everywhere that is $\ell(\mu)$ is a singular continuous function. In fact, the left or the right derivatives of $\ell(\mu)$ are infinite at the edge of

each step but this set of points have zero measure). When the devil's staircase is not complete, the sum of the steps width is obviously smaller than $(\mu_2 - \mu_1)$. The devil's staircase is called incomplete in the interval $[\mu_1, \mu_2]$. Then, the derivative of $\ell(\mu)$ does not vanish in the complementary set of the intervals $[\mu^-(\ell_r), \mu^+(\ell_r)]$ which has the finite measure $\mu_2 - \mu_1 - S(\mu_1, \mu_2)$ (this function $\ell(\mu)$ contains an absolutely continuous part).

The interacting energy between two discommensurations decreases exponentially with the distance n as $(\exp -\gamma n)$ in which the Lyapounov exponent γ is the inverse of the coherence length ξ of the commensurate configuration (i.e. the half width the discommensurations). It is readily shown that the behavior of the devil's staircase at the edge of each step is (see Ref. 15) for example for $\mu > \mu^+(\ell_r)$

$$\frac{\ell(\mu) - \ell_r}{2a} \cong \frac{-\gamma(\ell_r)}{s \ln(\mu - \mu^+(\ell_r))}$$

this Lyapounov exponent γ vanishes simultaneously with the PN barrier.* When $\lambda > \sup \lambda_c(\ell)$ with $\ell_1 = \ell(\mu_1)$ and $\ell_2 = \ell(\mu_2)$ $\ell_1 < \ell < \ell_2$, the PN barrier and the Lyapounov exponent remain finite when the order s of the rational ℓ_r goes to infinity. Since γ remains finite, the property (13) remains compelling for all commensurate ℓ_r .

It turns out that this only property is sufficient to prove that the devil's staircase is complete in the interval $[\mu_1, \mu_2]$ (see Ref. 15, Appendix 2). Conversely, when λ becomes smaller than $\sup \lambda_c(\ell)$ (in model (1) $\sup \lambda_c \neq 0.2$), the PN barrier strictly vanishes for many values

*When the PN barrier goes to zero, the width of a discommensuration $\xi = 1/\gamma$ goes to infinity.

of l . As a result, when l_r is approaching these values of l , $\gamma(l_r)$ goes to zero so that the behavior of $l(\mu)$ close to l_r is no longer logarithmic. The devil's staircase becomes incomplete. But as we noted in 2.2, in the vicinity of each commensurate $l_r/2a$, $\lambda_c(l)$ goes to zero and the PN barrier becomes finite. Consequently, at the edge of each step, the devil's staircase is in fact complete but only in a very small interval. The complementary set $\hat{G}$ of all these intervals in the interval $[\mu_1, \mu_2]$ turns out to have finite measure. When μ belongs to this set $\hat{G}$ the corresponding ground-state is incommensurate with a phason mode and the PN barrier rigorously vanishes. Moreover, when λ goes to zero, the measure of $\hat{G}$ goes to the full measure $(\mu_2 - \mu_1)$ of the interval so that $l(\mu)$ becomes a smooth differentiable curve. The net result is that the property of completeness of the devil's staircase is essentially the consequence of the non-analyticity (i.e., the existence of a PN barrier) of the incommensurate configurations which are passed through.

2.5 The devil's staircase in experimental observations

How a devil's staircase can be observed in experiments? What is the physical consequence of its completeness? In insulating incommensurate structures,⁽⁴⁾ the wave-vector of the periodic modulation generally varies with the temperature, pressure, electric field... etc. This FK model could be, in a first approach, a coarse model which can help to understand some aspects of this variation.

The FK model can be introduced for example by assuming that below the temperature T_0 (at which the structure becomes incommensurate) a distribution of parallel and smooth walls appears. For example, these walls can separate regions with a different electric polarization as in thiourea: $SC-(NH_2)_2$. The temperature T_0 is assumed to be equal to the

roughening transition temperature of an isolated wall in order that the position u_i of the i^{th} wall be well defined for $T < T_0$. The existence of these walls is explained by frustration effects (see the first remark of Ref. 15). They are interacting and by keeping only the first neighbour interaction energy between the wall $(i+1)$ at u_{i+1} and the wall i at u_i , this energy can be assumed to be $\frac{1}{2} C(u_{i+1} - u_i - \ell_0)^2$ where ℓ_0 is the distance between neighbouring walls at T_0 . Since the temperature is below their roughening transition temperature, the walls receive from the lattice a periodic potential which we assume to be $\lambda/2(1 - \cos \pi u_i/a)$ with the period $2a$ of the lattice in the direction perpendicular to the walls. When T is close to T_0 , the walls are very thick, the lattice effects are strongly averaged by their fluctuations. When the temperature decreases, the fluctuations of the wall also decrease while the interactions with the lattice increase. This effect can be easily calculated for a single wall in a standard self-consistent approach. As a result, λ increases from zero when T decreases from T_0 (the dependence of the constant C and ℓ_0 with respect to the temperature is disregarded in comparison with the dependence of λ). Consequently, within this model, the wall distribution will be given by the ground-state of a FK model. When the temperature decreases from T_0 , the mean distance ℓ between consecutive walls starts to vary from ℓ_0 essentially because of lattice effects. Its variation is a devil's staircase. Initially, this devil's staircase is incomplete with negligible steps and varies smoothly while λ is small. The interaction between the walls is sufficient to remove the PN barrier which would exist for a single wall. This structure should exhibit a phonon (which could be overdamped in experiments). Next, the devil's staircase becomes gradually complete and becomes to

exhibit steps at simple commensurability ratio which have a non negligible width, and simultaneously the PN barrier appears. Although continuous at the macroscopic scale, this transformation involves at the microscopic scale, a discontinuous sequences of configurations each of them being separated from the next one by a PN barrier. Indeed, a small change of $\frac{b}{2a}$ requires a large displacement of most discommensurations which must pass the PN barrier. (However, the nucleation process for this transformation should require an extra mechanism which is not considered here). The net result of the PN barrier is an hysteresis for the whole continuous transformation (global hysteresis) because this PN barrier remains finite even for the incommensurate structures. At lower temperature, the devil's staircase becomes steeper and steeper while its global hysteresis increases. The transformation generally ends by a lock-in at a simple commensurability ratio. However, in this phenomenological model, it can end at any stage of the above transformation since at zero K, any value of λ can be in principle reached.

Let us emphasize that this devil's staircase theory is essentially a qualitative theory. By varying the model inside the FK class, we get a wide variety of devil's staircase which essentially has the same above described topology despite the width of the steps can be considerably different. It is clear that it does not predict any critical exponent at T_G .

Experiments in thiourea^{(4-b)(4-c)} seem to exhibit some of the essential aspects of this qualitative behavior but also some discrepancies. Two lock-in at commensurability ratio $\frac{1}{9}$ and 0 are observed when varying the temperature at ambient pressure, but are first-order instead to be continuous. However, let us emphasize that the assumption

of an elastic (or more generally convex) interaction between the walls is not necessarily true. If the interaction between walls is not convex, then the model which must be studied does no longer belong to the FK class and our result does not apply. Indeed, it has been shown by J. Villain and M. Gordon⁽³⁾ that the wall interaction can be oscillating as a function of the distance which could explain first order lock-in transitions but also could introduce more complex structures as we will mention in the last section of this paper. Particularly, in the ANNNI model, the wall interaction is oscillating and it is now proved by M. Fisher and W. Selke⁽³²⁾ that at low temperature the commensurability ratio does not vary as a devil's staircase but as a "harmless staircase". These results are in contradistinction with those of Per Bak⁽³³⁾ who claims that the staircase of the ANNNI model is topologically the same as the one which exists in the FK class but he did not prove his assertion. (In fact what he did essentially, was to approximate the mean field equations of the ANNNI model by those of the FK model). Nevertheless, it seems that the phase diagram of the ANNNI model has some similarity to the one of the FK model although there is real first order transition when reaching each commensurate configurations but most of them are weak.⁽³⁴⁾ In fact, further studies are still necessary for the ANNNI model because more complex phases cannot be yet excluded at finite temperature.

Turning back, to experimental results, thiourea⁽⁴⁾⁽³⁵⁾ also exhibit under pressure a lock-in transition at the commensurability ratio $\frac{1}{7}$ which is continuous. Because of the crystal symmetry in thiourea, the lock-in at $\frac{1}{8}$ is expected to exist in a much smaller interval in temperature and pressure than the lock-in at $\frac{1}{9}$ and $\frac{1}{7}$. The magnitude of

this lock-in should have the same order than for the commensurability order $s = 16$). Under an electric field, the symmetry of thiourea is raised so that the lock-in at $\frac{1}{8}$ becomes experimentally observable. (36)

Let us emphasize now that the behavior* of $l(\mu)$ given by (13) at the edge of each step at commensurability ratio $\frac{l}{2a} = \frac{r}{s}$ is only valid when there is much less than one discommensuration per unit cell of length $2ra$. (If this condition is not satisfied, there exists another energy term due to an intracell rearrangement of the atomic position which modify (13). Then (13) is only true for

$$\frac{\delta l}{2a} \ll \frac{1}{s} \quad (14-a)$$

(for examples $s = 7$ yields $\delta l/2a \ll 1/63$). Moreover, for (13) to be valid, the distance between neighbouring discommensurations must be much larger than their thickness $2\ell = \frac{2}{\gamma}$. This condition yields another inequality.

$$\frac{\delta l}{2a} \ll \frac{\gamma}{2s} \quad (14-b)$$

When the devil's staircase is incomplete or complete with a small $\gamma(l)$ (14-b) implies that the interval of pressure or temperature in which law (13) can be observed is very small. This law becomes possibly observable in a non-negligible interval when the PN barrier (i.e. γ) becomes larger that is in the lowest temperature regions. Indeed, the exact calculation of devil's staircase given this paper, Appendix A, confirms inequalities (14). Otherwise, experiments in thiourea⁽³⁷⁾ agree with this law (13) only below the lock-in at $1/7$ but not above where γ is presumably smaller.

*It has been recently established by M. Fisher and D. Fisher and also by T. Natterman⁽³⁹⁾ that the logarithmic law (13) was not changed by the fluctuations in 3d systems (but it is changed in 2-d and 1d systems).

A crucial experimental problem in thiourea is to explain the origin of the small global hysteresis which is observed on the variation curve of the commensurability ratio. We believe that it is mostly due to lattice effects and thus that it is an intrinsic effect which would also exist in perfect samples. Indeed, the lock-in transitions which are observed in thiourea at such high order commensurability ratio $\frac{1}{9}$ and $\frac{1}{7}$, indicate that the lattice effects are important. Moreover, the periodic modulation in the temperature region where these lock-ins occur, is observed to be quite different from a pure sinus. Consequently, the lattice and the modulation which have comparable periods strongly interact and could produce this global hysteresis.

However, alternative explanations⁽³⁸⁾ are proposed by a phenomenological coupling of the periodic modulation either with dislocations or with impurities or point defects. From our point of view, we do not believe that the dislocations can play an important role because their size is much larger than the period of the modulation. Their main effect is probably to change locally the period of the modulation but not to lock substantially its phase. Conversely, in the case of quenched point defects, it has been argued by P. Lee and T. Rice⁽⁵¹⁾⁽⁴⁰⁾ that even a small amount of point defect can lock a sliding charge density wave and similarly a periodic modulation. The problem is to know how large is the locking due to isolated impurities compared to the lattice locking which extend coherently and uniformly all over the crystal. But let us point out an important difference between the locking due to the lattice and the locking due to impurities. As we already noted (see also appendix A) the lattice locking depends on λ and thus on the temperature. It should appear at a temperature T_L smaller than T_0 (T_L is in

fact a cross over temperature because the wave-vector varies so that $\lambda_c(0)$ is not well defined) and next should increase when the temperature decrease. By contrast, the locking due to impurities is not expected to be so much temperature dependent⁽⁵⁰⁾ and should still exist at T_0 .

Otherwise, non-quenched point defects (impurities or vacancies) when they can migrate (which requires a sufficiently high temperature) may produce a significant effect when the period of the modulation varies. (But this effect is not a really a locking of the periodic modulation). The argument is that their concentration in the crystal, which can only vary slowly in time, could be also modulated with the same period than the modulation of the crystal. Thus any change in the period of this modulation should produce a small migration of these points defects which is very slow. Nevertheless, the period of the modulation precedes the point defect migration and should vary much faster. It reaches almost its equilibrium value while a much longer time is necessary for the whole system to reach the real final state. In experiment, one should observe small memory effects depending on the story of the sample and on the speed at which the temperature or the pressure is varied. In thiourea, such effects could have been observed in very accurate experiments, but they are indeed very small.⁽⁴¹⁾ (By contrast, in Baryum Sodium Niobate in which the concentration of point defects due to non-stoichiometry⁽⁴²⁾ is quite large, this effect is perhaps much more important one and could explain the giant hysteresis which is observed in this compound.)

In another compound with chemical formula $(N-(CH_3)_4)_2 Zn Cl_4$, a devil's staircase versus the temperature seems to be observed. It exhibits without pressure more lock-in phases than thiourea and also a

global hysteresis. Moreover, in deuterated samples a complete devil's staircase is observed which is not monotonous which is in agreement with our theory for certain values of μ . It can be interpreted in terms of the biological variation of the devil's staircase which varies very slowly with μ and is negligible. In agreement with our theory, no phason mode has been observed (52) in deuterated samples. It has not yet been possible to observe a phason mode on the example of appendix A, on the curve 2(1) where μ is done. (order at all scales)

By contrast, biphenyl (52) does not exhibit a staircase. In this compound, the commensurate trajectory was either a staircase or a periodic cycle. The trajectory remains quasi sinusoidal. This observation is related to the existence of a phason mode in our terminology by assuming that the parameter λ is small which implies that the trajectory is a little and stays incomplete. Lattice effects are taken into account with this assumption a well defined phason mode exists in contrast with thiourea, in which it has not been possible to observe any phason mode.

3) Weakly periodic structures (i.e. local order)

In the above FK model, each ground-state trajectory $\mathcal{C}$ on a cylinder. The closure $\overline{\mathcal{C}}$ implies the devil's staircase which is a smooth manifold or a Cantor set or simply a possible situation precluding the discontinuity property of $\overline{\mathcal{C}}$ was essentially It is also interesting to note that the devil's staircase drastically changes with μ and it is not surprising because the balance between conflicting interactions is very sensitive to any change in the

step is to define for each ground-state of an arbitrary model, this topological set $\overline{\mathcal{C}}$. We first sketch the proof which allows to prove the existence of weakly periodic ground-states.

3-1 Minimal sets

We define the set of minimum energy configurations $\mathcal{Q}$ (m-e configurations) as the set of configurations such that any finite change of the atomic positions of any finite number of atoms necessarily increases the free energy Φ . (This set is non-void since m-e configurations can be obtained as limits of m.e configurations in finite boxes with increasing size). We distinguish m.e configurations from ground-states since for example in the FK model, elementary discommensurations are m.e configurations but are not genuine ground-state in the common sense. The atomic densities distribution of the configurations $\tilde{\mathcal{C}} = \{\tilde{u}_i^A, \tilde{u}_j^B, \dots\}$ have the standard definition

$$\rho_A(\tilde{r}) = \sum_i \delta(\tilde{r} - \tilde{u}_i^A) \quad (14-a)$$

$$\rho_B(\tilde{r}) = \sum_j \delta(\tilde{r} - \tilde{u}_j^B) \quad (14-b)$$

(δ is the Dirac distribution). These density functions allow to define the physical topology of $\mathcal{Q}$. By definition, a sequence of configuration $\mathcal{C}_n$ goes to a limit configuration $\mathcal{C}$, when the density distributions of $\mathcal{C}_n$ goes to the density distributions of $\mathcal{C}$ in the sense of the distribution convergence. (This topology is the vague topology). Within this topology, $\mathcal{Q}$ is shown to be closed. Now, we consider a m.e configuration $\mathcal{C}$. The set of translated configurations of $\mathcal{C}$ by all translations of the abelian group $\mathbb{R}^3$ is the orbit $\mathcal{C}$ (or trajectory) of $\mathcal{C}$. The closure of

this orbit $\overline{\mathcal{C}}$ is proved to be a set of configurations which is included in $\mathcal{Q}$. Taking another m-e configuration $\mathcal{C}'$ in $\overline{\mathcal{C}}$, the closed orbit $\overline{\mathcal{C}'}$ of $\mathcal{C}'$ is necessarily included in $\overline{\mathcal{C}}$ but is not necessarily identical to it. If it is not, $\mathcal{C}$ does not belong to $\overline{\mathcal{C}'}$ while $\mathcal{C}'$ does belong to $\overline{\mathcal{C}}$. As a result, the configuration $\mathcal{C}'$ can be approached infinitely close by translations of $\mathcal{C}$ but the configuration $\mathcal{C}$ cannot be approached by translations of $\mathcal{C}'$. The physical interpretation is that by taking the limit of translated configuration of $\mathcal{C}$, some of the defects of $\mathcal{C}$ have been swept away and eliminated. Thus, we consider that $\mathcal{C}'$ is more perfect than $\mathcal{C}$, if $\overline{\mathcal{C}'} \subset \overline{\mathcal{C}}$ (strictly). If $\overline{\mathcal{C}'} = \overline{\mathcal{C}}$, the two configurations are physically equivalent. (In the FK model they only differ by a phase shift). This property can be turned into mathematical terms by defining an order relation. For $\mathcal{C}$ and $\mathcal{C}'$ in $\mathcal{Q}$, we say that $\mathcal{C}' < \mathcal{C}$ is equivalent to $\overline{\mathcal{C}'} \subset \overline{\mathcal{C}}$. This order relation is not total because if $\mathcal{C} \not\subset \overline{\mathcal{C}'}$ and $\mathcal{C}' \not\subset \overline{\mathcal{C}}$, $\mathcal{C}$ and $\mathcal{C}'$ cannot be compared. Nevertheless, this order relation is shown to be inductive that is for any subset $\mathcal{E}$ of $\mathcal{Q}$ which is totally ordered (i.e. for any $\mathcal{C}$ and $\mathcal{C}'$ in $\mathcal{E}$ then, either $\mathcal{C} < \mathcal{C}'$ or $\mathcal{C}' < \mathcal{C}$) there exists a minorant $\mathcal{C}_E$ in $\mathcal{Q}$ which is such that for any $\mathcal{C}$ in $\mathcal{E}$, $\mathcal{C}_E < \mathcal{C}$. The next step of the theory is to use the Zorn lemma⁽⁴³⁾ which applies to inductive ordered sets. Here, it asserts that giving a configuration $\mathcal{C}$, there always exist a minimal configuration $\mathcal{C}^*$ such that $\mathcal{C}^* < \mathcal{C}$ (By definition, $\mathcal{C}^*$ minimal means that there exists no other $\mathcal{C}'$ in $\mathcal{Q}$ such that $\mathcal{C}' < \mathcal{C}^*$).

A consequence of the minimality of $\mathcal{C}^*$ is that for any $\mathcal{C}$ in $\overline{\mathcal{C}^*}$, $\overline{\mathcal{C}'} = \overline{\mathcal{C}^*}$. For a given $\mathcal{C}$, the minimal configuration is not necessarily unique but each of them have reached the maximum perfection which it could reach. We define the ground-states as m-e configurations which are minimal. ($\overline{\mathcal{C}^*}$ can be viewed as a non-linear irreducible representation of the group $\mathbb{R}^3$). Whatever is the model, there exists such

ground-states and moreover any minimum energy configuration can approach, by a sequence of translations, such a ground-state. It can be shown that they have a physical property that we call "weakly periodic" or equivalently "with local order at all scale" that we describe now.

3-2 Weakly periodic structures

Let us now describe what is local order at all scale. Let us consider an arbitrary neighbourhood $\mathcal{V}$ of the density distribution $\{\rho^A, \rho^B \dots\}$ of the configuration $\mathbb{C}$, then there exists a set of translations $\mathcal{T}$ which transform the density distribution of $\mathbb{C}$ into a density distribution which belong to $\mathcal{V}$, and moreover this set $\mathcal{T}$ is relatively dense which means that there exists a positive number $B(\mathcal{V})$ such that any ball in $\mathbb{R}^3$ with radius $B(\mathcal{V})$ contains vectors of $\mathcal{T}$. In physical terms, the configuration $\mathbb{C}$ reproduces the same local order at bounded distance because when a local configuration minimizes the energy of the system, the system reproduces the same ^{one} as close as possible, taking into account that the boundary energy between these two local configurations must also be minimized. This property remains true for all local configurations, at all scales, for which the system keeps the memory at an infinite distance. This is a new kind of long range order which is incompatible with randomness. Indeed, in case of randomness, a given local order is reproduced in probability but the distance at which it is reproduced is random and cannot be bounded.

With this definition, it is obvious that crystal and incommensurate structures are weakly periodic. In that case the set $\overline{\mathcal{C}}^*$ can be shown to be topologically isomorphic to a torus. For incommensurate structures $\overline{\mathcal{C}}^*$ turns out to be the superspace which is considered by Janer and Jansen. ⁽¹⁰⁾ Is it possible that $\overline{\mathcal{C}}^*$ be not a torus? The answer is yes. The FK

model provides such an example for incommensurate structures which are locked and thus without phason. The structure of $\overline{\mathcal{C}^*}$ is then a Cantor set (see Fig. 1-c in Ref. 14) but is still simple. In fact, there exists more surprising structures obtained by tiling the two dimensional plane with several kind of polygons. (We refer the reader to Ref. (44) for the description of the tiling problems of Robinson and Penrose).

Having several kinds of polygons of given shapes, the problem is to tile the infinite plane in order to have close packing with no overlap and no empty space. There is examples in which the problem is trivial (e.g. with squares), other examples in which the problem has no solution (e.g. with decagons) but there exists also problems which are undecidable like those of Robinson and Penrose. Undecidability means that it is not possible to decide whether there exists a recursive algorithm which allows to construct the solution or not. As a result, any finite surface of the plane can be covered by close-packed tiles because if some finite surface could not be covered, tiling the whole plane would be in fact impossible, there would exist no algorithm and the problem would be decidable. Otherwise, these tiling cannot be periodic (by reproducing the unit cell, it also would be decidable) or have any other kind of structure which can be regularly generated by an algorithm (for example a spiral structure). In fact, this undecidability property does not mean physically any more. (With a computer, it is possible to construct very large tiling by trying all possible configurations but in fact this brute-force non-recursive algorithm can be improved and made partially recursive but of course, we know that a purely recursive algorithm does not exist).

These tiling problems can be easily written as problems of minimum energy configuration. It is sufficient for that to consider that the interacting energy between two tiles which overlap is positive and for example proportional to their overlap surface, while if they do not overlap, this interacting energy is zero. (We disregard the configurations which are not close packing). Thus, it is clear that a close-packing configuration which cover the plane is a minimum energy configuration to which we can apply the above existence theorem: There always exists tiling of the plane which are weakly periodic. It is clear that for the tilings of Robinson and of Penrose, these ground-states structures cannot be periodic neither incommensurate with phason (Because the tiles cannot change continuously). The set $\overline{\mathcal{C}}^*$ which represent them have not the simple topology of a torus but is a more complex set from which we ignore the topology.

We know few properties of these structures. What is their entropy*? For the Robinson tiling, we have proved that its entropy is zero but the proof is rather fastidious and cumbersome. We conjecture that in general for an arbitrary model the entropy of the ground-state is zero (but of course there exist models in which this entropy is not zero for example the well-known Slater model for the ice. (However, this property cannot be the only consequence of the minimality of $\overline{\mathcal{C}}^*$ because it is possible to construct minimal sets which have finite entropy). Under the action of $\mathbb{R}^3$, it should be a consequence of the minimization of the free energy. But, we have not yet proved any general result about this entropy.

*The entropy of a single structure can be defined on the same footing as for information theory or the Kolmogorov entropy for dynamical systems. It can be shown that it is the genuine physical entropy.

Another question is what could be the property of the spectrum of such weakly periodic structures? We conjecture that the space-Fourier transform of the density-density correlation function, which is experimentally observable, have generally absolutely no continuous part.* Such a measure has the property to have a support which have a Lebesgue zero measure. In other words it contains either Dirac measures (i.e. Bragg peaks) or a singular continuous measure or both. Physically, this property means that in principle, all the peaks of the measure have zero width. If they are not Dirac peaks, these peaks should decompose with a thinner resolution into several other peaks. Each of these new peaks should decompose into several other peaks with a more thinner resolution and so on. This zero width should be a consequence of long range order without periodicity and then it would be perhaps not surprising to have space correlations which decrease as power law (but not exponentially).

How these ideal structures could be useful to understand physical structures. It is not obvious that a real system can reach such a weakly periodic structure. The reason is that since we know examples for which $\overline{\rho^2}$ have a Cantor-like structure, it should evolve discontinuously at the microscopic level with respect to the model parameters (for example the temperature). Consequently we should expect a global hysteresis in the transformation for the same reason than for the complete devil's staircase, and also configurations out of equilibrium with either an infinite or a very long relaxation time. (The locked "intrinsic defects" which should migrate during the structure transformation could also produce tunnelling centers which are expected for example in

*This property is perhaps connected with a zero entropy of the configuration (see the theorem of W. Parry in Ref. 45).

amorphous structures). Nevertheless, for a real system, it is not unreasonable that its ideal structure can be obtained up to a reasonable scale (for example several hundred $\text{\AA}$). Anyway, this theory brings the proof that there exists structures "with order without periodicity" which cannot be considered as chaotic despite it could be very difficult to distinguish experimentally between this new kind of order and a chaotic state. The Penrose tiling⁽⁴⁴⁾ is a nice example of a theoretical non stoichiometric compound because if we call atom A the kite-tile and B the Dart-tile, the net chemical formula of the tiled plane is just $A_x B$ where $x = 1.618 \dots$ is the golden mean.

We are now trying to find a one dimensional model in which an example of weakly periodic order could be studied at least numerically. We found good reasons to expect that when the converse potential of the FK model $\frac{1}{2}(u_{i+1} - u_i)^2$ in model (1) is replaced by a non-convex potential there should exist such kind of weakly periodic structures in some regions of the parameter space. We hope that this model will be useful to understand what could happen to the incommensurate structure when the wall interaction is not convex and for example oscillating, which is a situation which exists in real systems.

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Appendix A

Exact calculation of a devil's staircase

We report the results of an explicit calculation of a devil's staircase which can be done on a particular model (Ref. 15, Appendix 3). This model is similar to model (1) and has the energy

$$\begin{aligned} \phi(\{u_i\}) = \sum_i \left[\frac{1}{2}(u_{i+1} - u_i)^2 + \frac{\lambda}{2}(u_i - 2m_i a)^2 \right. \\ \left. - \mu \times (u_{i+1} - u_i) \right] \end{aligned} \quad (A-1)$$

$$\text{where } m_i = \text{Integer part of } \frac{u_i + a}{2a} \quad (A-2)$$

but the periodic potential with $\cos$ has been replaced by a piecewise parabola periodic potential which is not differentiable at each $(u_i + a)/2a$ which is an integer. Because of this pathology, there exist no incommensurate structures with phason and the devil's staircase is always complete. In comparison with model (1), this model overestimates the width of the steps of the devil's staircase and the PN barrier (this feature must be considered when comparing with experiments). Another pathology of the model is that the Lyapounov exponent γ does not depend on ℓ . However, the model has the advantage to allow exact calculations.

Defining

$$\eta(\lambda) = 1 + \frac{\lambda}{2} - \sqrt{4\lambda + \lambda^2} \quad (A-3)$$

the ground-state $\{u_i\}$ of this model with atomic mean distance ℓ and phase α is given by

$$u_i = \frac{2a\lambda}{\sqrt{4\lambda + \lambda^2}} \sum_{n=-\infty}^{+\infty} \text{Int} \left(\frac{(n+1)\ell + \alpha}{2a} \right) \eta^{|n|} \quad (A-4)$$

the equation of the devil's staircase $\ell(\mu, \lambda)$ is given by the implicit equation

$$\mu = \frac{a\lambda^2}{\sqrt{4\lambda+\lambda^2}} \sum_{n>0} n \left(1 + 2 \int_0^{\frac{n\ell}{2a}} \eta^n \right) \eta^n \quad (\text{A-5})$$

the width in μ of the step of the commensurate structure corresponding to the atomic mean distance $\ell = 2a \frac{r}{s}$ is

$$\delta\mu(2a \frac{r}{s}) = \frac{2a\lambda^2}{\sqrt{4\lambda+\lambda^2}} s \frac{\eta^s}{(1-\eta^s)^2}$$

(note a slight mistake in the formula A-3-16 of Ref. 15). The PN barrier can also be exactly calculated and is for a commensurate ground-state with $\ell = 2a \frac{r}{s}$ (r and s irreducible)

$$E_{PN} = \frac{1}{2} \frac{a^2\lambda^2}{\sqrt{4\lambda+\lambda^2}} \cdot \left(\frac{1+\eta^s}{1-\eta^2} \right)^2$$

For incommensurate ground-states, it is

$$E_{PN} = \frac{1}{2} \frac{a^2\lambda^2}{\sqrt{4\lambda+\lambda^2}}$$

which clearly is never zero.

For possible applications for the depinning of charge density wave under an electric field such as in NbSe_3 ⁽⁴⁸⁾ one also can calculate the depinning field of commensurate and incommensurate ground-state.

We assume that we apply a constant force on each atom which is F . (This force is the product of the electric field by the effective charge per unit cell of the charge density wave)

The minimum force F_c for depinning a commensurate ground-state is

$$F_c = \frac{a\lambda^2}{\sqrt{4\lambda+\lambda^2}} \frac{1+\eta^s}{1-\eta^s} \quad (\text{A-9})$$

and for the incommensurate ground-state

$$F_c = \frac{a\lambda^2}{\sqrt{4\lambda+\lambda^2}}$$

But let us emphasize that in the more physical model (1)

- 1) E_{PN} and F_c depend on the irrational $\frac{\ell}{2a}$
- 2) E_{PN} and F_c are zero for $0 < \lambda < \lambda_c(\ell)$

Appendix B

On the numerical problems for a reliable calculation of the ground-states and the metastable configurations by map technics.

This appendix is a comment to Ref. 25 which have been rejected for publication for obscure reasons. It also applies for Ref. 19. It should give useful information for the reader who would like to make numerical studies of the problems mentioned in this paper.

Per Bak⁽²⁵⁾ has studied the phase diagram of the anisotropic next nearest neighbour interaction model (ANNNI model) by transforming its mean field equations into those of a model which belong to the FK class defined by (5). The numerical results that he obtained seem to be partly in agreement with the analytical studies that we described in Ref. (13) and (15). This comment, however, focuses primarily on the numerical method which has been used in Ref. 25 despite this paper contains some other mistakes which are less essential.

The trajectories which are generated by all initial conditions in the map very often correspond to unstable configurations. (In order to avoid any confusion, it is very important that the reader distinguish between the stability of a trajectory in the map and the stability of the corresponding configuration, which is the physical stability.) To use the map representation for finding physical configurations, we need to elaborate on a method which allows one to discriminate between those trajectories which corresponds to stable configurations and the others which are unphysical. Although he did not state it explicitly in the text, Per Bak used a method which has been developed by J. Greene⁽¹⁷⁾ to find certain elliptic and hyperbolic periodic cycles by taking into account a symmetry of the model. This method does not generate all possible periodic cycles. However, although this was not noted in⁽²⁵⁾, it turns out that the trajectories of the model corresponding to the ground state configurations indeed belong to Greene's set of periodic cycles. Nevertheless, the above symmetry method is only practicable (as used by Greene) for calculating periodic cycles in the quasi integrable regions which are close to the KAM tori. Troubles arise in the chaotic regions when calculating high order periodic cycles with the Greene method or with other iterative methods. Indeed, as is well known since Poincaré's work, the chaotic trajectories are characterized by their high sensitivity to initial conditions. This sensitivity is measured by the Lyapunov exponent γ which is defined by the rate of separation of two trajectories which are initially at a small separation ϵ . After n iterations of the map, they separate to $\sim \epsilon \exp(\gamma n)$. For example, an initial discrepancy of 10^{-15} with a small Lyapunov exponent $\gamma = 0.05$ would become after 1000 iterations (in the

linear approximation) a discrepancy of $5 \cdot 10^6$! Thus although, a stationary configuration of the physical system is mathematically characterized by the initial point of its associated trajectory it cannot be numerically characterized by this point, since any small numerical error "explodes" after a finite number of iterations. As we noted elsewhere,^(13,15,24) these chaotic trajectories correspond physically to random distributions of defects which are locked on the lattice by the Peierls force. Approximate knowledge of the initial point of a trajectory corresponds only to a local knowledge of the corresponding defect configuration. It does not yield informations on the distribution and the density of distant defects. As a result, Greene's method, when it is used to calculate high order periodic cycles in the chaotic region, gives an uncontrolled limit which generally represents neither a ground-state nor a physically stable configuration. This physical instability can be simply explained. If a defect is moved through the lattice by one lattice spacing, its energy increases first, passes a maximum (Peierls-Nabarro barrier) and decreases again to the initial value. The maximum of its energy also corresponds to a stationary configuration, which we call a physically unstable defect, and which appears as a trajectory imbedded in the same chaotic region of the map. As a result, most chaotic trajectories of the map in fact correspond to configurations that contain with equal probability defects which are stable and unstable. It is then clear that the whole configuration is unstable.

It seems that the chaotic configurations which are found in Ref. (25) are such unstable configurations. In the ideal case, in which the computer had infinite accuracy, Greene's method would have given in the chaotic region high order periodic cycles similar to those of Fig. 1-c

in Ref. 14. Our method (which is previously unpublished) to find such configurations is now explained briefly. To find a stable configuration which is at least a local minimum of a free energy $\phi(\{u_j\})$ with respect to the variables u_j , we simply use the gradient method* by numerically integrating the set of equations $du_i/dt = -\partial\phi/\partial u_i(\{u_j\})$. For any initial conditions and after a certain evolution, $\{u_i\}$ becomes independent of t and is a stable configuration. For particular initial conditions given by theorem 1 in Ref. 14 we obtain the ground-state.

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*There exists faster algorithm which essentially gives the same result.

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