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INCOMMENSURATE STRUCTURE WITH NO AVERAGE LATTICE: AN EXAMPLE OF ONE DIMENSIONAL QUASI-CRYSTAL

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Introduction and summary

Quasi-crystals are characterized by a discrete Fourier spectrum with a symmetry incompatible with that of a crystal [1]. Unlike the standard incommensurate structures, they cannot be described as a crystal structure where the atomic positions are modulated as a periodic function of the space. These quasi-crystal structures can be considered as examples of "weakly periodic structures" the existence of which was conjectured in an earlier paper [2].

In the one dimensional case, the projection method consists in a projection of a strip of a two dimensional lattice on a line of arbitrary slope (Fig. 2). However, only standard one dimensional incommensurate structures with an average lattice periodically modulated in space are thus obtained, for an irrational slope. In that sense such structures cannot be considered as one-dimensional quasi-crystals.

This talk is devoted to some considerations on the type of order that one finds in a one-dimensional quasi-lattice or in an incommensurate structure with no average lattice. Details can be found in Ref. [14]. The main results are the following:

1. It is possible to find a simple structural model describing a chain of atoms such that, in the ground state, the fluctuation of the positions of the atoms around their average lattice diverges logarithmically. The Fourier spectrum is nevertheless discrete.
2. This property is related to a mathematical theorem due to Kesten in Discrepancy Theory. We give simple arguments which illustrate the theorem in physical terms.

3. The model is equivalent to a circle map with unusual mathematical properties: it is ergodic, mixing and has zero entropy.

4. This map is a natural generalization of the transformation obtained by the projection method in one dimension.

These results suggest extensions in higher dimension.

2. The model
We consider a chain of atoms \( j \) with coordinates \( u_j \) such that the distance between two consecutive atoms is \( l_0 \) or \( 2l_0 \), \( l_0 \) being an arbitrary given number. This chain is submitted to a periodic potential with period \( 2\pi \), that for simplicity we take sinusoidal (Fig. 1). For a given concentration \( c \) of links \( 2l_0 \) (not too large) we can find the ground state of the model.

We have to minimize the potential energy of the chain

\[
\Phi(u_j) = \sum_j \cos(u_j)
\]

(1)

on the space of configurations \( u_j \) fulfilling the constraints:

\[
u_{j+1} - u_j = l_0 \text{ or } 2l_0 \quad \text{and} \quad c = c_0 \text{ given.}
\]

(2)

Figure 1: The model. Black dots are atoms, white ones vacancies.

This model describes a distribution of vacancies with fixed concentration in a periodic incommensurate potential \((\frac{c}{l_0})/2\pi \text{ is in general an irrational number} \). It is a particular case of the model studied in Ref.[7] the purpose of which was the
understanding of the consequences of the non-convexity of the interactions in the Frenkel-Kontorova model [2]. It can also be viewed as a simplified one-dimensional model corresponding to systems in two dimensions, such as the adsorbed monolayers of a mixture of two rare gas. Considering the ad-atoms as non-interacting hard spheres which have two possible diameters, the problem of finding the ground-state of the close-compact monolayer is similar and consists in minimizing its energy in the periodic potential of the substrate.

3. Generation of the ground state by a circle map $T$

The sites $i$ are at the position $v_i = l_0 \alpha$ where $\alpha$ is the location of the first site. In order to have the smallest possible energy for the system, it is sufficient to choose the location $v_i$ of the vacancies at the sites $i$ which correspond to the largest possible energy $\cos(v_i)$. These sites are determined by a condition $\cos(v_i) > \cos(\Delta/2)$, which defines a symmetric interval mod $2\pi$, (called from now on the window): $W = [-\Delta/2, \Delta/2]$. Since the distribution of $v_i$ (mod $2\pi$) is uniform on the interval $[0,2\pi]$, one has: $\Delta = 2\pi c / (1+c)$. Therefore the sequence $\{u_j\}$ of atomic positions in the ground-state is obtained by renumbering the sequence $v_i = l_0 v_0$ after having withdrawn the terms $v_i$ which belong to $W$ (mod $2\pi$). For instance, one would find:

\[\begin{array}{ccccccccccc}
v_0 & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & \ldots & v_i & \ldots & v_N & \ldots \\
u_0 & u_1 & u_2 & u_3 & u_4 & u_5 & \ldots & u_j & \ldots & u_N & \ldots \\
\end{array}\]

$(u_0=v_0, u_1=v_1, u_2=v_3 \ldots)$ if $v_2, v_5 \ldots$ belong to $W$ mod $2\pi$. Considering this interval $W$ as an arc of the circle of length $2\pi$, the mapping $u'=T(u)$ of the circle onto itself defined as a piece-wise rotation by the following equations

\[\begin{align*}
u' &= u + l_0 & \text{when } u + l_0 & \text{ does not belong to } W & (3-a) \\
u' &= u + 2 \times l_0 & \text{when } u + l_0 & \text{ does belong to } W & (3-b) \\
\end{align*}\]

generates this sequence $\{u_j\}$. The first atom of the chain is at the arbitrary position $u_0=\alpha$, which produces negligible boundary effects in the limit of an infinite system. This sequence $\{u_j\}$ must fulfill for all $i$ the condition $u_{i+1} - u_i = l_0$ or $2l_0$ to be the ground-state of model Eq.(1-2). This means that there exists no consecutive vacancies, which implies

$\Delta < l_0$ and $\Delta < 2\pi - l_0$ or equivalently

$c < l_0 / (2\pi - l_0)$ and $c < (2\pi - l_0) / l_0$
4. Mathematical properties of the circle map \( T \)

Since \( \xi \) is irrational, the sequence \( \{v_i \text{ mod } 2\pi\} \) is uniformly distributed on the circle. Consequently the subsequence \( \{u_j \text{ mod } 2\pi\} \) is uniformly distributed on the complementary part \( W' \) of the window \( W \) on the circle.

This transformation \( T \) exchanges the order of three intervals, the union of which is \( W' \) (see Ref.[14]). The discrete dynamical system, the trajectories of which are defined by iterating the transformation \( T' \) on the initial point, has unusual properties. It is ergodic with respect to the usual Lebesgue measure on the real axis. For most choice (in probability) of \( \Delta \) and \( l_0 \), \( T' \) is also mixing as shown in ref.[10]. The mixing property of a dynamical system is usually associated with strongly chaotic trajectories and one usually expects in that case a finite Kolmogorov entropy [12]. In fact it can be shown that transformation \( T' \) has zero Kolmogorov entropy. This property can be related to the fact that its unique Lyapounov number is zero since transformation \( T' \) is measure-preserving (Pesin theorem (Ref.[11])). The behaviour of the trajectories is not sufficiently chaotic to produce a finite entropy. Transformation \( T' \) has also the property of being "minimal" [2]. This property means that the trajectories for all initial point are dense on the whole set \( W' \) and implies that the ground state structure has the property of "weak periodicity" or equivalently of "local order at all scales".

Fluctuation of the map \( T \) with respect to a uniform average rotation map.

Transformation \( T \) can also be written:

\[
\begin{align*}
u' &= T(u) = u + (1 + \chi(u + l_0)) l_0 \\
&= u + (1 + \chi(u + l_0)) l_0
\end{align*}
\]

where \( \chi(x) \) is the characteristic function of \( W \), equal to 1 when \( x \) belongs to \( W \) and to 0 when it does not. It is also defined as

\[
\chi(x) = \text{Int}((x + \Delta/2)/2\pi) - \text{Int}((x - \Delta/2)/2\pi)
\]

where \( \text{Int}(x) \) denotes the integer part of \( x \) i.e. the largest integer \( \leq x \).

The number of vacancies on the chain of sites \( \{v_i\} \) is \( \sum_{i=1}^{N} \chi(v_i) \) and consequently, the position \( u_n \) of atom \( n \) is equal to \( v_n = N l_0 + v_0 \) where \( N \) fulfills:

\[
n = N - \sum_{i=1}^{N} \chi(v_i)
\]

Because the distribution of the sequence \( \{v_i \text{ mod } 2\pi\} \) on the circle is uniform, the mean value of the characteristic function is

\[
\lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \chi(v_i) = \Delta/2\pi
\]
A theorem due to Kesten [8,9] asserts that the fluctuation
\[ \delta(N) = \frac{1}{N} \sum_{i=1}^{N} \chi(v_i) - N \Delta/2\pi \]
of the sum \( \sum_{i=1}^{N} \chi(v_i) \) with respect to its expected value \( N \Delta/2\pi \)
is bounded in \( N \) if and only if the width \( \Delta \) of \( W \) is a multiple mod \( 2\pi \) of the rotation
angle \( l_0 \) that is when \( \Delta = r l_0 \mod 2\pi \) for some integer \( r \). If \( \Delta \) does not fulfill this
condition, other theorems [9] assert that \( \delta(N) \) diverges logarithmically as \( N \) grows.

5. Ground-state hull function

The ground-state of model (1-2) appears as an incommensurate periodic modulation of
the vacancy density. It is similar to the kind of incommensurate structures which are
formed for example in certain alloys by antiphase boundaries [13]. By contrast, a
standard displacive incommensurate structure is described by a hull function which
describes the modulation of the atomic positions from their average lattice site.
In one dimension, the simplest incommensurate structure \( \{u_n\} \) with one atom per unit
cell, is given by:
\[ u_n = u_0 + n l + g(q n) \]  
(6)
where \( l \) is the interatomic mean distance \( l = \langle u_{n+1} - u_n \rangle \) which determines the average
lattice \( \langle u_n \rangle = u_0 + n l \), \( g(x) \) is a 2\( \pi \)-periodic function which describes the modulation
and \( q \) is the wave-vector of this modulation. In order to have a physical meaning, this
function \( g(x) \) cannot be too pathological. In the case of standard displacive
incommensurate structures, this function \( g(x) \) is bounded and square summable in
order to have a discrete Fourier spectrum.

We show below that the ground-state of model (1-2) cannot be described by a form (6)
where \( g(x) \) is a bounded function. The atomic mean distance is a function of the
concentration \( c \) of bounds \( 2 l_0 \) and is related to \( \Delta \) by \( \Delta = 2\pi c/(1+c) : l = (1-c) l_0 + c 2 l_0 = 2\pi/(2\pi-\Delta) l_0 \). The modulated average lattice, if it exists, is defined by:
\( \langle u_j \rangle = j l + u_0 \). Suppose now that there exists a hull function \( g(x) \) such the ground-state be
described by Eq.(6) for some wave-vector \( q \). From Eq.(4) and (5), it comes out that \( g(x) \)
is given for \( x = qn \) by:
\[ g(q n) = N l_0 - n l = 1 \delta(N) \]  
where \( \delta(N) \) is the fluctuation
considered by the Kesten theorem. When \( \Delta \neq r l_0 \mod 2\pi \), this fluctuation \( \delta(N) \), and
consequently the displacements of the atoms from their average position, are not
bounded, which means that a bounded hull function \( g(x) \) does not exist. This result is
better understood by doing the analysis of the case where \( \Delta = r \mod 2\pi = r \mod \pi \) for some integer \( r \). In that case, Eq.(4-b) gives:

\[
\delta(N) = \sum_{i=1}^{N} \chi(v_i) - N \Delta / 2\pi
\]

\[
= \sum_{i=1}^{N} \left[ \frac{\text{Fract}(\frac{i l_0 + v_i - \Delta/2)}{2\pi}) - \frac{\text{Fract}((i+N) l_0 + v_i - \Delta/2)}{2\pi})}{2\pi} \right]
\]

where Fract(x) = x modulo 1. Thus: \( \delta(N) = - \left[ G_r(N l_0 + v_0) - G_r(v_0) \right] \)

The function \( G_r(x) \) is defined by \( G_r(x) = \sum_{i=1}^{r} \left[ \text{Fract}(\frac{x + i l_0 - \Delta/2)}{2\pi}) \right] \)

and has period \( 2\pi \). It is a “saw tooth” function, linear by part with a slope equal to \( r/2\pi \) and \( r \) discontinuities of amplitude \(-1\) per period located at \( x_n = (r/2 - m) l_0 \mod 2\pi (m=1,2,...,r) \). Hence, when \( r \to \infty \), functions \( G(x) \) and \( \delta(N) \), if they exist, have non-bounded variations.

6. Fourier spectrum of the ground state

Since the vacancy density defined by \( T \) is periodically modulated, the Fourier spectrum of the ground state of model \( (1-2) \) is discrete. The atomic density

\[
\rho(r) = \sum_i \delta(r - u_i) = \sum_j \delta(r - j l_0 - \alpha) [1 - \chi(j l_0 + \alpha)]
\]

is the product of two periodic functions which have the periods \( 2\pi \) and \( l_0 \) respectively. Consequently the structure factor

\[
S(K) = \int \exp(i K r) \rho(r) \, dr
\]

\[
= 1/n \sum_{j=0}^{N} [1 - \chi(j l_0 + u_0)] \exp[i K(j l_0 + u_0)]
\]

can be written as:

\[
S(K) = \frac{N}{n} \times \frac{1}{N} \sum_p \sum_m a_p \exp \left[ i(p+K)(m l_0 + u_0) \right]
\]

where \( a_p \) are the Fourier coefficient of the \( 2\pi \)-periodic function

\[
1 - \chi(x) = \sum_{p=-\infty}^{\infty} a_p \exp(ipx)
\]

defined by

\[
a_p = 1/2\pi \int_0^{2\pi} (1 - \chi(x)) \exp(-ipx) \, dx
\]

\[
= \frac{-\sin(p\Delta/2)}{p\pi} \quad \text{for } p \neq 0
\]

\[
= 1 - \Delta/2\pi \quad \text{for } p = 0
\]

Therefore the Fourier spectrum \( S(K) \) of the atomic density is a sum of Dirac peaks located at \( K_{p,q} = -p+2qn/l_0 \) with intensities proportional to \( |S(K_{p,q})|^2 = (1+c)^2 |a_p|^2 \). As is the case for usual incommensurate structures, these vectors \( K_{p,q} \) are obtained by
the rational combinations of two vectors of the reciprocal lattice:

\[ K_{0,1} = \frac{2\pi}{l_0}, \text{ wave-vector of the one dimensional lattice in the absence of any} \]

vacancies and \( K_{1,0} = 1, \text{ wave vector of the modulating } 2\pi \text{ periodic sine potential.} \)

Assuming that the ground-state \( \{u_n\} \) can also be described as a displacive incommensurate structure, it is possible to prove that the width of the window \( \mathcal{W} \) can be written in the form \( \Delta = r \mod 2\pi \) [14]. In other words there cannot exist any summable periodic hull function for the ground-state when \( \Delta \) is not a multiple of \( l_0 \) (mod \( 2\pi \)) and that there exists one when \( \Delta \) is a multiple of \( l_0 \).

### 7. Connection with the projection method

Finally let us note that, in the simple case \( \Delta = l_0 \), the ground-state of our model is an incommensurate structure isomorphic to the one obtained by the projection method [3-6]. The projection method in one dimension first consists in defining the strip of points of a two dimensional square lattice which are covered by all the translations of the unit square, parallel to a given straight line \( D \) of slope \( t = \tan(\theta) \). Next, the points contained in this strip are projected on the line \( D \) (Fig. 2). The distances between the consecutive points on the line are either \( c = \cos(\theta) \) or \( s = \sin(\theta) \).

It is also possible to obtain the sequence of links \( \{c, s\} \) by a rotation on a circle. The length \( l + t \) of the circle is equal to the width of the section of the strip by the vertical axis. On this circle one defines a window of width unity (Fig. 2). The rotation with a unit angle on the circle generates a sequence of points. By associating the links \( c \) to the points which belong to the window and the links \( s \) to the other points, one obtains the same sequence of links as with the projection method. In conclusion, the sequence of links \( \{c, s\} \) is generated by the transformation \( T \) defined in Eq.(3) for \( l_0 = \Delta = 1/(1 + \tan \theta) \) (except that now the length of the links are not double one from another).

One can describe more precisely the sequence of links denoted by \( \{l_i, \} \) as follows.

\[ l_i = c \quad \text{if } v_i \in \mathcal{W} \quad \text{and} \quad l_i = s \quad \text{if } v_i \notin \mathcal{W} \]

where

\[ v_i = \frac{1}{l_0} (l_0 = 1/(1+t)). \]

Or:

\[ l_i = s(1-\chi(v_i)) + c\chi(v_i) \]

where \( \chi \) is the characteristic function of \( \mathcal{W} \) defined as:

\[ \chi(x) = \text{Int}(x) - \text{Int}(x-l_0). \]

\( l \) is given by:
Figure 2: Equivalence between the projection method in one dimension and a rotation on a circle. Δ is the window.

\[ l = \lim_{N \to \infty} (1/N) \sum_{i=1}^{N} l_i \]
\[ = s+(c-s)x = s+(c-s)/(1+t) = 1/(s+c) \]

In the same manner one finds the hull function for the sequence of links:
\[ g(N) = \sum_{i=1}^{N} l_i - N l = \sum_{i=1}^{N} \left( s+(c-s)x_i \right) - N l \]
\[ = Ns + (c-s)\text{int}(N/(1+t)) - N l = (s-c)\text{Frac}(N/(1+t)) \]
\[ = (s-c)\text{Frac}(N c l) \]

Therefore the structure generated by the projection method in the one dimensional case is a standard incommensurate structure with a bounded periodic modulation. For that reason it is not the analogous of a quasi-crystal.
8. Concluding remarks

We studied here a model for which the ground-state is obtained as an incommensurate modulation of a vacancy density (compositional modulation). For a discrete sequence of vacancy concentrations the same structure can also be described by a periodic crystal with an incommensurate displacive modulation. For other concentrations, corresponding to the general case, the structure configuration is generated by a one-dimensional map having unusual properties. The map is ergodic, mixing and has zero Kolmogorov entropy. Thus, the type of order found in the ground-state can be considered as intermediate between that of a standard incommensurate structure and that of a chaotic disordered structure.

The nature of the fluctuation of the position of the $i^{th}$ atom, defined by the distance between its actual position $u_i$ and its average position $i 1+\alpha$ (where $l$ is the average distance between consecutive atoms), permits to distinguish between those degrees of order. In the case of a standard incommensurate structure this fluctuation, described as a smooth function of the atomic position, is bounded. For the model studied here, this fluctuation is generally not bounded but its root mean square diverges proportionally to $\log(L)$ as a function of the size $L$ of the system. By contrast, this root mean square diverges much faster and proportionally to $\sqrt{L}$ in the case of a chaotic distribution of atoms.

Although the model studied here is very crude, it points out important aspects of the difference between the compositional incommensurate structures and the displacive incommensurate structures. Extensions of this study to two and three dimensions could help to understand the formation of incommensurate antiphase structures and of quasicrystals which both occur in metallic alloys (e.g. AlTi and AlMn respectively).

References


