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Excitation spectrum, extended states, gap closing : some exact results for codimension one quasicrystals

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Résumé. — Dans cet article, nous étudions un hamiltonien de liaisons fortes pour les quasicristaux de codimension un. Nous utilisons une nouvelle numérotation des sites, qui les ordonne selon leur environnement géométrique. Ceci nous permet de trouver analytiquement des états étendus pour la chaîne linéaire quasi périodique, et de leur associer un pseudo-vecteur de Bloch. Ces états qui s'avèrent dégénérés, correspondent à des énergies pour lesquelles un gap du spectre se referme, quand les paramètres du hamiltonien varient. De plus, nous exhibons une surface de l'espace des paramètres qui coupe le spectre de toutes les chaînes linéaires construites à partir de 2D dans le cadre de la méthode de coupe et projection. Les conséquences de ces résultats sur le comportement de certaines quantités physiques sont brièvement abordées. Enfin, bien que généraux, nous illustrons ces résultats sur la chaîne de Fibonacci.

Abstract. — In this paper, we study a tight-binding Hamiltonian for codimension one quasicrystals by means of a new numbering which orders the sites according to their environment. This includes the general 1D quasiperiodic chain. We exhibit exact extended wave functions on approximants for the general quasiperiodic chain, for which we define a « quasi-Bloch » vector. These extended states can be shown to be degenerate. Moreover, some of them correspond to energies where gaps disappear, when the tight-binding parameters vary. We also exhibit a surface of the three dimensional space of parameters, which intersects the spectrum of all 1D quasiperiodic chains which can be generated by the standard cut and projection algorithm from 2D. The consequences of these properties on physical quantities such as the conductivity are briefly discussed. These results, although being general, are illustrated on the Fibonacci chain.

1. Introduction.

The properties of the Schrödinger operator with a quasiperiodic potential are of considerable interest since the discovery of quasicrystals. In 1D, quasiperiodic tight binding models have very interesting properties [1]. For instance, the spectrum is known to be a Cantor set whose Lebesgue measure is always zero independently of the involved irrational number [2]. There is an infinite number of gaps and the wave functions are in general critical, that is, neither extended nor localized by the disorder. Nevertheless, it has never been shown that extended states cannot exist. In fact, we exhibit exact degenerate extended wave functions, which turn

out to correspond to energies for which a gap disappears in the spectrum. In higher dimensions, there are very few exact results. Numerical simulations on the Penrose lattice seem to show that the spectrum is singular [3]. Moreover, it was found, for a non-trivial subtiling of the standard octagonal tiling, that there can be any number of gaps (including zero and infinity), and the Lebesgue measure of the spectrum can be zero or finite, depending on the hopping parameters [4]. In the next section, we define a new numbering for codimension one quasicrystals which turns out to be relevant in order to study a tight-binding Hamiltonian on such structures.

2. Codimension one quasicrystal approximant.

Recently, a new set of coordinates has been introduced for vertices of approximants of codimension one quasicrystals [5]. Codimension one quasicrystals (COQ), are quasiperiodic tilings in a d -dimensional space (the « physical » space), which can be obtained from \mathbb{Z}^{d+1} , by means of the standard cut and project method [6]. This includes 1D quasiperiodic chains as well as 2D or 3D quasicrystals. When the d -dimensional plane is not parallel to a reticular plane of the $(d+1)$ -dimensional hypercubic lattice (it is the generic case), a structure is obtained which is not invariant under any translation. It represents the simplest model for quasicrystalline structures. Whenever it is parallel to a reticular plane, a periodic structure is obtained. Note that its unit cell can be very large with respect to the hypercubic lattice edge, when the corresponding d -dimensional reticular plane has a low density. We shall not consider the intermediate cases where the physical space is parallel to subspaces of lower dimension ; the generated structure presents both periodic and quasiperiodic characters. Note finally that, from a mathematical point of view, a periodic function is a special case of a quasiperiodic one. In the following, however, we shall make the distinction between the two cases, denoted by COQA and COQ. The letter A stands for approximant. Indeed, as it is possible to approach irrational numbers by rational approximants, the COQ can be approximated by a series of COQA.

So, let d be a non-zero integer. In \mathbb{R}^{d+1} with the canonical basis $\{\mathbf{e}_1, \dots, \mathbf{e}_{d+1}\}$, we define \mathcal{F} , the rational d -dimensional hyperplane spanned by the \mathbf{a}_i 's, $1 \leq i \leq d$:

$$\mathbf{a}_i = (0, \dots, 0, p_i, 0, \dots, 0, -r_i) \quad 1 \leq i \leq d \quad (1)$$

where p_i is at the i -th row. One can easily see that $\alpha_i = -p_i/r_i$ is the slope of the intersection of \mathcal{F} and the plane $(\mathbf{e}_i, \mathbf{e}_{d+1})$, which is a line. Now, we define the strip \mathcal{B} which is obtained by translating the unit hypercube of \mathbb{R}^{d+1} along \mathcal{F} . Inside \mathcal{B} , there is a unique corrugated d -dimensional surface which will give an approximant of a quasicrystal after projection on \mathcal{F} . In order to introduce the new numbering, we define another vector \mathbf{a}_{d+1} . If $a_{d+1}^{(j)}$ is the j -th component of \mathbf{a}_{d+1} , we have

$$\begin{aligned} a_{d+1}^{(j)} &= r_j \prod_{i \neq j} p_i \quad 1 \leq j \leq d \\ a_{d+1}^{(d+1)} &= \prod_{1 \leq i \leq d} p_i. \end{aligned} \quad (2)$$

With this definition, it is clear that \mathbf{a}_{d+1} is orthogonal to \mathcal{F} . Now, let p be the g.c.d. of the $a_{d+1}^{(j)}$'s and \mathbf{q} the vector with coordinates $q_j = |a_{d+1}^{(j)}/p|$. Then, since the q_i 's are mutually prime, by using the Bézout theorem, there exists an integer vector $\mathbf{h} = (h_i)$, we shall call it the generator, so that

$$\langle \mathbf{h} | \mathbf{q} \rangle = \sum_{i=1}^{d+1} h_i q_i = 1. \quad (3)$$

With all these definitions, we verify that the \mathbf{x}_j 's defined below are the coordinates of all points of the approximant unit cell.

$$\mathbf{x}_j = j\mathbf{h} [\mathbf{a}_1, \dots, \mathbf{a}_d] \quad 0 \leq j < \sum_{i=1}^{d+1} q_i = n. \tag{4}$$

Here, $[\]$ denotes the modulo operation with respect to the \mathbb{Z} -module spanned by the \mathbf{a}_i 's. The above coordinates correspond to vertices selected in the strip defined by the sum of the physical space and a unit hypercube in \mathbb{Z}^{d+1} . Usually (as in Fig. 1), the sites are orthogonally mapped onto the physical space. Such a mapping amounts to inserting a projection operator in the formula and does not change anything in the problem treated here (the excitation spectrum). Thus, in any dimension, we have found a one dimensional dynamics, which will turn out to be the relevant way to index the sites of a COQA. One can show that there exists a unique \mathbf{h} (modulo the above \mathbb{Z} -module) so that this numbering consists in ordering vertices with respect to their distance from \mathcal{F} or, in an equivalent way, according to their local environment. Moreover, in this numbering (which we shall call the CO-numbering), using the property $\langle \mathbf{h} | \mathbf{q} \rangle = 1$, one can show that if $j + \varepsilon q_i \in [0, n - 1]$, with $\varepsilon \in \{-1, 1\}$, then the site whose CO-number is $j + \varepsilon q_i$ is one of the nearest neighbours of site j . This is obtained from the identity

$$(j + \varepsilon q_i) \mathbf{h} = j\mathbf{h} \pm (0, \dots, 0, 1, 0, \dots, 0) [\mathbf{a}_1, \dots, \mathbf{a}_d]. \tag{5}$$

This shows that the connectivity matrix is a multidagonal matrix when sites are indexed according to the CO-numbering and if we apply periodic boundary conditions to the unit cell itself. Moreover, we note that (5) implies that the q_i 's are all different. In figure 1, we show an example of such a 2D tiling. The two slopes are some approximants for the golden mean $(\sqrt{5} - 1)/2$ and the silver mean $\sqrt{2} - 1$.

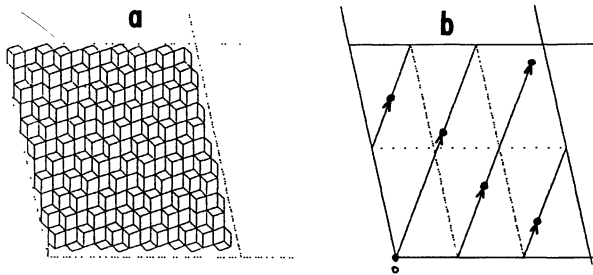


Fig. 1. — A 2D quasiperiodic tiling, defined from the golden and silver means. We have also shown some site indices in the CO-numbering.

3. The Hamiltonian.

Now, we shall see the consequences of such a property on the study of tight-binding model for a COQ, whose general form is

$$\mathcal{H} = \sum_i x_i |i\rangle \langle i| + \sum_{i \neq j} t_{i,j} (|i\rangle \langle j| + |j\rangle \langle i|) \tag{6}$$

where i and j label the sites of the quasicrystal. We call $\{n_i\}$ the set of the q_i 's reordered in the increasing order, since they are all different (5). Then, one can naturally define a Hamiltonian \mathcal{H} in the following way.

$$t_{i,j} = \langle i | \mathcal{H} | j \rangle = \rho_k \quad 1 \leq k \leq d + 1, \quad 0 \leq i \neq j \leq n - 1 \tag{7}$$

when sites i and j are nearest neighbours, so that the vector joining the vertices i and j in the strip defined in \mathbb{Z}^{d+1} is $\pm \mathbf{e}_k$. Thus, after projection on \mathcal{F} , these sites will be considered as nearest neighbours linked by the bond ρ_k . In addition, we define a set $\{V_i\}$ of on-site potentials, one for each local environment, this set being finite when $n \rightarrow +\infty$, since a site has no more than $2(d+1)$ nearest neighbours. Thus, in the CO-numbering, as for the connectivity matrix, \mathcal{K} is a symmetric multidagonal matrix, with ρ_k on the n_k -th diagonal. On the main diagonal, the V_i 's of each kind are gathered in a same region. It is clear that, if we consider interactions up to second or third neighbours, the Hamiltonian will keep its property of being a multidagonal matrix.

Now, since our present paper is specially devoted to the 1D case, we shall study it explicitly. Thus, consider an irrational number ρ_0 , and (p, q) such that p/q is an approximant of τ_0 . In the following, we use the notation $n = p + q$ which will play the same role as in (4), $\tau = p/q$ and $\theta = \tau/(1 + \tau)$. We call S_n the linear chain obtained by associating a 1 with a horizontal and a ρ with a vertical bond (so we have $\rho_1 = 1$ and $\rho_2 = \rho$ in the above notation), for each bond of the broken line drawn along the edges of a \mathbb{Z}^2 lattice selected in the strip

$$0 \leq y - \tau x < 1 + \tau \quad (x, y) \in \mathbb{Z}^2. \tag{8}$$

This is exactly the well known cut and project method. S_∞ is defined in the same way by replacing τ by τ_0 in (8). We take $0 < \tau, \tau_0 < 1$ without any loss of generality since $S_\infty(1/\tau_0)$ is obtained from $S_\infty(\tau_0)$ by inverting vertical and horizontal bonds. S_n is a periodic chain whose elementary cell contains $p + q = n$ atoms. We have shown that the coordinates of points in a unit cell of S_n , in the strip (before mapping), can be written as follows

$$\begin{aligned} \mathbf{x}_\ell &= \ell \mathbf{h} [\mathbf{a}_1] \quad \text{with } m \in \mathbb{Z}, \ell = 0, 1, \dots, n - 1 \\ \mathbf{h} &= \begin{pmatrix} q' \\ p' \end{pmatrix} \quad \mathbf{a}_1 = \begin{pmatrix} q \\ p \end{pmatrix} \end{aligned} \tag{9}$$

where $(\mathbf{h}, \mathbf{a}_1)$ is a unit basis of \mathbb{Z}^2 , since we have the Bézout condition

$$p'q - pq' = 1 \tag{10}$$

\mathbf{a}_1 defines the unit cell of the approximant periodic structure and \mathbf{h} is the generator. In a subsequence of n sites in S_n , we find one and only one \mathbf{x}_ℓ , labelled with a fixed ℓ . We give the example of the Fibonacci chain approximant in figure 2. In this numbering, it can be shown that the two nearest neighbours of \mathbf{x}_ℓ are the two in the set

$$\{\mathbf{x}_{\ell \mp p}, \mathbf{x}_{\ell \mp q}\} \tag{11}$$

for which the first coordinate is between 0 and $n - 1$. These two coordinates are $\ell + p[n]$ and $\ell + q[n]$ (where $[]$ denotes the modulo operator). This result can be written in the following way. Let \mathfrak{J} be $[0, n - 1]$.

- * if $\ell - p \in \mathfrak{J}$ and $\ell + p \in \mathfrak{J}$ the site ℓ is surrounded by two 1.
- * if $\ell \pm p \in \mathfrak{J}$ and $\ell \pm q \in \mathfrak{J}$, the site ℓ is surrounded by a 1 and a ρ .

The case $\ell - q \in \mathfrak{J}$ and $\ell + q \in \mathfrak{J}$ is impossible since we took $\tau, \tau_0 < 1$. Thus, this numbering orders the sites according to their local environment which is the relevant ordering in this case. This is also the true case in higher dimension.

Now, the above tight-binding model on S_n reads

$$t_{i,i-1} \Psi_{i-1} + x_i \Psi_i + t_{i,i+1} \Psi_{i+1} = E \Psi_i \tag{12}$$

to be critical, wich is an intermediate state between localized and extended. More precisely, in order to study the localization of the eigenstate (Ψ_i), one can introduce (following [12]) a kind of free energy function $F(x)$, which is a commonly used quantity in the multifractal formalism. $F(x)$ is trivial when the wave vector is extended ($F(x) = 0$), but proves to be useful for the characterization of critical states :

$$\begin{aligned}
 F(x) &= \lim_{n \rightarrow +\infty} F_n(x) \\
 &= \lim_{n \rightarrow +\infty} \frac{1}{n} \ln \left[\frac{\sum_{i=1}^n |\Psi_i|^{2x}}{\left(\sum_{i=1}^n |\Psi_i|^2\right)^x} \right].
 \end{aligned}
 \tag{15}$$

Since our numbering seems very efficient in reordering the Hamiltonian matrix, we expect the wave functions to have a simpler expression in this ordering than in the geometric one. Thus, we look for Ψ_i of the type $\Psi_i = f(i/n)$ where $f(x)$ is a smooth continuous function. If such a state exists, it must be extended since

$$\sum_{i=1}^n |\Psi_i|^{2x} = n \left(\int_0^1 f^{2x}(t) dt + O(1/n) \right)
 \tag{16}$$

is proportional to n for large n , and then, one finds easily that $F_n(x)$ goes to zero like $\ln n/n$.

Now, we rewrite the system of equations (13) for $k = 0$.

$$\begin{aligned}
 \Psi_{i+p} + \rho \Psi_{i+q} &= (E - V_{1\rho}) \Psi_i \quad 1 \leq i \leq p \\
 \Psi_{i-p} + \Psi_{i+p} &= (E - V_{11}) \Psi_i \quad p < i \leq q \\
 \rho \Psi_{i-q} + \Psi_{i-p} &= (E - V_{\rho 1}) \Psi_i \quad q < i \leq p + q = n
 \end{aligned}
 \tag{17}$$

and give two examples of such a kind of extended state, the second one being more interesting.

* $\Psi_\ell = a^{\ell/n}$: defining $\theta = p/n = \tau/(1 + \tau)$, this ansatz gives immediately

$$\begin{aligned}
 a^\theta + \rho a^{1-\theta} &= E - V_{1\rho} \\
 a^{-\theta} + a^\theta &= E - V_{11} \\
 \rho a^{\theta-1} + a^{-\theta} &= E - V_{\rho 1}.
 \end{aligned}
 \tag{18}$$

We see that, in general, there is no solution, except if $(\rho, E - V_{1\rho}, E - V_{11}, E - V_{\rho 1})$ belongs to the curve $\mathcal{B}(a)$ defined by (18), in the four dimensional space of parameters. We note that, except when $a = 1$, for which we recover the upper energy of the periodic chain ($\Psi_i = 1$), we have $V_{1\rho} \neq V_{\rho 1}$. A typical state of this kind is shown in figure 3. One can see that, by increasing a so that $V_{1\rho}/V_{\rho 1}$ becomes large compared to 1, the wave function seems to be more and more localized, although when $n \rightarrow \infty$, for a fixed a , the wave function remains extended *stricto sensu*. We note that these states which are extended from the analysis of (15) and (16), have a self-similar structure related to τ . These states still exist even in higher dimension for the general COQ. For instance, in 2D, one can obtain a similar system of seven equations (or less for some α_i 's) which correspond to two kinds of sites with 3, 4, 5 and one kind with 6 (the latter kind can disappear for some α_i 's). Although this first set of extended states is interesting, we do not investigate it any longer.

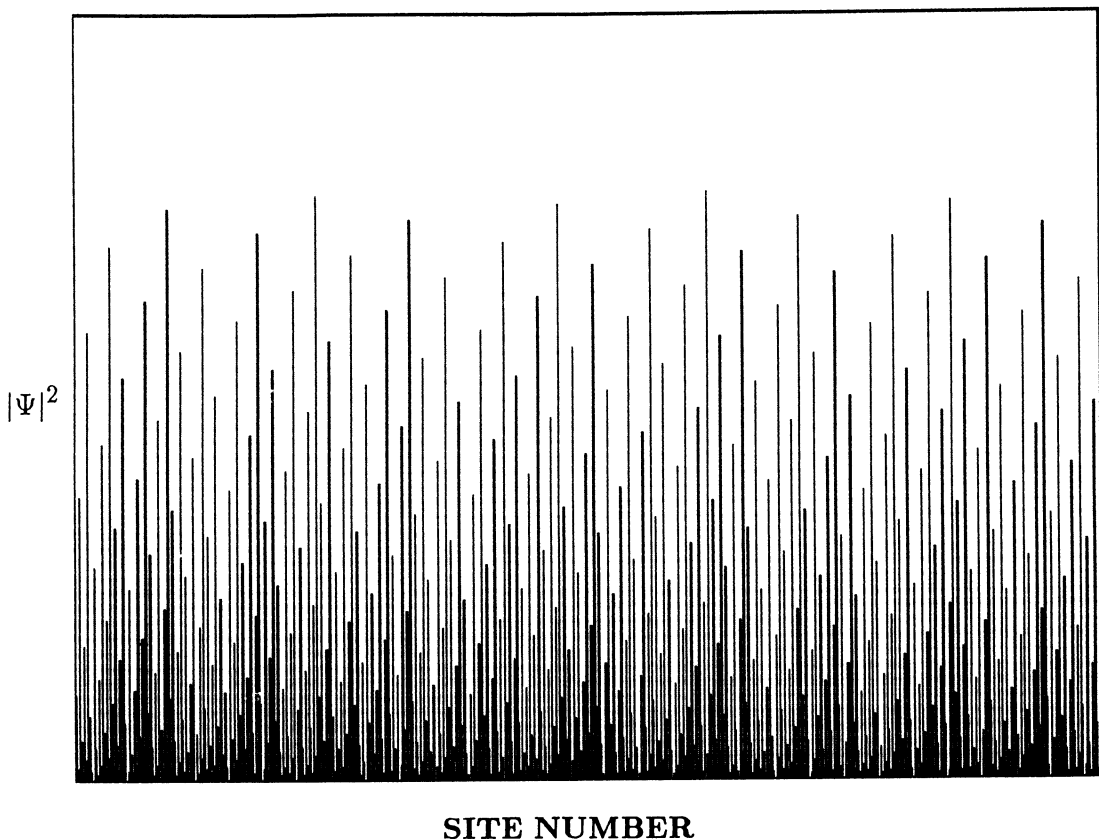


Fig. 3. — An extended state of the first type as defined in section 3. $|\Psi|^2$ is represented against the site number of a Fibonacci chain.

* $\Psi_\ell = e^{\pm i\alpha \frac{\ell}{n}}$: one finds from (17)

$$\begin{aligned} E - V_{1\rho} &= E - V_{\rho 1} \\ &= \cos(\alpha\theta) + \rho \cos(\alpha(1-\theta)) \\ E - V_{11} &= 2 \cos(\alpha\theta) \end{aligned} \tag{19}$$

and

$$\sin(\alpha\theta) + \rho \sin(\alpha(1-\theta)) = 0.$$

Since a global shift of $E, V_{1\rho}, V_{\rho 1}$ and V_{11} leaves the problem invariant, using (19), we take from now on $V_{1\rho} = V_{\rho 1} = \lambda/2$ and $V_{11} = -\lambda/2$. In this way, we have defined a three dimensional space of parameters $\delta = (\lambda, \rho, E)$. Then, we can rewrite (19) in a more efficient way and define the curve $C_+(\alpha)$ (the + recalls that this result holds for $k = 0$) of δ by

$$\begin{aligned} \lambda(\alpha) &= \frac{\sin(\alpha)}{\sin(\alpha(1-\theta))} \\ C_+(\alpha): \quad \rho(\alpha) &= -\frac{\sin(\alpha\theta)}{\sin(\alpha(1-\theta))} \quad \alpha \in [0, 2\pi n] \\ E(\alpha) &= 2 \cos(\alpha\theta) - \frac{\sin(\alpha)}{2 \sin(\alpha(1-\theta))}. \end{aligned} \tag{20}$$

Since $(\lambda(-\alpha), \rho(-\alpha), E(-\alpha)) = (\lambda(\alpha), \rho(\alpha), E(\alpha))$, the state of energy $E(\alpha)$ is degenerate. We will see the consequences of such a property on the electronic spectrum in the next section. In figure 4 a typical wave function of this kind is shown. We note that for $\alpha \rightarrow 0$ (or $\alpha \rightarrow n\pi$), the tight-binding model reduces to a constant plus a Laplacian-like operator, for which the diagonal term of site i is the sum of the two hopping parameters surrounding the i -th site. Thus, we find that for $\rho = \pm p/q$, the edge state is degenerate. The two wave functions are $\Psi_\ell = 1$ or $\Psi_\ell = (-1)^\ell$ (which is a classical result), and $\Psi_\ell = \ell$ or $(-1)^\ell \ell$. The modulus of this last wave functions grows proportionally to ℓ in our numbering. In classical geometric ordering, this wave function has a more complicated structure than a simple Bloch wave (Fig. 4). Now, we show that even for $k \neq 0, \pi$, there exists a curve $C_k(\alpha)$ whose points are extended states inside a band. For the periodic chain ($\rho = 1, \lambda = 0$), for $k \neq 0$, the eigenstate indexed by k in the j -th band has the following energy and wave function at site ℓ

$$E_j(k) = 2 \cos \left(\frac{2 \pi q j}{n} + \frac{k}{n} \right), \quad \Psi_\ell^{(j)}(k) = e^{\frac{2 i \pi \ell j}{n} + i \frac{k}{n} (\ell n' [n])} \quad (21)$$

$$= e^{\frac{2 i \pi \ell j}{n} + i k (\ell \tau' [1])}$$

where $n' = p' + q'$ (see Sect. 2 and (9)) and $\tau' = n'/n \rightarrow \tau_0$ when $n, n' \rightarrow +\infty$. This can be verified directly by noting that $n'q - nq' = 1$. So, in the same way as for $k = 0$ we try the ansatz

$$\Psi_\ell(k) = e^{\frac{i \alpha \ell}{n} + i \frac{k}{n} (\ell n' [n])} \quad (22)$$

$$= e^{\frac{i \alpha \ell}{n} + i k (\ell \tau' [1])}$$

where $k \in]0, \pi]$. After some manipulations which repeat the above calculations of (19) (20), we find that this vector is indeed a wave function for the energy E , if and only if the point (E, λ, ρ) is on the curve $C_k(\alpha)$ with

$$\lambda(\alpha) = \frac{\sin(\alpha)}{\sin(\alpha(1-\theta) + k/n)}$$

$$C_k(\alpha): \quad \rho(\alpha) = - \frac{\sin(\alpha\theta - k/n)}{\sin(\alpha(1-\theta) + k/n)} \quad \alpha \in [0, 2\pi n] \quad (23)$$

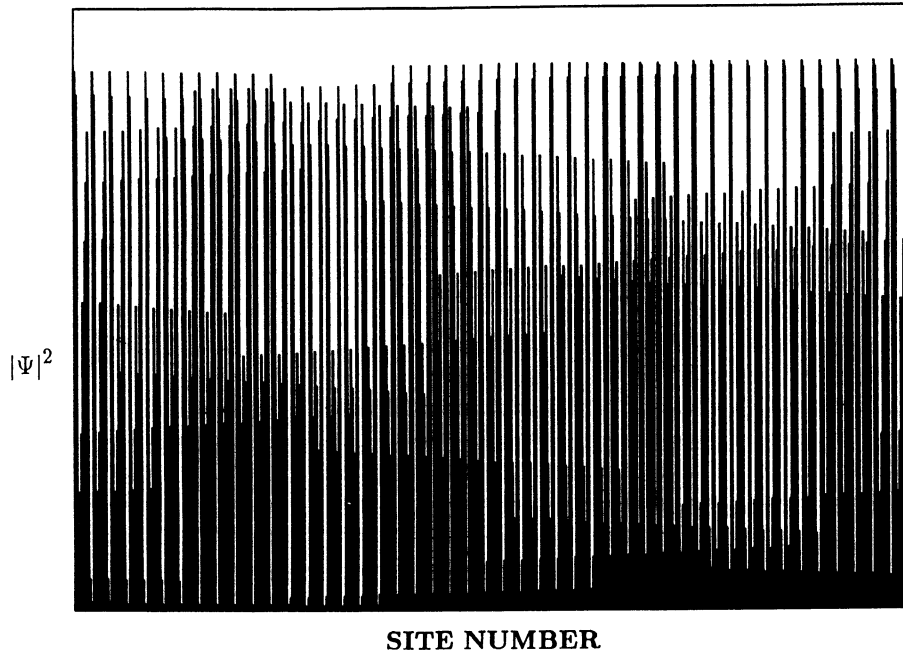
$$E(\alpha) = 2 \cos(\alpha\theta - k/n) - \frac{\sin(\alpha)}{2 \sin(\alpha(1-\theta) + k/n)}$$

Of course, for $k = 0$, we recover C_+ . In addition, we define $C_- = C_\pi$ and $C = C_+ \cup C_-$. Thus, in this section we have exhibited quasiperiodic solutions for a Hamiltonian on a COQA [11].

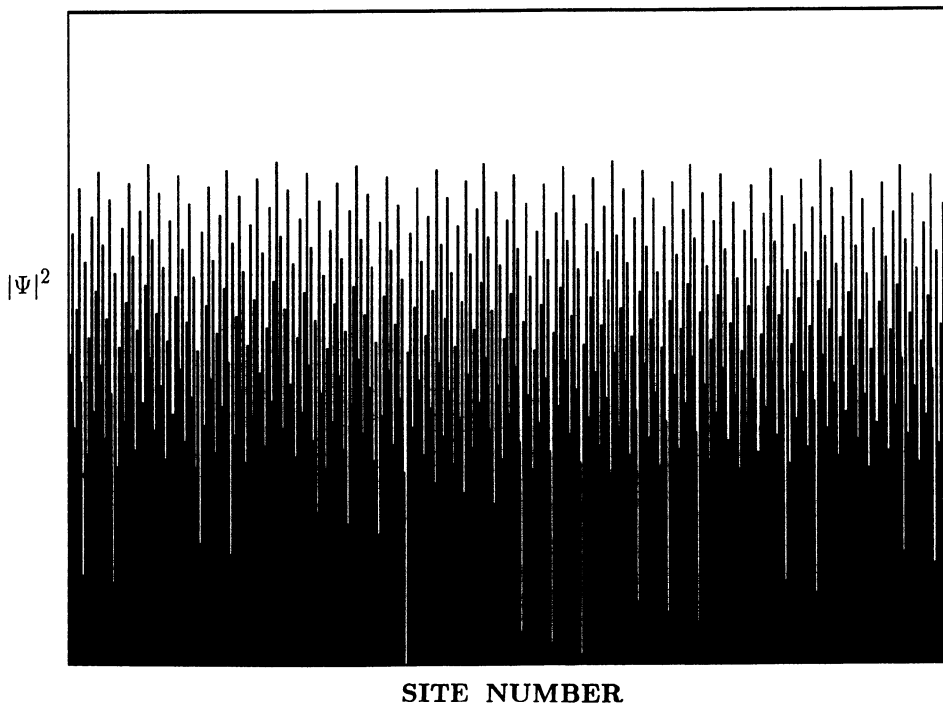
5. Gap closing.

In the discussion of section 3, we have shown that the states corresponding to $k = 0$ and $k = \pi$ are the band edges. In section 4, we have shown that there is a curve $C(\lambda(\alpha), \rho(\alpha), E(\alpha))$, depending on θ , whose points are some degenerate band edge states. This implies that for a fixed α , the gap which would normally exist at $E(\alpha)$ vanishes. This gap appears again if λ and ρ are shifted by an infinitesimal amount from $\lambda(\alpha)$ and $\rho(\alpha)$. In order to test our result, we take $p = F_{\ell-2}$ and $q = F_{\ell-1}$, where F_ℓ is the ℓ -th Fibonacci number defined by

$$F_0 = 1, \quad F_1 = 1 \quad \text{and} \quad F_{\ell+2} = F_{\ell+1} + F_\ell. \quad (24)$$



(i)



(ii)

Fig. 4. — (i) A typical « quasi-Bloch » state and (ii) the edge state for the Laplacian-like Hamiltonian defined in section 3 (Fibonacci chain).

It defines a periodic linear chain S_ℓ , whose elementary cell contains F_ℓ atoms. Its spectrum will be called $\text{Sp}\{S_\ell\}$. A trace mapping can be found which allows us to describe the spectrum numerically in a very simple way (a similar mapping has been found in [1]). It reads

$$\begin{aligned}
 & \text{with } x_0(E) = \frac{1}{2\rho} \left(E - \frac{3}{2}\lambda \right) \\
 & E \in \text{Sp}\{S_\ell\} \leftrightarrow |x_\ell(E)| \leq 1 \quad \begin{aligned} x_1(E) &= \frac{1}{2} \left(E + \frac{\lambda}{2} \right) \\ x_2(E) &= \frac{1}{2\rho} \left(\left(E - \frac{\lambda}{2} \right)^2 - 1 - \rho^2 \right) \end{aligned} \quad (25) \\
 & \text{and } x_{\ell+3} = 2x_{\ell+2}x_{\ell+1} - x_\ell.
 \end{aligned}$$

The band edges verify $x_\ell(E) = 1$ for $k = 0$, and $x_\ell(E) = -1$ for $k = \pi$ since one can easily show that $x_\ell(E) = \cos k$, where k is the Bloch vector. For a fixed λ , we show in figure 5 a part of the diagram (E, ρ) . The gap closing can be easily seen.

Now, in order to understand the meaning of α , we try to evaluate it when ρ is close enough to 1 and λ to 0, that is, near the periodic linear chain. In addition, we set $k = 0$ since the case $k = \pi$ can be studied in the same way. Under these conditions, from the form of the eigenvector, we see that α must go to a real of the type $2j\pi$ in such a way that α/n is a Bloch vector of the linear periodic chain. Now using the third equation of (20), we find

$$\alpha_j = 2j\pi + (\rho - 1) \tan(2j\pi\theta) + o(\rho - 1). \quad (26)$$

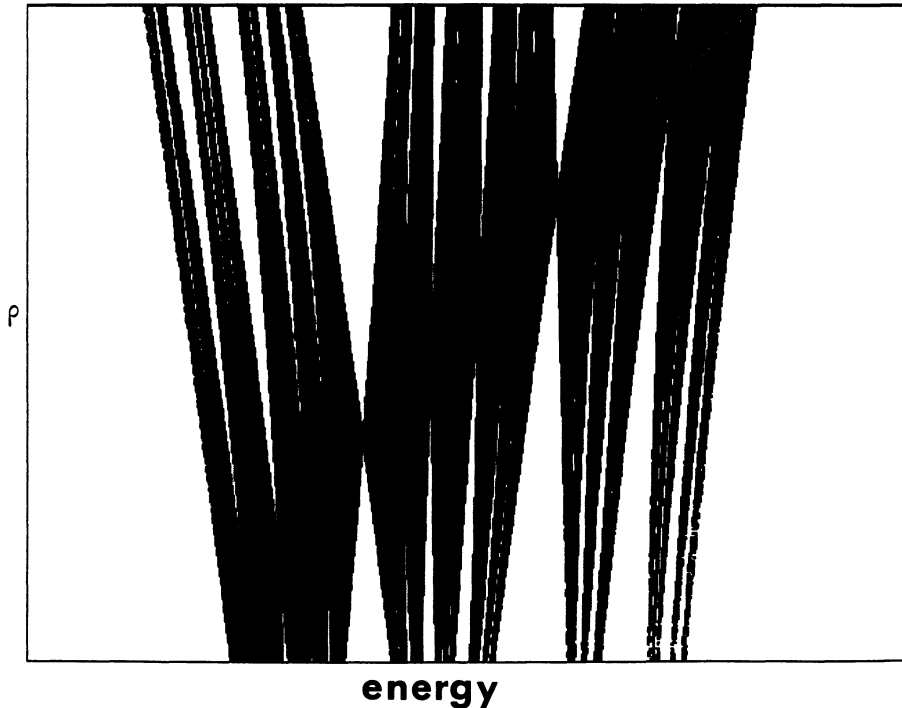


Fig. 5. — For a fixed $\lambda = -0.2$, we show the energy spectrum for $\rho \in [0.6, 1.4]$. The gap closings are easily seen and are located on the intersection of the surface \mathcal{S} and the 2D plane $\lambda = -0.2$.

Then, using the other two equations (20) we find that a gap disappears at E_j if

$$\begin{aligned} \lambda &= \frac{1 - \rho}{\cos(2j\pi\theta)} \\ E_j &= 2 \cos(2j\pi\theta)(1 - \theta(1 - \rho)) + \frac{\lambda}{2}(4\theta - 1) \end{aligned} \tag{27}$$

which are exactly the two expressions one would obtain by applying the perturbative approach described in [7]. Indeed, by means of a perturbative formalism, we have shown that for the general 1D quasiperiodic chain, a gap appears at $2\varepsilon \cos(\pi j\theta)$ in the spectrum of the 1D periodic chain, and the edges of this gap are given by

$$\begin{aligned} 2\varepsilon \cos(\pi j\theta)(1 - (1 - \rho)\theta) + \lambda \left(2\theta - \frac{1}{2}\right) + \\ + \frac{2\varepsilon'}{\pi j} \left[(1 - \rho) \sin(\pi j\theta) - \varepsilon \frac{\lambda}{2} \sin(2\pi j\theta) \right] \end{aligned} \tag{28}$$

where $\varepsilon, \varepsilon' \in \{-1, 1\}$. Indeed, we see that the condition for a gap closing in the perturbative approach is exactly (27). Thus, we have shown that for any (λ, ρ, E) which obey (20), one can define a « quasi-Bloch » vector α/n , which reduces to the Bloch vector of the linear chain for $\rho = 1$ and $\lambda = 0$, according to (26) and the expression of E_j in (27).

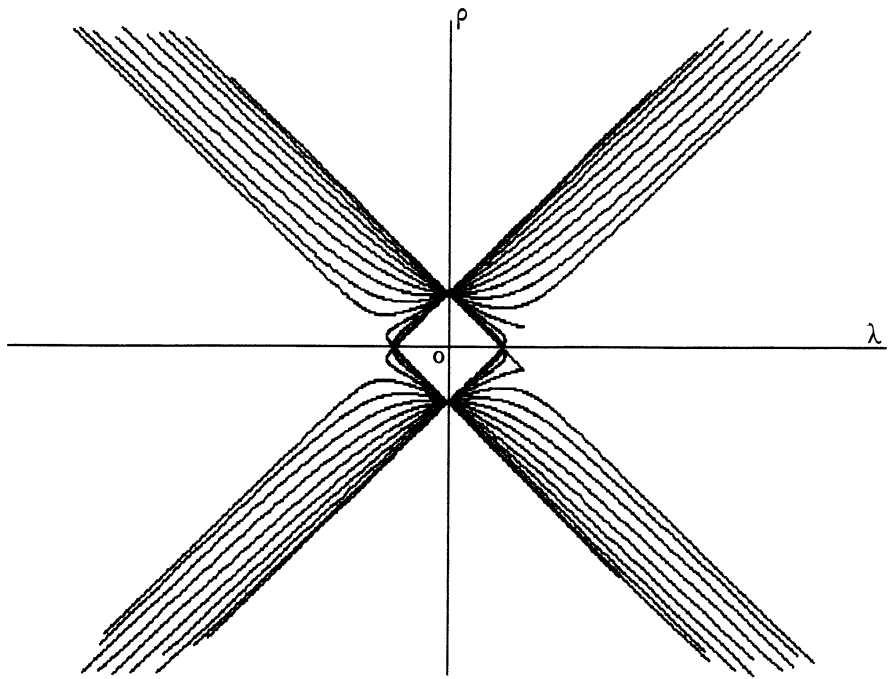
In the following, we study the curve $\mathcal{C}(\lambda(\alpha), \rho(\alpha), E(\alpha))$. First of all, from (23), it is easy to show that for any k , $\mathcal{C}_k(\alpha)$ lies on the 2D-surface \mathcal{S} of \mathfrak{E} defined by

$$E = \frac{1 - \rho^2}{\lambda} + \frac{\lambda}{2} \quad (\lambda, \rho) \in \Delta \tag{29}$$

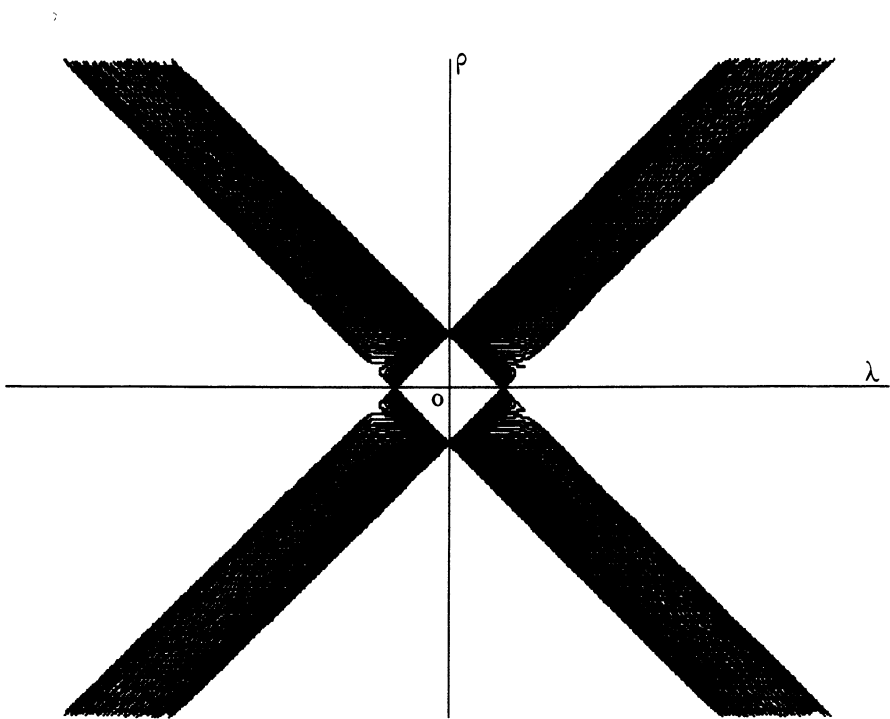
where Δ is the set limited by the four lines $\lambda = \pm(\rho \pm 1)$ excluding the internal square. In figure 6, we show Δ and the projection of $\mathcal{C}(\alpha)$ on the plane (λ, ρ) . If θ (or τ) is an irrational number, $\mathcal{C}(\alpha)$ is dense on \mathcal{S} , and its projection is dense on Δ (Fig. 6). In figure 6, we show that \mathcal{S} is made of four branches. Each of them can be deduced from the one in the space $\rho \geq 0, \lambda \geq 0$ by very simple symmetries. Thus, in figure 7, we have only shown this last branch. The vertical segment, $E \in [-2, 2], \lambda = 0$ and $\rho = 1$ corresponds to the gap closing (of all gaps) near the linear chain. The point $(\lambda = 1, \rho = 0, E = 3/2)$, is a molecular state, since for $\rho = 0$, the chain splits into an assembly of molecules (made of 2 or 3 atoms for the golden number). For this value of λ , the upper energies of both molecules ($E_3 = \sqrt{2 + \lambda^2}/4, E_2 = \lambda/2 + 1$) are the same. It is interesting to note that although $\mathcal{C}_k(\alpha)$ depends explicitly on τ , this is not the case for \mathcal{S} . Moreover, \mathcal{S} is contained in the intersection of all τ -spectra, τ being any real number, irrational or not. Indeed, although \mathcal{C}_k is of zero measure on \mathcal{S} , for any point P of \mathcal{S} , one can find k and α such that $P \in \mathcal{C}_k$ with parameter α . We conjecture that \mathcal{S} is exactly the intersection of all energy spectra. More precisely, we define $\text{Sp}(\tau, \lambda, \rho)$, the spectrum of the linear chain, built from τ , rational or not, with tight-binding parameters λ and ρ . Then, we have proved that

$$\mathcal{S} \subset \bigcap_{\tau \in \mathbb{R}} \left\{ \bigcup_{\lambda, \rho \in \Delta} \text{Sp}(\tau, \lambda, \rho) \right\} \subset \bigcap_{\tau \in \mathbb{R}} \left\{ \bigcup_{\lambda, \rho \in \mathbb{R}} \text{Sp}(\tau, \lambda, \rho) \right\}. \tag{30}$$

Our assumption is that both inclusions are in fact equalities. Moreover, we have shown that, for a fixed τ , on \mathcal{S} , the states are extended, with a dense set which corresponds to gap closings. In the next section, we show the origin of these states in terms of a dynamical system. This will provide a solid argument that we have found all the extended states of our model.



(i)



(ii)

Fig. 6. — The region Δ and the projection of the curve C for $\theta = 8/21$ (upper) and $\theta = 34/89$ (lower). For an irrational value of θ , C is dense on S and Δ .

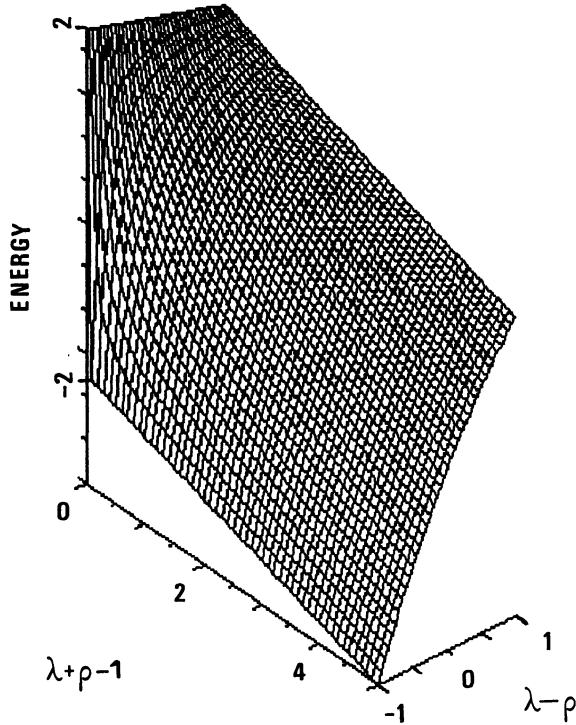


Fig. 7. — The branch of \mathcal{S} in the region $(\lambda > 0, \rho > 0)$ in the variables $(\lambda + \rho - 1, \lambda - \rho, E)$.

6. Origin of the surface \mathcal{S} .

It has been shown that the spectrum of any 1D quasiperiodic chain can be obtained from a dynamical system [8]. More precisely, (13) can be studied in terms of transfer-matrices. The important result is that, for any τ , there is a mapping involving some traces of certain products of transfer-matrices. For example, when τ is the golden mean, this mapping Φ has already been given in (25) and reads :

$$\Phi(x, y, z) = (y, z, 2zy - x) . \tag{31}$$

The initial conditions for this mapping depend on λ, ρ and E . Then, E is in the spectrum, if the iterations of the map Φ do not go to a fixed point including infinity. Moreover, there is an invariant, which is the same for any τ , provided x, y and z are properly defined (in the simplest case, for the golden mean x, y, z are the x_i 's in (25) ; the general expression is more complicated). So for any τ , one can prove that Φ leaves the following surface invariant

$$\begin{aligned} \mathfrak{J}(x, y, z) &= x^2 + y^2 + z^2 - 2xyz = \mathfrak{J}(\lambda, \rho, E) \\ \mathfrak{J}(\lambda, \rho, E) &= 1 + \frac{1}{4} \left[\frac{\lambda \left(E - \frac{\lambda}{2} \right)}{\rho} + \rho - \frac{1}{\rho} \right]^2 . \end{aligned} \tag{32}$$

When $\lambda = 0, \rho = 1$ (periodic chain), $\mathfrak{J} = 1$. However, even for other values of the parameter, \mathfrak{J} can be equal to 1. It occurs if, and only if, the square in (32) vanishes. It is clear that this condition implies that $(\lambda, \rho, E) \in \mathcal{S}$. So, we have found that there are some initial

values of the energy (and the parameters) for which the iterations of the mapping Φ remain on the surface corresponding to the periodic chain. Thus, we are not surprised that these states are extended ones. In higher dimension, it can be shown that, although the extended states of first kind (18) still exist, this is not the case for the second ones (except of course for the square and cubic lattices). In fact, since, in higher dimensions, there is no equivalent of the 1D periodic chain (that is a topologically equivalent periodic structure), that could explain why this type of « quasi-Bloch » extended states does not exist. We show now that such degeneracies lead to the appearance of a Berry phase. For a general real Hamiltonian, Wigner and Von Neumann [9] have shown that generically, one needs at least two parameters to make degeneracies appear. We see that this is exactly the case for the Hamiltonian (13). Moreover, following Berry [10], we define a closed path in the space of parameters (λ, ρ) . Then, if this path encloses a degeneracy (we recall that \mathcal{C} on \mathcal{S} is precisely the set of degeneracies) for one specified state, the corresponding wavefunction will transform into its opposite. This is the so-called Berry phase. In our problem, if the circuit intercepts the set Δ previously defined (see Fig. 6), then, it contains generically an infinite set of energy levels (or only a large set for large approximants), since the projection of \mathcal{C} on Δ is dense. Thus, instead of only one wave function, such a circuit will cause the change of sign for an infinite (or large) number of eigenfunctions.

To end this section, let us stress that the existence of the surface \mathcal{S} may lead to some interesting properties of some physical quantities such as conductivity. When λ and $(1 - \rho)$ are very small, we expect the physical properties of the quasiperiodic chain to be very close to those of the periodic chain. In the same way, when, for a given ρ and λ (even far from the periodic case), \mathcal{S} intercepts the energy spectrum, there exists one extended state and the wave functions of the states near this energy, though critical, behave like extended states, with a fractal dimension very close to 1. Therefore, in this range of energies, the physical properties (conductivity) should be very close to what is found in a crystal.

7. Conclusion.

In this paper, we have presented some exact results concerning codimension one quasicrystals. We first introduced a new numbering of the sites which by reordering the rows and columns of the Hamiltonian matrix, reveals an underlying simpler structure. This approach allows us to find exact extended states, for a quasiperiodic Hamiltonian. This implies that, for well chosen tight-binding constants, the vicinity of these states should consist in « almost extended » states, that is, critical, but with fractal dimension very close to 1. This could lead to crystal-like physical properties. The occurrence of some degeneracies has been exhibited and corresponds to gap closing. We note that these results can be found in a similar way when studying a vibrational problem instead of the excitation spectrum of a linear quasiperiodic chain.

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Note added :

Some related results concerning the existence of extended states have been recently published in the Fibonacci chain case (V. Kumar, in Proc. of conference on Quasicrystals, ICTP, Trieste (World Scientific, 1990) p. 391). Our results are more general since they apply to any rational or irrational number governing the chain geometry and also because the eigenfunctions are given explicitly here.

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