Classification
Physics Abstracts
72.15N - 64.60

Short Communication

Renormalization group for a quasiperiodic Schrödinger operator

L.S. Levitov

L.D. Landau Institute for Theoretical Physics, Moscow, U.S.S.R.

(Reçu le 13 octobre 1988, accepté sous forme définitive le 8 février 1989)

Résumé.– Nous construisons un groupe de renormalisation dans l'espace réel pour hamiltonien de Fibonacci généralisé. Nous montrons que le spectre a la structure hiérarchique d'un ensemble de Cantor de mesure nulle lié à la représentation en fraction continue de la fréquence incommensurable du problème. Nous discutons des propriétés fractales du spectre.

Abstract.– The real-space renormalization group for a generalized Fibonacci Hamiltonian is constructed. The spectrum is shown to have the hierarchical structure of a zero-measure Cantor set guided by the continuous fraction representation of the incommensurate frequency ω of the problem. The fractal properties of the spectrum are discussed.

1. Introduction.

In this work we study the one-dimensional discrete Schrödinger equation

$$E\,\psi_k = t_k\,\psi_{k-1} + t_{k+1}\,\psi_{k+1} \tag{1.a}$$

with a quasiperiodic sequence of hopping amplitudes t_k :

$$t_k = V\,(\omega\,k\,+\,\varphi) \tag{1.b}$$

where ω is an irrational number and $V(x)$ is a periodic function ($V(x+1) = V(x)$) taking two values :

$$V(x) = \begin{cases} V_1, & 0 \le x < \omega \\ V_2, & \omega \le x < 1 \end{cases} \tag{1.c}$$

This problem and related ones were intensively studied recently in connection with quasicrystals both analytically [1, 3-8, 11, 14] and numerically [2, 4, 8-13]. The works [1-14] mainly concern the "golden mean" case : $w = (\sqrt{5}-1)/2$.

The most important analytic result obtained for this problem is that the recursion relation for the traces of the transfer matrices has an invariant function J (Kohmoto, Kadanoff, Tang [1]). This "conservation law" results in nonuniversal scaling properties of the spectrum and eigenfunctions of the problem (1), since the invariant J for it is given by

$$J = \frac{1}{2}\left[\left(\frac{V_1}{V_2}\right)^2 + \left(\frac{V_2}{V_1}\right)^2\right]. \tag{2}$$

It was pointed out in section 2 of [4] that the conservation law found in [1] exists not only for $\omega = (\sqrt{5}-1)/2$ but for all irrational ω as well. Thus one can expect nonuniversal scaling results for the problem (1) with an arbitrary ω.

In this Letter the $J \gg 1$ limit of the problem (1) is studied. Treating $1/J$ as a small parameter we extend the renormalization scheme developed in [4] for $\omega = (\sqrt{5}-1)/2$ to all irrational ω.

2. Geometrical formulation of the problem.

Let us consider the interger lattice Z^2 in the plane R^2. We define an (α, c)-strip as the set of points (x, y) such that

$$\alpha x + c < y < \alpha x + c + 1 + \alpha \tag{3}$$

(α is irrational, c is chosen so that no integer points belong to the boundary of the strip). Then we find a continuous chain consisting of horizontal and vertical segments of Z^2 (denoted "h-segments" and "v-segments") lying inside the strip. This chain always exists and is defined unambiguously. One can see that the alternation order of h-segments and v-segments in the chain coincides exactly with the alternation law for the hopping amplitudes V_1, V_2 given by (1.b, c) provided $\omega = 1/(1+\alpha)$.

Hence, instead of problem (1) we can consider the tight binding problem for an electron moving along the chain so that a) it is allowed to stay at the vertices of the chain only ; b) the amplitudes of hopping across the segments are V_1 (for h-segments) and V_2 (for v-segments).

Remark.– Our results will depend neither on the phase φ in (1.b) nor on the strip position c in (3). Therefore we neglect φ and c everywhere below for the sake of brevity (e.g. we write "α-strip" instead of "(α, c)-strip").

In accordance with this remark any problem (1) is completely defined by three numbers : V_1, V_2, α. It is convenient to use the following parametrization : $V_1 = \lambda V$, $V_2 = V$, $\alpha = n_1 + 1/(n_2 + \ldots = (n_1, n_2 \ldots))$ (the continued fraction expansion). We will work with triplets $[V_1/V_2, V_2, \alpha] = [\lambda, V, (n_1, n_2 \ldots)]$.

We are going to study the $J \gg 1$ -sector of the problem. This implies $\lambda \ll 1$ or $\lambda \gg 1$ since $J = \frac{1}{2}(\lambda^2 + \lambda^{-2})$ (see (2)). The problems $[V_1/V_2, V_2, \alpha]$ and $[V_2/V_1, V_1, 1/\alpha]$ are equivalent (they are related by the permutation of the x-axis

and the y-axis), so we will study the $\lambda \ll 1$ -case only, i.e. we assume that the coupling across h-segments is much weaker that that across v-segments.

3. Renormalization procedure.

We study separately two possible situations : $\alpha < 1$ and $\alpha > 1$.

I. $\underline{\alpha > 1}$ $(n_1 \neq 0)$.– Let us consider the problem $[\lambda,\ V,\ (n_1,\ n_2, ...)]$ $(\lambda \ll 1)$ in the zero-order approximation, i.e. put $\lambda = 0$. This means that all h-segments are erased and we are left with "molecules" consisting of n_1 and $n_1 + 1$ v-segments as shown in figure 1 (denote them "n_1 – molecules" and "$n_1 + 1$ – molecules"). Their energy levels are given by

$$E_m = 2V \cos\left(\frac{\pi m}{n}\right) \quad m = 1, ..., n-1, \tag{4}$$

where $n = n_1 + 2$ for n_1 – molecules, $n = n_1 + 3$ for $(n_1 + 1)$ – molecules. The normalized eigenfunction corresponding to the m-th level (4) is given by

$$\psi_m(k) = \sqrt{\frac{2}{n}} \sin\left(\frac{\pi m}{n} k\right) \quad k = 1, ..., n-1 \tag{5}$$

where k is the number of the site.

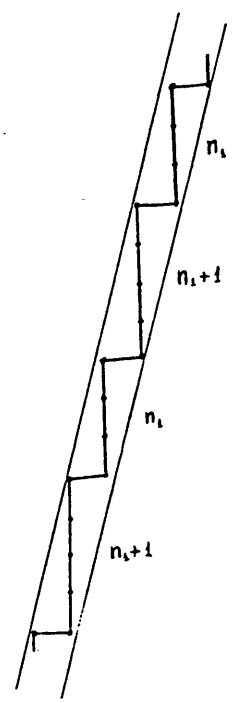

Fig. 1.– The strip (3) with the corresponding chain of horizontal and vertical segments is shown. Vertical segments form n_1–molecules and $(n_1 + 1)$–molecules ($n_1 = 3$ in the picture).

Since $\lambda \neq 0$ but very small, each of $2n_1 + 3$ levels (4) splits into subbands. To find this splitting we apply the standard quantum mechanical perturbation procedure : we treat exactly the interaction of degenerated levels, whereas the interaction of nonresonance levels is taken in the lowest nonvanishing order of λ-expansion. This method is reliable if

$$\left|\left\langle m \left| \hat{H} \right| m' \right\rangle\right| \ll |E_m - E_{m'}| \tag{6}$$

for all eigenstates $|m\rangle$, $|m'\rangle$ such that $E_m \neq E_{m'}$. Let us estimate the LHS and RHS of (6). For the levels E_m and $E_{m'}$ of the neighboring n_1-molecule and $(n_1+1)-$molecule we obtain

$$E_m - E_{m'} = 2V\left(\cos\left(\frac{\pi m}{n_1+2}\right) - \cos\left(\frac{\pi m'}{n_1+3}\right)\right) \tag{7.a}$$

$$\left\langle m \left| \hat{H} \right| m' \right\rangle = \lambda V\ \psi_m(1)\ \psi_{m'}(n_1+2) =$$

$$= (-1)^{m'+1}\ \lambda V\ \frac{2\sin\left(\frac{\pi m}{n_1+2}\right)\ \sin\left(\frac{\pi m'}{n_1+3}\right)}{\sqrt{(n_1+2)(n_1+3)}} \tag{7.b}$$

Easy but long calculations show that

$$\left|\frac{\left\langle m \left| \hat{H} \right| m' \right\rangle}{E_m - E_{m'}}\right| < 2\lambda \tag{7.c}$$

Since $\lambda \ll 1$ we can apply the perturbation theory to derive the effective Hamiltonians for the subbands (4).

First we sutdy how n_1-molecules and $(n_1+1)-$molecules alternate in the chain. Let us attribute the vectors

$$e_1 = \left\| \begin{matrix} 1 \\ \\ n_1+1 \end{matrix} \right\|, \quad e_2 = \left\| \begin{matrix} 1 \\ \\ n_1 \end{matrix} \right\| \tag{8}$$

to the molecules. The chain of segments (8) shown in figure 2 gives the alternation law we are interested in. After the coordinates are changed so that $e_1 \longrightarrow \left\| \begin{matrix} 1 \\ \\ 0 \end{matrix} \right\|$, $e_2 \longrightarrow \left\| \begin{matrix} 0 \\ \\ 1 \end{matrix} \right\|$ we obtain the chain corresponding to the standard strip (2) with α replaced by $\beta = (n_2 - 1,\ n_3, \ldots)$. The v-segments and h-segments of the β-strip obtained represent n_1-molecules and $(n_1+1)-$molecules respectively. Two different situations for β are possible : $\beta < 1$ $(n_2 = 1)$ and $\beta > 1$ $(n_2 \neq 1)$. They must be studied separately.

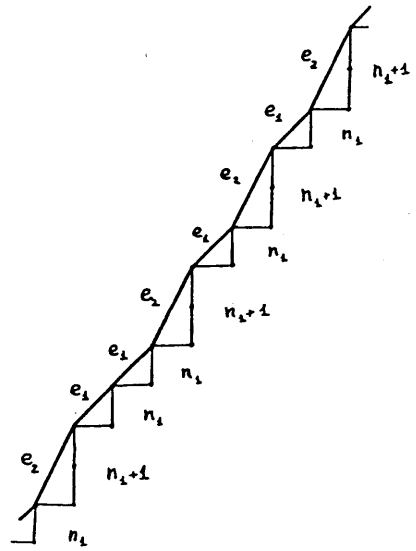

Fig. 2.– The chain of the segments e_1, e_2 given by (8) gives the law for the alternation of n_1 – molecules and $(n_1 + 1)$ – molecules in the standard chain.

a) $\underline{\beta < 1}$.– Let us take the m-th level of $(n_1 + 1)$ – molecules and find the effective Hamiltonian for the corresponding subband.

The neighboring $(n_1 + 1)$ – molecules are either adjacent or separated by one n_1 – molecule. The amplitude V'_m of hopping to the adjacent $(n_1 + 1)$ – molecule is given by

$$V'_m = \lambda V \, \psi_m(1) \, \psi_m(n_1 + 2) = (-1)^{m+1} \lambda V \frac{2}{n_1 + 3} \sin^2\left(\frac{\pi m}{n_1 + 3}\right) \tag{9}$$

The amplitude $\lambda'_m V'_m$ of hoping across one n_1 – molecule is given by

$$\lambda'_m V'_m = \lambda^2 V^2 \, \psi_m(1) \, \psi_m(n_1 + 2) \, g_{n_1}(E_m), \tag{10}$$

where

$$g_n(E) = \sum_{p=1,\ldots,n-1} \frac{\psi_p(1) \, \psi_p(n-1)}{E - E_p}, \tag{11}$$

$n = n_1 + 2$, the eigenstates ψ_p and the energy levels E_p of n_1 – molecule are defined by (4), (5). One can prove the remarkable identity

$$g_{n_1}(E_m) = \frac{(-1)^{m+1}}{V} \tag{12}$$

(see Appendix). Taking (10), (11), (12), into account, we obtain

$$\lambda'_m = (-1)^{m+1} \lambda, \tag{13}$$

i.e. the absolute value of the ratio V_1/V_2 of the hopping amplitudes is *not renormalized.*

Let us find how the amplitudes (9), (10) alternate in the sequence of $(n_1 + 1)$ – molecules. We introduce the vectors

$$e_1 = \begin{Vmatrix} 1 \\ 1 \end{Vmatrix}, \quad e_2 = \begin{Vmatrix} 1 \\ 0 \end{Vmatrix} \tag{14}$$

and the chain of segments (14) shown in figure 3. This chain gives the alternation of the amplitudes (9), (10), e_1 – segments and e_2 – segments corresponding to $\lambda'_m V'_m$ and V'_m respectively. One finds immediately that, after the coordinates are changed so that $e_1 \longrightarrow \begin{Vmatrix} 1 \\ 0 \end{Vmatrix}$, $e_2 \longrightarrow \begin{Vmatrix} 0 \\ 1 \end{Vmatrix}$, our chain is transformed into the standard chain corresponding to the α'-strip, where

$$\alpha' = (n_3 - 1,\ n_4, \ldots) \tag{15}$$

We see that the Hamiltonian for the m-th band corresponds to the triplet $[\lambda'_m,\ V'_m,\ \alpha']$ given by (9), (13) and (15).

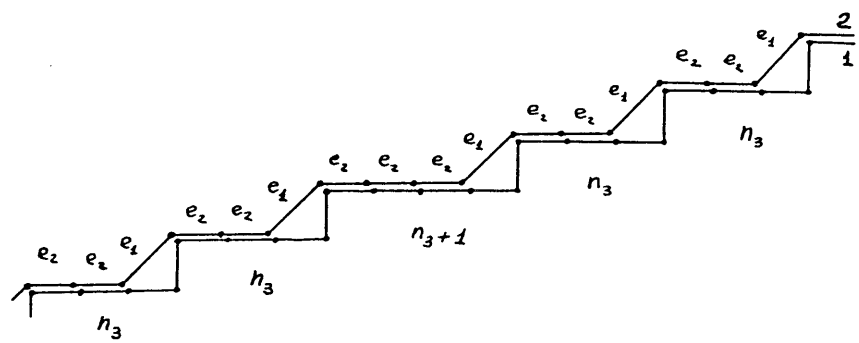

Fig. 3.– The ordering of the segments of the chain 1 gives the law for the alternation of $(n_1 + 1)$ – molecules (h-segments) and n_1 – molecules (v-segments). The chain 2 corresponds to the sequence of $(n_1 + 1)$ – molecules : a) the vertices are associated with $(n_1 + 1)$ – molecules ; b) the segments e_1, e_2 given by (14) correspond to the hopping amplitudes V'_m (e_2 – segment) and $\lambda'_m V'_m$ (e_1 – segment).

Remark.– The perturbation theory gives not only the hopping amplitudes but also the corrections to the energy levels E_m. One can see that these corrections coincide for all $(n_1 + 1)$ – molecules to our accuracy, so they only shift the levels slightly

$$E_m \longrightarrow E'_m = E_m + \Delta E_m,\ |\Delta E_m| \ll |E_m - E_{m\pm1}|$$

but do not contribute to the splitting.

Now we have to consider n_1 – molecules. Each two neighboring n_1 – molecules are separated by n_3 or $n_3 + 1$ $(n_1 + 1)$ – molecules. Let us find the hopping amplitudes for the m-th level of n_1 – molecules. The amplitude V'_m of hopping across n_3 $(n_1 + 1)$ – molecules is given by

$$V'_m = (\lambda V)^{n_3+1} \psi_m(1) \psi_m(n_1 + 1) [g_{n_1+1}(E_m)]^{n_3} \tag{16}$$

where ψ_m is the eigenfunction of the m-th level, $g_{n_1+1}(E)$ is given by (11) with $n = n_1 + 3$, E_p and ψ_p being the energy levels and eigenstates of the $(n_1 + 1)$ – molecule. The amplitude $\lambda'_m V'_m$ of hopping across the $n_3 + 1$ $(n_1 + 1)$ – molecules is given by

$$\lambda'_m V'_m = (\lambda V)^{n_3+2} \psi_m(1) \psi_m(n_1 + 1) [g_{n_1+1}(E)_m]^{n_3+1} \tag{17}$$

Taking into account the identity

$$g_{n_1+1}(E_m) = \frac{(-1)^m}{V} \tag{18}$$

we find the renormalized values of λ'_m V'_m:

$$\lambda'_m = (-1)^m \lambda$$

$$V'_m = \lambda^{n_3+1} V (-1)^{m(n_3+1)+1} \frac{2}{n_1 + 2} \sin^2\left(\frac{\pi m}{n_1 + 2}\right) \tag{19}$$

One checks easily that the alternation of the amplitudes $\lambda'_m V'_m$ and V'_m coincides exactly with the sequence of the h-segments and v-segments of the chain corresponding to the α'-strip, where

$$\alpha' = (n_4 - 1, n_5, \ldots) \tag{20}$$

We see that the m-th band is described by the Hamiltonian associated with the triplet $[\lambda'_m, V'_m, \alpha']$ given by (19) and (20) (note that the absolute value of λ is *not renormlaized* again).

b) $\underline{\beta > 1}$.– The calculations are quite analogous to those for $\beta < 1$, so we only quote the result.

The neighboring n_1 – molecules are either adjacent or separated by one $(n_1 + 1)$ – molecule. The splitting of the m-th band of n_1 – molecules is described by the Hamiltonian associated with the triplet $[\lambda'_m, V'_m, \alpha']$:

$$\lambda'_m = (-1)^m \lambda$$

$$V'_m = \lambda V (-1)^{m+1} \frac{2}{n_1 + 2} \sin^2\left(\frac{\pi m}{n_1 + 2}\right) \tag{21}$$

$$\alpha' = (n_2 - 2, n_3, n_4, \ldots)$$

The neighboring $(n_1 + 1)$ – molecules are separated by $n_2 - 1$ or n_2 n_1 – molecules. The corresponding triplet $[\lambda'_m, V'_m, \alpha']$ is given by

$$\lambda'_m = (-1)^{m+1}$$

$$V'_m = \lambda^{n_2} V (-1)^{n_2(m+1)} \frac{2}{n_1 + 3} \sin^2\left(\frac{\pi m}{n_1 + 3}\right) \tag{22}$$

$$\alpha' = (n_3 - 1, n_4, \ldots)$$

II. $\alpha < 1$. — We start with the zero-approximation : $\alpha = 0$. The chain consists of 1-molecules (v-segments) and single "atoms" (vertices having 2 horizontal neighbors). The energy levels are $E_{\pm} = \pm V$ (for molecules) and $E_0 = 0$ (for atoms).

Let us find the splitting of the molecular levels $E'_{\pm}$. Two adjacent molecules are separated by n_2 or $n_2 - 1$ atoms. Calculations similar to those presented in Part I ($\alpha > 1$) give the result

$$[\lambda'_+, V'_+, \alpha'_+] = \left[\lambda, \frac{1}{2} V \lambda^{n_2}, (n_3 - 1, n_4, \ldots)\right]$$
$$[\lambda'_-, V'_-, \alpha'_-] = \left[-\lambda, (-1)^{n_2} \frac{1}{2} V \lambda^{n_2}, (n_3 - 1, n_4, \ldots)\right] \tag{23}$$

For the $E_0 = 0$ band one has to study two different situations : $n_2 > 1$ and $n_2 = 1$. When $n_2 > 1$ the neighboring atoms are either adjacent or separated by one molecule. We find

$$[\lambda', V', \alpha'] = [-\lambda, \lambda V, (n_2 - 1, n_3, \ldots)] \tag{24}$$

When $n_2 = 1$ the neighboring atoms are separated by n_3 or $n_3 + 1$ molecules. We find

$$[\lambda', V', \alpha'] = [-\lambda, (-1)^{n_3} \lambda^{n_3+1} V, (n_4 - 1, n_5, n_6, \ldots)] \tag{25}$$

4. Self-consistency of the renormalization.

We see that the splitting of all bands is described by effective Hamiltonians corresponding to the triplets $[\lambda', V', \alpha']$ such that $\lambda' \neq \lambda$, i.e. $|\lambda|$ is *not renormalized*. Consequently, $\lambda \ll 1$ implies $\lambda' \ll 1$ and, hence, the renormalization procedure can be repeated step by step infinitely many times.

Analyzing the expression (9), (19), (21)-(25) for V' we find that the width of each subband ($\sim V'$) is at least λ^{-1} times smaller than the distance to the nearest energy level obtained at the preceding step of the iteration (in agreement with the estimate (7.c)). Thus the bands obtained by the splitting do not overlap. We conclude that the spectrum is a zero measure fractal of Cantor set type organized hierarchically.

An important remark should be made here. We found that the absolute value of the parameter λ is not renormalized at the first order of the perturbative theory. Probably, this is an approximate result. One can expect that, if higher order perturbation is taken into account, then $|\lambda|$ changes from one step of the iteration to another : $\lambda_1, \lambda_2, \lambda_3, \ldots$ where $|\lambda_i| \neq |\lambda_j|$, $(\lambda_1 = \lambda)$. Then an important quantity is $\lambda^* = \lim_{k \to \infty} \lambda_k$. Two situations are possible :

a) if $\lambda^* \ll 1$ for $\lambda \ll 1$ then the renormalization is self-consistent, since starting from weak coupling we never go out of this region ;

b) on the other hand, if $\lambda^* \geq 1$ or $\lambda^* = \infty$ then the iterative procedure developed in section 3 breaks down at some step of the iteration.

In the author's opinion, case a) takes place, although this is not proven yet. The reason for such a belief is that the problem has a conservation law (see [4]). One can think that the conservation of $|\lambda|$ obtained at the first order of perturbative approximation reveals the (exact) conservation of the quantity $J = \mathrm{tr}\left(ABA^{-1}\,B^{-1}\right)$ (A, B are transfer-matrices – see [1, 4]. Assuming that this is true we conjecture that $\lambda^* \neq 0$ and moreover $\frac{|\lambda_k|-|\lambda|}{|\lambda|} \longrightarrow 0$ uniformly for all k when $\lambda \longrightarrow 0$.

To conclude we make some remarks on the dependence of fractal properties of the spectrum on the choice of ω (or α). Using the above established hierarchical structure of the spectrum one can calculate its fractal dimension as well as the critical exponents for eigenstates. We review the results for two interesting cases.

1) "good" irrational α (the sequence n_i is uniformly bounded : $n_i <$ const. for all i). The fractal dimension d of the spectrum is a nonuniversal function of λ such that $d \sim$ const. $[\ln(\lambda^{-1})]^{-1}$ at very small λ. The eigenstates are critical, i.e. on every large piece of the chain having length L an eigenfunction is effectively supported by L^{γ} sites ($0 < \gamma < 1$).

2) "bad" irrational α (the sequence n_i grows : $\lim_{i \longrightarrow \infty} n_i = \infty$). The fractal dimension of the spectrum is one (this does not contradict the zero-measure property). The eigenfunctions are extende (detailed calculations will be reported elsewhere).

Acknowledgements.

I am grateful to A. Kitaev for interesting and fruitful discussions.

Appendix.

Let us prove the identity

$$\frac{1}{n}\sum_{k}\frac{(-1)^{k+1}\,\sin^2\left(\frac{\pi k}{n}\right)}{\cos\theta\;-\;\cos\left(\frac{\pi k}{n}\right)} = \frac{\sin\theta}{\sin(n\,\theta)} \tag{A1}$$

(the sum is taken over $k = 1,\ldots, n-1$).

Proof.– Let us replace $\exp(i\theta)$ by z in (A1). Both the LHS and RHS of (A1) are rational analytic functions of z taken as a complex variable. It is known that two analytic functions $f_1(z)$, $f_2(z)$ such that $\lim_{z \longrightarrow \infty} f_1(z) = 0$, $\lim_{z \longrightarrow \infty} f_2(z) = 0$ coincide if and only if their poles and corresponding residues coincide. A simple calculation shows that this is true for the RHS and LHS of (A1). The identity is proven.

The identities (12), (18) are immediately obtained by substituting $\theta_m = \frac{\pi m}{n \pm 1}$ in (A1), since

$$\frac{\sin\theta_m}{\sin(n\,\theta_m)} = \mp\,(-1)^m \tag{A2}$$

References

[1] KADANOFF L.P., TANG Chao, KOHMOTO M., *Phys. Rev. Lett.* **50** (1983) 1870-1872.

[2] OSTLUND S., PANDIT R., RAND D., SCHELLNHUBER H.J., SIGGIA E.D., *Phys. Rev. Lett.* **50** (1983) 1873-1876.

[3] KOHMOTO M., OONO Y., *Phys. Lett.* **102A** (1984) 145-148.

[4] KALUGIN P.A., KITAEV A.Yu., LEVITOV L.S., Electron Spectrum of a One-Dimensional Quasicrystal (Landau Institute preprint, 1985), *Zh. Eksp. Teor. Fiz.* **91** (1986) 692 ;
translation : *Sov. Phys. JETP* **64** (1986) 410.

[5] CASDAGLY M., *Commun. Math. Phys.* **107** (1986) 295-318.

[6] DELYON F., PETRITIS D., *Commun. Math. Phys.* **103** (1986) 441-444.

[7] SUTO A., *Commun. Math. Phys.* **111** (1987) 409-415.

[8] LUCK J.M.,Workshop on Aperiodic Crystals, *J. Phys. Colloq. France* **47** (1986) C3-205.

[9] OSTLUND S., PANDIT R., *Phys. Rev. B* **29** (1984) 1394.

[10] FUJITA M., MACHIDA K., *Solid State Commun.* **59** (1986) 61.

[11] LUCK J.M., PETRITIS D., *J. Stat. Phys.* **42** (1986) 289.

[12] KOHMOTO M., BANAVAR J., *Phys. Rev. B* **34** (1986) 563.

[13] NORI F., RODRIGUEZ J.P., *Phys. Rev. B* **34** (1986) 2207-2211.

[14] SUTHERLAND B., *Phys. Rev. Lett.* **57** (1986) 770.