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1993 J. Phys.: Condens. Matter 5 2769

(http://iopscience.iop.org/0953-8984/5/17/011)

J. Phys.: Condens. Matter 5 (1993) 2769–2778. Printed in the UK

Gap-labelling properties of the energy spectrum for the on-site model of one-dimensional Fibonacci quasi-lattices

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Received 9 June 1992, in final form 4 January 1993

Abstract. We study the gap-labelling properties of the energy spectrum for the on-site model of one-dimensional Fibonacci quasi-periodic lattices; we have obtained the occupation probabilities on subbands of the hierarchical energy spectrum and the step heights of the integrated density of states. It is analytically proved that the step height is equal to $\{m\tau\}$, where the braces denote the fractional part, and m is an integer which can be used to label the corresponding energy gap. Numerical simulations confirm these results.

1. Introduction

Since the experimental study by Schechtman *et al* [1] of an Al–Mn alloy that exhibits a diffraction pattern with peaks showing icosahedral symmetry, much attention has been focused on studies of quasi-periodic systems. The study of one-dimensional quasi-periodic systems has become particularly relevant since the success in growing Fibonacci superlattices [2–4] and the discovery [5] of one-dimensional quasi-crystals in rapidly solidified $Al_{80}Ni_{14}Si_6$, $Al_{65}Cu_{20}Mn_{15}$ and $Al_{65}Cu_{20}Co_5$. A large number of theoretical studies have been devoted to the physical properties of one-dimensional quasi-crystals of the Fibonacci type [6–16]. By means of the weak-bond approximation, Niu and Nori [9] first used the renormalization group method to investigate the electronic energy spectrum of one-dimensional Fibonacci quasi-crystals. By the use of the direct diagonalization method, Liu and Riklund [11] found that for the on-site model the energy spectrum exhibits a four-subband global structure, each of which further trifurcates following the hierarchy of splitting from one to three subsubbands. Subsequently, Liu and Sritrakool [15] used the renormalization group approach analytically to calculate the occupation probabilities of the electronic spectrum and to locate the absolute heights of the steps in the integrated density of states (IDOS) of the on-site model for one-dimensional Fibonacci quasi-crystals. The IDOS is an important parameter, which shows the structure of a Cantor-like spectrum and appears to have a devil's-staircase structure. The steps (or plateaux) of the IDOS correspond to the gaps in the energy spectrum and show their widths. The regular splitting of the spectrum allows us to investigate the gap-labelling rules. Luck and Petritis [7] have defined an almost periodic Laplace operator to describe the Fibonacci chain and to study the gap-labelling rules.

0953-8984/93/172769+10$07.50

More recently, Luck [17] has analysed perturbatively the IDOS of an arbitrary deterministic aperiodic sequence and found that the gaps in the energy spectrum can be 'labelled' by the singularities of the Fourier transform of the sequence of potentials. Ashraff *et al* [18] have found numerically that in two-dimensional Fibonacci quasi-lattices the steps in the IDOS curve for the electron and phonon cases occur at ordinate values, some of which have the form $I = \{m\tau\}$, where m is a non-zero integer. Bellissard *et al* [19] have obtained the exact labelling of all spectral gaps for the period-doubling sequence. Recently, the gap-labelling properties of the energy spectrum for the transfer model of one-dimensional Fibonacci quasi-lattices was studied by Liu *et al* [16].

In fact, the gap-labelling properties were studied earlier for incommensurate potential systems that are defined by the Harper equation $-f_{n+1} - f_{n-1} + v(n\theta L)f_n = Ef_n$, where $v(n\theta L)$ is a periodic function and θ is the wavevector of the underlying periodic lattices with atomic spacing L and is an irrational number. The spectrum of this kind of one-dimensional system also has a devil's-staircase structure [22–25]. Claro and Wannier [22] proved that any gap in the spectrum can be labelled by a pair of integers n and m (positive or negative) and the IDOS below that gap is equal to

$$I = L|n\theta + m(2\pi/L)|/2\pi. \tag{1}$$

Equation (1) has been referred as a 'gap-labelling theorem' [24] because it gives a way of labelling the infinite hierarchy of gaps in the spectrum of the incommensurate systems. Subsequently the 'gap-labelling theorem' has been studied mathematically by Bellissard and co-workers [20, 21]. In this paper, we prove analytically the gap-labelling theorem for the energy spectrum of the on-site model of one-dimensional Fibonacci quasi-lattices, for which the equation of motion is

$$T_{n+1}f_{n+1} + T_nf_{n-1} = (E - E_n)f_n. \tag{2}$$

For the on-site model the T_n values ($n = 1, 2, \ldots$) take the values unity, and the site energies E_n take two values E_A and $E_B = -E_A$, which are arranged in a Fibonacci sequence [6–16]. The theorem states that the steps of the IDOS rigorously are equal to $\{m\tau\}$, and m is a progressively increasing natural integer corresponding to different hierarchies of gaps of the spectrum.

In section 2, we obtain the occupation probabilities (OPs) on subbands of the hierarchical energy spectrum and the step heights of the IDOS. In section 3, we find that an integer can be used to label the corresponding energy gap.

2. Electronic energy spectrum and occupation probability

The energy spectrum for the Fibonacci on-site model has been explained by different analytical methods and confirmed by the numerical simulations. The decomposition–decimation method based on the renormalization group technique [9, 15] may give the clearest physical picture for the formation of the pattern. Figure 1 exhibits the four-subband global structure and the trifurcation rule in the following hierarchies. From this figure we can see that the formation rules are as follows.

(1) The formation of a four-subband global structure is $F_{17} = F_{15} + F_{14} + F_{13} + F_{14}$ which suggests that, for an nth-generation Fibonacci lattice, the global branching rule is

$$F_n = F_{n-2} + F_{n-3} + F_{n-4} + F_{n-3}. \tag{3}$$

(2) For the subband structure, the formation rule is

$$F_i = F_{i-2} + F_{i-3} + F_{i-2}. \tag{4}$$

Both of the above two rules can be analytically obtained by the following analysis. Because the golden mean τ is greatly involved in the calculation, it is very helpful to write down the formulae concerned with τ here.

(1) $\tau^2 + \tau - 1 = 0$, where $\tau = (\sqrt{5} - 1)/2 = 0.618\,033\,98$.
(2) The recursion relation

$$\tau^n + \tau^{n-1} = \tau^{n-2}(\tau^2 + \tau) = \tau^{n-2}. \tag{5}$$

We consider the studied one-dimensional model of the lattice as a chain of atoms, which contains two kinds of atom: A and B. The on-site model, such as ABAABABAABAAB for the seventh generation of Fibonacci chain, can be considered to be built up of three kinds of construction element: A, AA and B. For the nth-generation sequence, let N_A^n, N_{AA}^n and N_B^n be the numbers of construction elements, respectively. We have found the following distribution rule [11]:

$$N_A^n = F_{n-4} \qquad N_B^n = F_{n-2} \qquad N_{AA}^n = F_{n-3} \qquad \text{odd } n$$
$$N_A^n = F_{n-4} + 2 \qquad N_B^n = F_{n-2} \qquad N_{AA}^n = F_{n-3} - 1 \qquad \text{even } n.$$

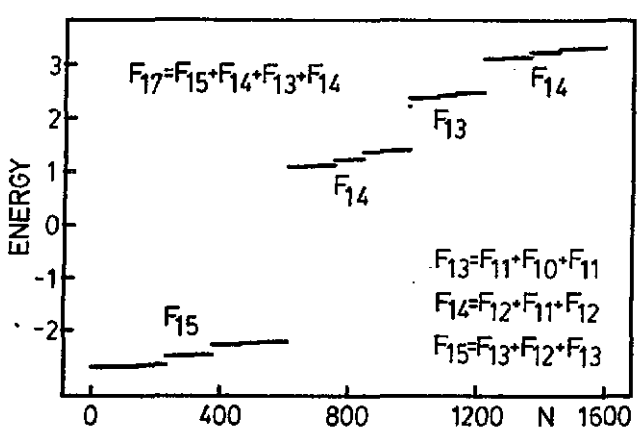

Figure 1. Electronic spectrum for an on-site model with two site energies $E_A = -E_B = 2$, for a seventeenth-generation Fibonacci chain with $N = 1597$. The four-subband global structure and the distribution rules are shown.

Let $P(\mathrm{B})$ represent the OP for a B atom in an infinite Fibonacci chain, and similarly $P(\mathrm{A})$ the OP for an isolated atom A, $P(\mathrm{AA})$ the OP for a molecule AA, and $P(\mathrm{A}+\mathrm{AA})$ the OP for atom species A. Therefore, we have

$$P(\mathrm{B})/P(\mathrm{A}+\mathrm{AA}) = \lim_{n\to\infty}[F_{n-2}/(F_{n-4}+2F_{n-3})] = \tau = 0.618\,033\,98\ldots.$$

Because $P(\mathrm{A}+\mathrm{AA}) + P(\mathrm{B}) = 1$, we have

$$P(\mathrm{B}) = \tau^2$$

and

$$P(\mathrm{A}+\mathrm{AA}) = \tau. \tag{6}$$

On the other hand, the molecules AA can be decomposed into bonding and antibonding biatomic molecular state subchains, the OPs of which are $P^+(\mathrm{AA})$ and $P^-(\mathrm{AA})$, respectively; they are equal to $P(\mathrm{AA})$. Because $P(\mathrm{AA})/P(\mathrm{B}) = \lim_{n\to\infty}(F_{n-3}/F_{n-2}) = \tau$, then the OPs for the four main subbands are as follows:

$$\begin{aligned} P(\mathrm{B}) &= \tau^2 \qquad & P^+(\mathrm{AA}) &= \tau^3 \\ P(\mathrm{A}) &= \tau^4 \qquad & P^-(\mathrm{AA}) &= \tau^3 \end{aligned} \tag{7}$$

which can be confirmed by the equality $\tau^2+\tau^3+\tau^4+\tau^3 = \tau^2+\tau = 1$.

This analytical result confirms the suggested global branching rule shown by equation (3), because, for an infinite Fibonacci chain, the proportion of constructing elements between two successive generations equals $F_{n-1}/F_n = \tau$. Therefore, equation (3) satisfies the general equation (7).

To explain the trifurcation appearing in the following hierarchies, Liu and Sritakool [15] noted that the on-site model chain can be decomposed into four transfer model subchains with bond lengths arranged in a Fibonacci sequence. The energy spectrum of each subchain would further trifurcate indefinitely. This conclusion for the transfer model can be easily obtained if we follow the deduction performed by Niu and Nori [9]. Now we shall study the distribution of OPs for the trifurcating subsubbands. Using the notation N_{S} and N_{L} to label the numbers of short bonds and long bonds, we have $N_{\mathrm{S}}/N_{\mathrm{L}} = \tau$. For each subband split into three subsubbands, a simple calculation shows that

$$\begin{aligned} &P(\text{middle subsubband}) = \tau^3 \\ &P(\text{side subsubband}) = \tau^2 \end{aligned} \tag{8}$$

which can be confirmed by the equality $\tau^2+\tau^3+\tau^2 = \tau^2+\tau = 1$. Consequently, we obtain the second conclusion that the side subband: middle subband OP ratio is $\tau^2 : \tau^3$. From the relation $F_{n-1}/F_n = \tau$ again, we can see that the formation rule (4) is exactly the same as the analytical result

$$F_{i-2} : F_{i-3} : F_{i-2} = \tau^2 : \tau^3 : \tau^2.$$

Using the above two distribution rules (7) and (8) and recursion relations (5), we can easily calculate the OP on any subband to a high branching hierarchy. For the first branching hierarchy, the OPs of the four main subbands are τ^2, τ^3, τ^4 and τ^3, respectively, as proved above. Table 1 shows the OPs of all subsubbands up to the second hierarchy of the energy spectrum. On the basis of the above results on the OPs of the subbands, we can obtain analytically the step heights of the IDOS by the use of the following formula:

$$I(E_n) = \sum_{i=1}^{n} P(i) \tag{9}$$

where $P(i)$ is the OP of the ith subsubband in the hierarchy studied, and E_n is the highest energy of the nth subsubband (lower edge of the ith gap). $I(E_n)$ is the IDOS up to the energy E_n and corresponds to a step in the IDOS 'stairs' curve. Table 1 gives the absolute heights of steps in the IDOS as well as the OP of the subsubbands for an infinite Fibonacci chain up to the second hierarchy of the spectrum.

Table 1. The occupation probabilities on the subbands and the step heights of the IDOS expressed by $(n + m\tau)$.

OP	
First hierarchy	Second hierarchy
τ^3	τ^5
	$4 - 5\tau$
	τ^6
	$-1 + 3\tau$
	τ^5
$2 - 2\tau$	τ^6
	$-3 + 6\tau$
τ^4	τ^7
	$5 - 7\tau$
	τ^6
τ	τ^5
	$3 - 4\tau$
τ^3	τ^6
	$-2 + 4\tau$
	τ^5
$1 - \tau$	τ^4
	$-1 + 2\tau$
τ^2	τ^5
	$2 - 3\tau$
	τ^4

3. Gap labelling

Now we study the gap-labelling property. Using the recursion relation of the Fibonacci number $F_n = F_{n-1} + F_{n-2}$ with $F_1 = 1$ and $F_2 = 1$, we have obtained the following recursion relationship between the golden mean τ and F_n:

$$\tau^n = (-1)^n(F_{n-1} - F_n\tau) \tag{10}$$

which is a key formula in the proof of the gap-labelling theorem and also is an interesting relationship connecting the golden mean and Fibonacci numbers.

We can use a sequence 1, 2, 3, 4 to label the first hierarchy of the spectrum and $\bar{1}, 0, 1$ for the higher hierarchy. A subband of the nth hierarchy can be labelled $(l_1, l_2, l_3, \ldots, l_n)$ with $l_1 = 1, 2, 3, 4$ and $l_i = \bar{1}, 0, 1$ $(i = 2, 3, \ldots, n)$. Let E_b and $P(l_1, l_2, \ldots, l_n)$ denote the highest energy and OP of the subband $(l_1, l_2, \ldots, l_n)$. The step height $I(E_b; l_1, l_2, \ldots, l_n)$ of the IDOS, which corresponds to the low edge of the gap located above the subband studied, can be calculated by the following method.

First it is easy to see that, with $P(1) = \tau^2$, $P(2) = \tau^3$, $P(3) = \tau^4$ and $P(4) = \tau^3$,

$$P(l_1, l_2, \ldots, l_n) = P(l_1)P(l_2)\ldots P(l_n). \tag{11}$$

On the other hand, for the four subbands of the first hierarchy of the spectrum we have

$$I(E_b;1) = P(1) = \tau^2$$
$$I(E_b;2) = P(1) + P(2) = \tau^2 + \tau^3 = \tau$$
$$I(E_b;3) = P(1) + P(2) + P(3) = \tau^2 + \tau^3 + \tau^4 = 2\tau^2$$
$$I(E_b;4) = P(1) + P(2) + P(3) + P(4) = \tau^2 + \tau^3 + \tau^3 + \tau^3 = 1.$$

For the (l_1, l_2) subband of the second hierarchy, we have

$$I(E_b; l_1, l_2) = I(l_1 - 1) + P(l_1, l_2 - 2) + P(l_1, l_2 - 1) + P(l_1, l_2).$$

If $l_2 - i < -1$, $P(l_1, l_2 - i)$ is taken to be zero.

In general, for the $(l_1, l_2, \ldots, l_n)$ subband of the nth hierarchy the step height of the IDOS is equal to

$$I(E_b; l_1, l_2, \ldots, l_{n-1}, l_n) = I(l_1, l_2, \ldots, l_{n-1} - 1) + P(l_1, l_2, \ldots, l_{n-1}, l_n - 2) + P(l_1, l_2, \ldots, l_{n-1}, l_n - 1) + P(l_1, l_2, \ldots, l_{n-1}, l_n) \tag{12}$$

where $l_1 = 1, 2, 3, 4$ and $l_i = \bar{1}, 0, 1$ $(i = 2, 3, \ldots, n)$. If $l_n - i < -1$, $P(l_1, l_2, \ldots, l_n - i)$ is taken to be zero.

The proof of the above formulae is straightforward. Equations (11) and (12) can be used to obtain the OP and the step height of the IDOS for any subband of any hierarchy.

From equation (11) we can see that the OP of every subband in any hierarchy has a τ^i form. Therefore, equation (12) can be rewritten as

$$I = \sum_i k_i \tau^i \tag{13}$$

where k_i is a positive integer; the range of the parameter i depends on the hierarchy and subband studied. On the other hand, because $0 < I \leqslant 1$, from equations (10) and (13) we can conclude that the step height of the IDOS can be written as

$$I = n + m\tau = \{m\tau\} \tag{14}$$

Table 2. The characteristic number m of the gap.

Hierarchy	m_1 (positive)	m_2 (negative)
First	1	$-1, -2$
Second	2–4, 6	$-(m_1+1)$
Third	5, 7–12, 14, 16, 17, 19, 27	$-(m_1+1)$
Fourth	13, 15, 18, 20–26, 28–33, 35, 37, 38, 40, 42–46, 48, 50, 51, 53, 61, 69, 71, 72, 74, 82, 116	$-(m_1+1)$
Fifth	34, 36, 39, 41, 47, 49, 52, 54–60, 62–68, 70, 73, 75–81, 83–88, 90, 92–93, 95, 97–101, 103, 105, 106, 108, 110–115, 117–122, 124, 126, 127, 129, 131–135, 137, 139, 140, 142, 150, 158, 160, 161, 163, 171, 179, 181, 182, 184, 186–190, 192, 194, 195, 197, 205, 213, 215, 216, 218, 226, 260, 294, 302, 304, 305, 307, 315, 349, 493	$-(m_1+1)$

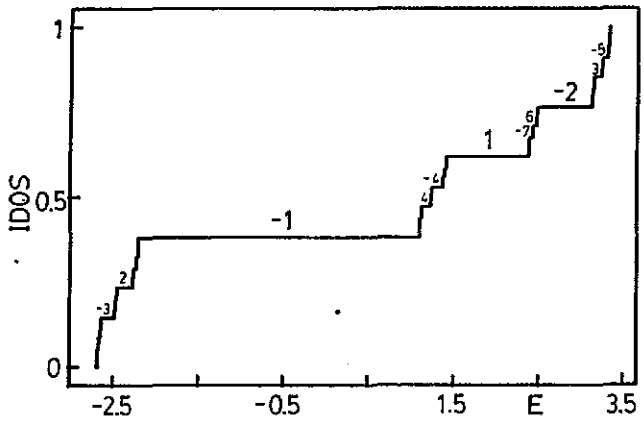

Figure 2. The IDOS as a function of energy for a seventeenth-generation Fibonacci chain with site number $N = 1597$. The characteristic numbers m are marked in the corresponding steps (gaps).

where n and m are both sums of Fibonacci numbers; therefore they are integers.

Because τ is an irrational number, from equation (12) for the step height we can see that the $\{m\tau\}$ for different gaps are absolutely different. This point is also guaranteed by the Cantor-like hierarchical structure of the spectrum. Consequently, every gap of any hierarchy of the spectrum, which corresponds to a step of the IDOS, is a uniquely characteristic number of a gap; so we can use m to label the gaps. Table 1 gives the OPs of subbands and the step heights of the IDOS expressed as $n + m\tau$. Table 2 presents the corresponding characteristic numbers of the IDOS up to the fifth hierarchy of the spectrum for an infinite Fibonacci chain. Unlike the transfer model, for the on-site model the spectrum is asymmetrical with respect to $E = 0$. Consequently, in the IDOS curve the steps are not symmetric either, which implies that the characteristic numbers m are not asymmetric with respect to $E = 0$. This result is different from that of the transfer model, for which Liu *et al* [16] have proved that the

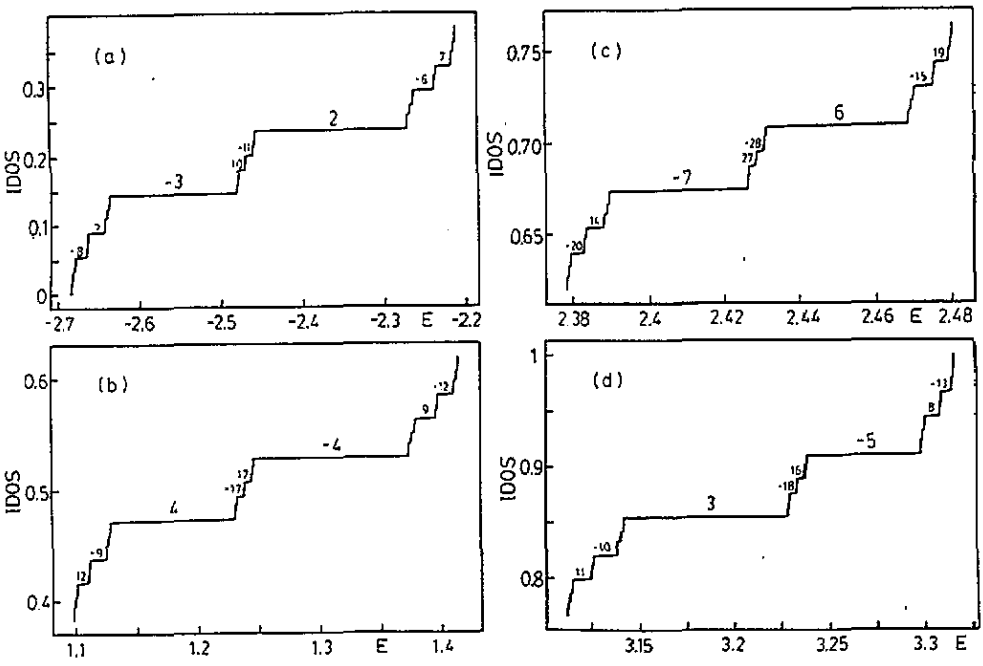

Figure 3. Enlarged figures for the four main subbands (shown in figure 2). The characteristic numbers m are marked in the corresponding gaps.

Table 3. The analytical and numerical results of the step heights of the IDOS for a one-dimensional Fibonacci chain. The results are for a Fibonacci chain with site number $N = 1597$.

First hierarchy			Second hierarchy		
m	$\{m\tau\}$	Numerical result	m	$\{m\tau\}$	Numerical result
			-5	0.909 830	0.909 831
			3	0.854 102	0.854 101
-2	0.763 932	0.763 933			
			6	0.708 204	0.708 203
			-7	0.673 762	0.673 763
1	0.618 034	0.618 034			
			-4	0.527 864	0.527 865
			4	0.472 136	0.472 135
-1	0.381 966	0.381 966			
			2	0.236 068	0.236 067
			-3	0.145 898	0.145 899

values of m are asymmetric with respect to $E = 0$. From the m-values shown in table 2, we note that, on going to a higher hierarchy, the integer m progressively increases in a natural-number sequence starting from 1. In the same hierarchy, for the transfer model the positive integer m_1 and the negative integer m_2 satisfy $m_2 = -m_1$ [16], but for the on-site model the relation is $m_2 = -(m_1+1)$. m does not continuously increase from one hierarchy to the next hierarchy but in jumps; before the fourth hierarchy the natural numbers missing

in the m-values of a hierarchy appear immediately in the following hierarchy, but in the higher hierarchies this does not hold.

The numerical results on the IDOS are shown in figures 2 and 3 for the seventeenth-generation Fibonacci chain with site number $N = 1597$; here, we have chosen the site energy $E_B = -E_A = 2.0$. In figure 2 we plot the entire spectrum, in which we can clearly see the hierarchical four-main-subband structure of the energy spectrum and the steps of the IDOS. Figures 3(a), 3(b), 3(c) and 3(d) are the enlarged plots of the four subbands, respectively. Even though the numerical simulation is performed for a small size of Fibonacci chain, the results are in good agreement with the analytical results for an infinite Fibonacci chain; the comparison between them is presented in table 3.

4. Brief summary

We have studied the gap-labelling properties of the energy spectrum of the on-site model for one-dimensional Fibonacci quasi-crystals. We obtained the OPs on subbands of the hierarchical energy spectrum and the step heights of the IDOS and found that an integer m can be used to label the corresponding energy gap. The numerical simulations confirm these results very well. The theoretical and numerical results show that the gap-labelling property of the on-site model is different from that of the transfer model.

Acknowledgments

This work is supported by the National Science Foundation of China, and in part by the International Program in Physical Science, Uppsala, Sweden.

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