PHYSICAL REVIEW B VOLUME 51, NUMBER 6 1 FEBRUARY 1995-II

Hierarchical mobility edges in a class of one-dimensional generalized Fibonacci quasilattices

Xiujun Fu and Youyan Liu
Department of Physics, South China University of Technology, Guangzhou 510641, China

Zizheng Guo and Peiqin Zhou
Department of Physics, Inner Mongolia Normal University, Huhhot 010022, China

Xiuqing Huang
Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box. 8730, Beijing 100080, China and Department of Physics, Zhongshan University, Guangzhou 510275, China

(Received 31 January 1994; revised manuscript received 29 September 1994)

The electronic energy spectrum and localization of the wave functions for a class of one-dimensional generalized Fibonacci quasilattices, whose substitution rules are $A \rightarrow ABB$ and $B \rightarrow A$, have been studied. It has been found that the spectrum has a peculiar trifurcating structure and there are three kinds of wave functions in the spectrum: extended, localized, and intermediate states. The middle part of the central subband in every hierarchy of the spectra is always continuous and the corresponding wave functions are all extended while the rest of the wave functions are intermediate or localized, i.e., there exist mobility edges in the subband. For the whole spectra the mobility edges possess a type of hierarchical structure.

As a one-dimensional version of quasicrystals, the Fibonacci chain has been extensively studied since the experimental discovery by Schechtman *et al.*[1] Its main feature is the Cantor set character of the energy spectrum.[2–5] For recent years the theoretical interest has been shifting towards other one-dimensional quasiperiodic systems, such as the generalized Fibonacci quasilattices,[6–9] Thue-Morse and generalized Thue-Morse models,[10,11] and the three-tile SML model.[12] The so-called generalized Fibonacci sequence is best described by successive application of the substitution rules $A \rightarrow A^m B^n$ and $B \rightarrow A$, with m,n being positive integers, which is denoted as $GF(m,n)$ here. In this paper we concentrate on the study of $GF(1,2)$ quasilattices, which is also referred to as the twins model or the copper mean lattice.[6–9]

Most studied physical properties of the one-dimensional generalized Fibonacci quasilattices are concentrated on the spectral structure. On the other hand, the localization of the electronic states has not been much investigated. But, following the discovery of the quasisemiconductor,[13] the localization problem is likely to attract more and more interest. It is well known that for one- and two-dimensional disordered systems the electronic states are all localized, but for three-dimensional ones there are mobility edges, which separate the conducting region (extended state region) from the nonconducting one (localized state region). In a one-dimensional system, no matter whether quasiperiodic or aperiodic, whether there exist mobility edges is a very attractive problem. For the one-dimensional quasilattices, the extended states have been found at individual energies.[8] Recently, Sil *et al.*[9] have analytically shown that there is an infinite number of extended states in the $GF(1,2)$ chain. For the $GF(1,2)$ model studied in this article, we found that the spectrum has a trifurcating structure. For the central subband of every hierarchy of the spectrum, the middle part is always continuous. Because the continuous spectrum corresponds to the extended state band, we can expect that not only are there mobility edges, but that furthermore the mobility edges would have a hierarchical structure. This conjecture has been confirmed by the numerical calculations. To the best of the authors' knowledge this is the first time that a hierarchical structure of mobility edges is discovered.

In order to study the spectral properties of quasiperiodic systems, many approaches have been developed. The analytical methods based on the trace maps and real-space renormalization-group technique have played a central role in the understanding of the problem.[2–4] Liu and Sritrakool[5] have developed a decomposition-decimation (DD) method to study the Fibonacci chain and have given a simple and clear physical picture of the electronic spectral behavior. Because the geometric self-similarity also exists in the present model, we can use the DD method to analyze the spectral behavior of the $GF(1,2)$ quasilattices.

Let us consider the transfer model of the $GF(1,2)$ chain shown in Fig. 1(a), where the site energies are set to be zero and the transfer-matrix elements take one of the two values t_A and t_B according to the $GF(1,2)$ sequence. Assume $t_A \ll t_B$, first, in the absence of the weak bonds, i.e., let $t_A = 0$, the chain is broken into two kinds of isolated clusters: the isolated atoms (IA's) and triatomic molecules (TM's) as shown in Fig. 1(b). The eigenenergy of the isolated atom is simply $E = 0$ and those of triatomic molecule are $E = 0, \pm\sqrt{2}t_B$. Consequently, in the first approximation the spectrum consists of three levels $E = 0$ and $E = \pm\sqrt{2}t_B$, which determines that the energy spectrum should have a three-main-subband structure.[5] The numerical results shown in Fig. 2 confirm this conclusion.

Now we consider the side subband with $E = \sqrt{2}t_B$ re-

0163-1829/95/51(6)/3910(4)/$06.00

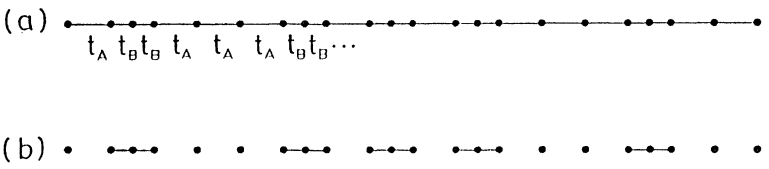

FIG. 1. (a) The $GF(1,2)$ chain of the fifth generation. All of the sites are the same, but there are two kinds of hopping integrals t_A and t_B. (b) If the weak bonds t_A are cut, the $GF(1,2)$ chain is broken into two kinds of clusters: isolated atoms and triatomic molecules.

sulting from the TM's, for which there are two coupling cases (see Fig. 1). The effective coupling strengths can be obtained as $t'_A = t_A^3/8t_B^2$ for two TM's connected by three t_A bonds, and $t'_B = t_A/4$ for two TM's connected by one t_A bond.

If we take the TM with energy $E=\sqrt{2}t_B$ as a "superatom" and two effective coupling bonds t'_A and t'_B are denoted by A' and B', respectively, then the superatoms construct a new chain $A'B'B'A'A'A'B'B'A'B'B'\ldots$, which is again a $GF(1,2)$ sequence with renormalized coupling strengths $t'_A = t_A^3/8t_B^2$ and $t'_B = t_A/4$. Consequently, if we break off the new weak bond t'_A to perform the second approximation, the level $E=\sqrt{2}t_B$ will split to three new levels, $E=\sqrt{2}t_B$ and $E=\sqrt{2}t_B \pm \sqrt{2}t'_B = \sqrt{2}t_B \pm \sqrt{2}t_A^3/8t_B^2$. From the first renormalization procedure we know that the further splitting pattern of these three subsubbands should be the same as their corresponding main subbands, individually. The numerical results shown in Fig. 2 are coincident with the above analysis.

Because of the symmetry of the spectrum, the structure of another side subband related with eigenenergy $E=-\sqrt{2}t_B$ in the first approximation is exactly the same as that of $E=\sqrt{2}t_B$. Now we turn to investigate the central subband with eigenenergy $E=0$ resulting from IA's and TM's in the first approximation. When t_A is taken into account, the coupling interactions among these states have three cases (see Fig. 1). They are all connected by a weak bond t_A, and their resonant coupling strengths are as follows:

(a) between two IA's: $t'_1 = t_A$,

(b) between an IA and a TM: $t'_2 = \sqrt{2}t_A/2$, (1)

(c) between two TM's: $t'_3 = -t_A/2$.

Even though the sequence constructed by t'_1, t'_2, and t'_3 is still quasiperiodic, $|t'_1|$, $|t'_2|$, and $|t'_3|$ are same order of significance, i.e., there is no weak bond. Consequently, the spectral structure around $E=0$ should be much more like that of a periodic system than that of a quasiperiodic one. It suggests that the middle part of the central subband should be a continuous spectrum. This conjecture is strongly supported by the numerical calculations shown in Fig. 2. From the analysis on the triatomic molecule with eigenenergy $E=\sqrt{2}t_B$ we know that the relations (1) should always hold for every central subband of any hierarchy of the spectrum. Therefore, the continuous spectrum behavior also exists in the middle part of all the subbands in the following hierarchies. Figures 2(a) and 2(b) give the enlarged plots of two central subbands labeled by A and B, respectively, where we can clearly see that the middle part of each central subband is continuous.

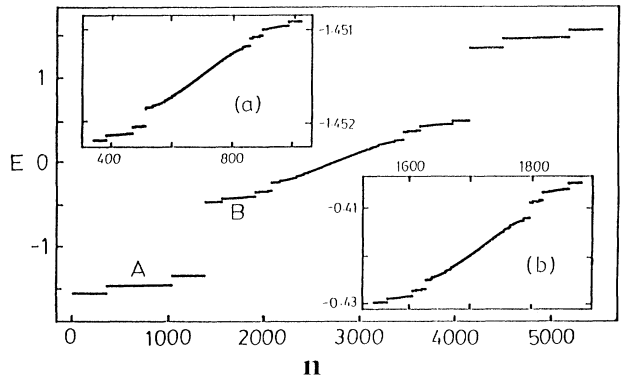

FIG. 2. The electronic spectrum of the $GF(1,2)$ quasilattice with $t_A=-0.3$, $t_B=-1$, and $N=5462$ sites. The trifurcating self-similar structure and the continuous behavior around $E=0$ are clearly seen. (a) and (b) are the enlarged plots of the central subbands A and B, respectively, of which the same spectral properties as that of the global spectrum are clearly shown.

Summarizing the above results, we can finally figure out the whole spectral structure of the $GF(1,2)$ quasilattice. The spectrum is grossly trifurcating and self-similar and the side subbands in every hierarchy will further trifurcate, but the middle part of the central subband stays continuous.

To describe the splitting pattern of the spectrum, we can code a subband in the nth hierarchy by a symbolic string $(p_1, p_2, \ldots, p_n)$, where the p_i's $(i=1,2,\ldots,n)$ take values of 1, 0, and -1, corresponding to the top, central, and bottom branch, respectively. For instance, if the subband successively belongs to the central main subband, the top subsubband of the central main subband, ..., the bottom branch of the $(n-1)$th-stage subband, then we associate with it a string $(0,1,\ldots,-1)$. By the numerical simulation we find that if more than three symbols on the tail are all 0, the corresponding subband is completely continuous. But if a subband has 1 or -1 as its last symbol it will further trifurcate.

Now we turn to study the localization of the electronic states for the $GF(1,2)$ model. If we take the atom spacing as the unit of length, then the inverse participation ratio (IPR) for the ith eigenstate is defined as[4]

$$IPR(i) = \sum_{j=1}^{N} |B_{ij}|^4 ,$$

where B_{ij} is the jth component of the wave function. The IPR is a measure of the reciprocal (inverse) of the number of sites occupied by the wave function. Generally, the smaller the IPR is, the more extended the state is. For a

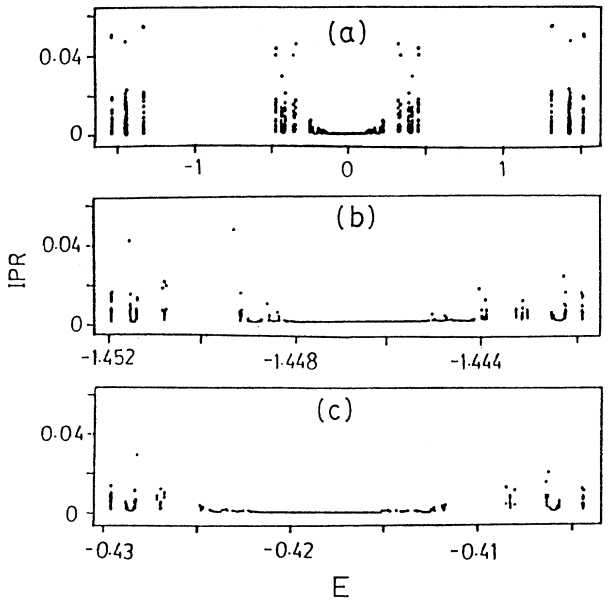

FIG. 3. The inverse participation ratio (IPR) vs energy E for the $N=5462$ site system with $t_A=-0.3$, and $t_B=-1$. (a) is for the whole spectrum; (b) and (c) are the enlarged plots of subband $(-1,0)$ and $(0,-1,0)$, respectively.

system with N sites, the IPR of an extended state would be the order of $1/N$, but for a localized state the IPR is of order 0.1–0.01. The IPR values of the intermediate states are between both of them, which responds to the unusual behavior of its wave function, decaying practically to zero and recovering to a large amplitude then decaying again alternately.

Figure 3(a) shows the numerical results of IPR versus eigenenergy E. We find that for the states located in the continuous band around $E=0$ the points form a straight line, and the corresponding IPR values are of order 10^{-4}, which suggests that the eigenstates are extended. Two enlarged plots corresponding to subbands $(-1,0)$ and $(0,-1,0)$ are given in Figs. 3(b) and 3(c), and the IPR in the middle part of the two subbands have the same values as that listed above. The points also form a straight line in the picture, which shows that these states are also extended. Furthermore, the localization parameters of IPR in the next hierarchy of the spectrum also exhibit the same features as those in Fig. 3. The facts stated above reveal that the localization of electronic states has a hierarchical structure: the side subbands of the spectrum in every hierarchy are trifurcating, but the middle part of the central subband is always continuous, and the corresponding wave functions are extended. The existence of such a hierarchical structure of mobility edges, i.e., the extended-state subbands, is a very interesting result.

More solid evidence of the localization is the behavior of the wave functions themselves. We have investigated the spatial distribution for a large number of wave functions; the results are also in very good agreement with the above analysis. We find that the wave functions with eigenenergy from -0.118 to 0.118 are all extended, examples of which are presented in Figs. 4(a) and 4(b). The intermediate and localized states exist in the edges of each subband in every hierarchy; the examples are shown in Figs. 4(c) and 4(d), respectively. It should be noted that the extended state shown in Fig. 4(a) is even periodic. In fact, we have found many such states with a variety of periods in our calculation.

In brief summary, we have studied the spectral structure and localization of the electronic states for the $GF(1,2)$ quasilattices. The spectrum has a very special hierarchical and self-similar structure: in every hierarchy, the side subbands are trifurcating, but the middle part of the central subband is a continuous spectrum. The existence of the energy region with continuous spectrum suggests to us that its corresponding eigenstates should be extended. This conjecture is strongly supported by the numerical calculations. In the edges of every

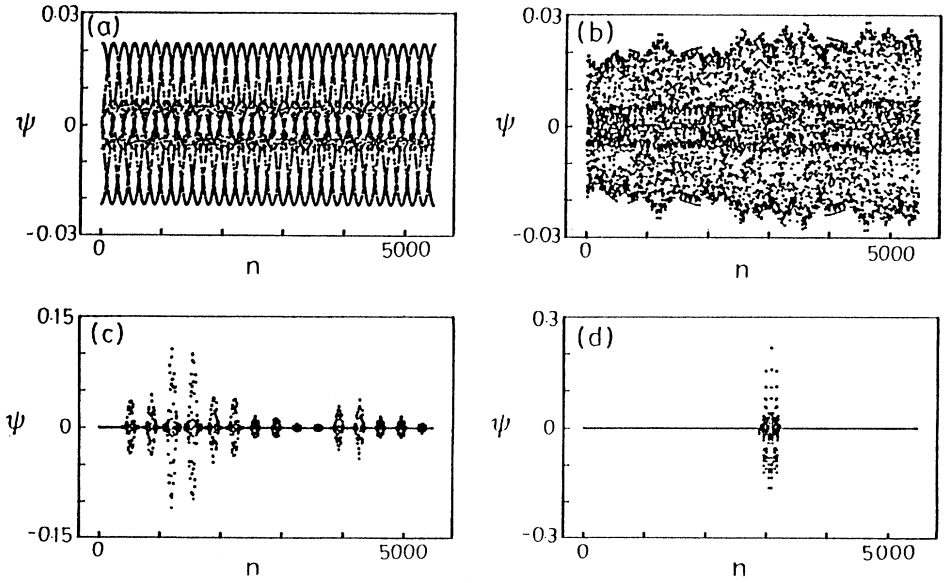

FIG. 4. Examples of three kinds of states in the central main subband. (a) An extended state in the middle part with $E=-0.006\,921\,502$. (b) Extended state in the edge of the continuous region with $E=-0.094\,022\,177$. (c) Intermediate state in the side subsubband with $E=-0.245\,420\,319$. (d) Localized state in the side subsubband with $E=-0.337\,636\,907$.

subband the spectrum is of pure point or singular continuous, so the corresponding eigenstates are either localized or intermediate. For whole spectra the mobility edges possess a hierarchical structure.

This work was supported by the National Science Foundation of China, Grant No. 19134020, and in part by the International Program in the Physical Science, Sweden.

[1]D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).
[2]M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).
[3]Q. Niu and F. Nori, Phys. Rev. Lett. **57**, 2057 (1986).
[4]Youyan Liu and R. Riklund, Phys. Rev. B **35**, 6034 (1987).
[5]Youyan Liu and W. Sritrakool, Phys. Rev. B **43**, 1110 (1991).
[6]G. Gumbs and M. K. Ali, Phys. Rev. Lett. **60**, 1081 (1988); J. Phys. A **21**, L517 (1988); **22**, 951 (1989).
[7]M. Holzer, Phys. Rev. B **38**, 1709 (1988); **38**, 5756 (1988).
[8]J. Q. You and Q. B. Yang, J. Phys. Condens. Matter **2**, 2093 (1990).
[9]S. Sil, S. N. Karmakar, R. K. Moitra, and A. Chakrabarti, Phys. Rev. B **48**, 4192 (1993).
[10]R. Riklund, M. Severin, and Youyan Liu, Int. J. Mod. Phys. B **1**, 121 (1987).
[11]M. Kolar, M. K. Ali, and F. Nori, Phys. Rev. B **43**, 1034 (1991).
[12]Youyan Liu, Xiujun Fu, Hui Han, Bolin Cheng, and Changfu Luan, Phys. Rev. B **43**, 13 204 (1991).
[13]A. Carlsson, Nature (London) **353**, 15 (1991).