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ELECTRONIC PROPERTIES FOR A CLASS OF ONE-DIMENSIONAL QUASILATTICES*

HUANG XIU-QING(黄秀清) and MO DANG(莫 党)
Department of Physics, Zhongshan University, Guangzhou 510275, China
LIU YOU-YAN(刘有延)
International Center for Materials Physics, Academia Sinica, Shenyang 110015; Department of Physics, South China University of Technology, Guangzhou 510641, China

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We have studied a new class of one-dimensional quasiperiodic lattices, for which the substitution rules are $B \to BA$, and $A \to BAB$. The Kohmoto-Kadanoff-Tang (KKT) renormalization group method has been used to study the asymptotical behavior of the spectrum. It is found that the energy spectra are Cantor-like but have different self-similarity from that of Fibonacci lattice. By use of several different criteria, three kinds of wave function behavior (extended, localized, and intermediate states) are clearly observed.

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I. INTRODUCTION

Since the fundamental experimental discovery of the diffraction pattern with five-fold symmetry by Shechtman *et al.*[1], the one-dimensional quasiperiodic systems have attracted much attention of both physicists and mathematicians for many years. As a one-dimensional version of quasicrystals, the Fibonacci chain has been extensively studied in many aspects. Its main feature is the Cantor set character of the energy spectrum[2-12]. In recent years, the theoretical study has been shifting towards other one-dimensional quasiperiodic systems, such as generalized Fibonacci quasilattices[13-16], Thue-Morse model[17,18] and the three-tile SML model[19]. To our knowledge, unlike the Fibonacci lattice these models cannot be obtained by high-dimensional projection method. Therefore, rigorously say, they are not quasiperiodic lattice. Consequently, they have no perfect physical properties as the Fibonacci quasilattices do. Recently, we suggested and studied a new one-dimensional two-tile[20] model with rigorous quasiperiodic property, which is generated by substitution rules: $B \to BA$, and $A \to BAB$, or by matrix expression

$$\begin{bmatrix} A \\ B \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} B \\ A \end{bmatrix}, \tag{1}$$

where A and B correspond to two kinds of atomic spacings: long and short. The first four sequences are as follows: $S_1=\{B\}, S_2=\{BA\}, S_3=\{BABAB\}, S_4=\{BABABBABABBA\}$. Let S_n denote the nth sequence, which obeys the recursion relation

$$S_n = 2S_{n-1} + S_{n-2}, \qquad n > 2. \tag{2}$$

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Let F_n be the number of elements contained in the nth sequence, and $\alpha = \lim_{n\to\infty}(F_{n-1}/F_n)$, then α is the positive root of the quadratic equation

$$\alpha^2 + 2\alpha = 1\ , \quad \text{and} \quad \alpha = \sqrt{2} - 1 = 0.414213562\cdots \tag{3}$$

We propose to call α the "Intergrowth mean" and the corresponding sequence (2) as the "Intergrowth sequence" (IS), which can be obtained by projection from a 2D periodic lattice. The α can be expressed as the following continued fraction number: $\alpha = 1/(2+1/(2+1/\cdots))$.

By using the *decomposition-decimation* (DD) method, for the transfer model of IS, a perfect multifractal spectral structure is found[20], which displays an interesting multifractal spectral structure that is different from the monofractal self-similarity of the Fibonacci quasilattices[9]. Recently, we studied the diffraction pattern and indexing problems for IS model, the theoretical results showed that the strongest peaks display an interesting self-similarity property[21]. In sec. II, we use Kohmoto-Kadanoff-Tang (KKT) renormalization group method to study the electronic properties of the IS model. It is found that the energy spectra are Cantor-like, but have different self-similarity from that of the Fibonacci quasicrystals[4]. In sec. III, we calculate the first moment, second moment, inverse participation ratio to examine the localization of the electronic wave function. The three kinds of wave function behavior (extended state, localized state, and intermediate state) are definitely found.

II. TRANSFER MATRIX AND THE CANTOR-LIKE SPECTRA

To deal with the electronic properties of IS quasilattices (Fig.1), Schrödinger equation for single electron can be written

$$T_n\psi_{n+1} + T_{n-1}\psi_{n-1} + \varepsilon_n\psi_n = E\psi_n\ . \tag{4}$$

In the matrix form, the above equation can be expressed as

$$\begin{aligned} \Phi_n &= \underline{M}(T_n,\ T_{n-1})\Phi_{n-1}\ , \\ \underline{M}(T_n,\ T_{n-1}) &= \begin{bmatrix} (E-\varepsilon_n)/T_n & -T_{n-1}/T_n \\ 1 & 0 \end{bmatrix}\ , \quad \Phi_n = \begin{bmatrix} \psi_{n+1} \\ \psi_n \end{bmatrix}\ , \end{aligned} \tag{5}$$

where ψ_n denotes the wave function in the Wannier representation, T_n is the hopping matrix element from the Wannier state $|n\rangle$ to $|n+1\rangle$, and ε_n is the site energy. The wave function on an arbitrary site N is determined by

$$\begin{aligned} \Phi_N &= \underline{M}^{(N)}\Phi_1\ , \\ \underline{M}^{(N)} &= \underline{M}(T_N,\ T_{N-1})\underline{M}(T_{N-1},\ T_{N-2})\cdots\underline{M}(T_2,\ T_1)\ . \end{aligned} \tag{6}$$

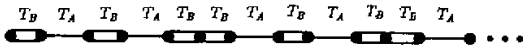

Fig. 1. A schematic representation for the transfer model. Two kinds of interactions are arranged by IS.

For the transfer version of IS model, we set site energy $\varepsilon_n = 0$ for all sites. The transfer matrix in formula (5) is simplified as

$$\underline{M}(T_n,\ T_{n-1}) = \begin{bmatrix} E/T_n & -T_{n-1}/T_n \\ 1 & 0 \end{bmatrix}, \tag{7}$$

where $\{T_n\}$ is arranged according to IS sequence with two kinds of hopping matrix elements T_A and T_B, which are arranged in the intergrowth sequence (see Fig.1). It is found that the transfer matrices $\underline{M}_j \equiv \underline{M}^{(F_j)}$ obeys the following recursion relation:

$$\underline{M}_{j+2} = \underline{M}_{j+1}\underline{M}_{j+1}\underline{M}_j\ , \qquad j \geq 1\ . \tag{8}$$

Here F_j denotes the number of the elements in the jth IS sequence S_j and is determined by $F_{j+2} = 2F_{j+1} + F_j$ with $F_1 = 1$, $F_2 = 2$. The corresponding initial conditions can be simply written as

$$\begin{aligned} \underline{M}_1 &= \underline{M}(T_B;\ T_B)\ , \\ \underline{M}_2 &= \underline{M}(T_B,\ T_A)\underline{M}(T_A,\ T_B)\ . \end{aligned} \tag{9}$$

The KKT method is at first developed to study the electronic problem of the Fibonacci lattice. Consider a sequence of periodic systems with progressively large unit cells, then the sequence asymptotically approaches the quasiperiodic lattice[2,3]. For the present IS model, the unit cell of the periodic system is simply the jth generation IS sequence S_j, so the relevant period of the system is P_j. A periodic system with period P_j can be solved with the help of the Bloch theorem. By the use of the periodic condition $\varphi_{p_j+1} = \exp(\mathrm{i}kP_j)\varphi_1$, where k is the Bloch index, then the allowed energies are just the same as the eigenvalues of the corresponding $P_j \times P_j$ Hermitian matrices $\underline{H}_j$. For the transfer version, the nonzero elements are written as follows: $(\underline{H}_j)_{i,i+1} = (\underline{H}_j)_{i+1,i} = T_i$, and $(\underline{H}_j)_{p_j,1} = (\underline{H}_j)^*_{1,p_j} = T_{p_j}\exp(\mathrm{i}kP_j)$. For a fixed index k, the Hermitian matrix $\underline{H}_j$ has P_j eigenvalues. All of these eigenvalues form P_j energy bands with k varying in the first Brillouin zone $[-\pi/P_j,\ \pi/P_j]$, and $k = 0,\ \pm\pi/P_j$ correspond to the band edges. One can rigorously prove that any energy E in the bands must satisfy $\mathrm{Tr}\underline{M}/2 = \cos(kP_j)$ and the energy E in the gaps does not. Because of the continuity of the Bloch index, the conditions for bands and gaps in the energy spectrum are, respectively[2]

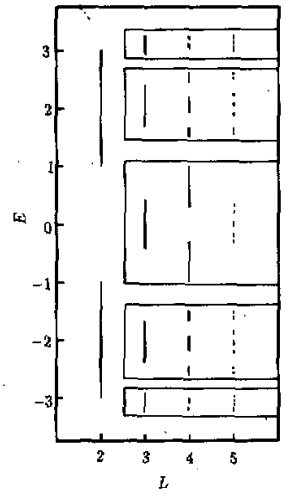

Fig. 2. The band structures of Eq.(8) with $T_A = 1$, $T_B = 2$. The two side-spectra and the central-spectrum have same structure as the whole spectra, but the two intermediate-spectra do not.

$$\begin{aligned} &\text{bands:} \quad |X_j| \le 1 \,, \\ &\text{gaps:} \quad |X_j| > 1 \,. \end{aligned} \tag{10}$$

The spectrum for the IS quasiperiodic lattices is obtained in the limit $j \to +\infty$. After a choice of $T_A = 1$ and $T_B = 2$, Fig.2 shows the band structure obtained by KKT method for the one-dimensional two-tile IS model. It can be clearly seen that the jth spectrum consists of P_j bands and $P_j - 1$ gaps. In the limit $j \to +\infty$, it displays a Cantor-like behavior. In addition, Fig.2 shows an interesting self-similarity characterized by that the two side-spectra and the central-spectrum have same structure as the whole spectra, but the two intermediate-spectra do not. To display this point, we list the numbers of subband for the whole and branching spectra in the following:

$$\begin{aligned} &1,\ 2,\ 5,\ 12,\ 29,\ 70,\ \cdots && \text{(whole-spectra)} \\ &1,\ 2,\ 5,\ 12,\ \cdots && \text{(side-spectra)} \\ &1,\ 3,\ 7,\ 17,\ \cdots && \text{(intermediate-spectra)} \\ &1,\ 2,\ 5,\ 12,\ \cdots && \text{(central-spectra)} \\ &1,\ 3,\ 7,\ 17,\ \cdots && \text{(intermediate-spectra)} \\ &1,\ 2,\ 5,\ 12,\ \cdots && \text{(side-spectra)} \end{aligned}$$

Let F_n be the number of elements contained in the nth intergrowth sequence, then the above spectral self-similarity can be expressed by F_n as follows:

$$\begin{aligned} &F_1,\ F_2,\ F_3,\ F_4,\ F_5,\ F_6,\ \cdots && \text{(whole-spectra)} \\ &F_1,\ F_2,\ F_3,\ F_4,\ \cdots && \text{(side-spectra)} \\ &(F_0+F_1),\ (F_1+F_2),\ (F_2+F_3),\ (F_3+F_4),\ \cdots && \text{(intermediate-spectra)} \\ &F_1,\ F_2,\ F_3,\ F_4,\ \cdots && \text{(central-spectra)} \\ &(F_0+F_1),\ (F_1+F_2),\ (F_2+F_3),\ (F_3+F_4),\ \cdots && \text{(intermediate-spectra)} \\ &F_1,\ F_2,\ F_3,\ F_4,\ \cdots && \text{(side-spectra)} \end{aligned} \tag{11}$$

here $F_0 = 0$, the self-similar band structure shown above can be written as $F_n = F_{n-2} + (F_{n-2} + F_{n-3}) + F_{n-2} + (F_{n-2} + F_{n-3}) + F_{n-2}$, which is exactly the same as the results obtained by decomposition-decimation (DD) method and the numerical simulation[20]. This kind of self-similarity is different from that of the Fibonacci quasilattices, for which there are only three branching spectra which have same structure as the whole spectra[4].

III. LOCALIZATION OF THE ELECTRONIC STATES

In the framework of the single-particle tight-binding model, the electronic states in a one-dimensional periodic system are all extented, but they are all localized if the system is disordered[22]. There is a general expectation that since quasiperiodic systems are between

the periodic and disordered ones, the wave functions would be neither localized nor extended. A typical spatial distribution of the wave function is decaying practically to zero and recovering to large values, then decaying again alternately. The term "critical" or "intermediate" is usually used to describe this kind of wave function behavior which corresponds to a singular continuous spectrum. But for a finite system Liu and Riklund[10] have numerically shown that in Fibonacci quasicrystals the extended, localized, and intermediate states may coexist. Later, Severin *et al.*[11] performed a multifractal analysis of the wave function and found the coexistence of localized, critical, and extended states in a non-Fibonacci quasilattice. In this section we numerically study the localization of the electronic states for the model by several criteria: the first moment and second moment, the inverse participation ratio, and the spatial distribution of the wave functions. All of the calculations display the coexistence of the extended states, localized states, and intermediate states. This kind of coexistence, in fact, is characteristic of quasiperiodic structures.

In the Wannier representation the ith normalized eigenfunction can be expressed as

$$|\Psi_i\rangle = \sum_{j=1}^{N} B_{ij}|j\rangle \ , \tag{12}$$

where B_{ij} is the amplitude of the ith wave function in the jth site, and $|j\rangle$ is the Wannier state centered at site j. If we take the atomic spacing as the unit of length, then the first moment (FM), which gives the center of gravity of wave function, is defined as[10]

$$\mathrm{FM}(i) = (1/N)\sum_{j=1}^{N} j|B_{ij}|^2 \ , \tag{13}$$

and the second moment (SM), which gives the effective width of wave function, is defined as[10]

$$\mathrm{SM}(i) = (1/N)\left[\sum_{j=1}^{N} j^2|B_{ij}|^2 - (\sum_{j=1}^{N} j|B_{ij}|^2)^2\right]^{1/2} \ . \tag{14}$$

The corresponding inverse participation ratio (IPR) is defined as[10]

$$\mathrm{IPR}(i) = \sum_{j=1}^{N} |B_{ij}|^4 \ . \tag{15}$$

The FM gives the average position of the wave function. The SM and IPR, from different aspects, measure the localization of the wave function. For an extended state, if the distribution of amplitude is homogeneous, the FM should equal 0.5, even though it is not a sufficient condition for the extended state. The SM is a measure of the extension of the wave function in the system. For the bound state, which is certainly extended, in a one-dimensional infinite potential well, we can easily prove[23] that its SM equals exactly $1/\sqrt{12} = 0.288675\cdots$,

which is a characteristic number to distinguish the extended states from other states. It means that the state with the SM close to 0.2887 is a reasonable candidate of the extended state. Evidently, for a localized state the SM is a small number roughly under 0.1, which corresponds to the small extension of wave function. The candidates of intermediate states are those with SM from 0.1 to 0.2887. The IPR is a measure of the reciprocal (inverse) of the number of sites occupied by the wave function. Generally, the smaller the IPR, the more extended the state. For a 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 the order of 0.1 to 0.01. The IPR values of the intermediate states are in between these two values, which responds to the unusual behavior of its wave function, decaying practically to zero and recovering to a large amplitude, then decaying again alterantely.

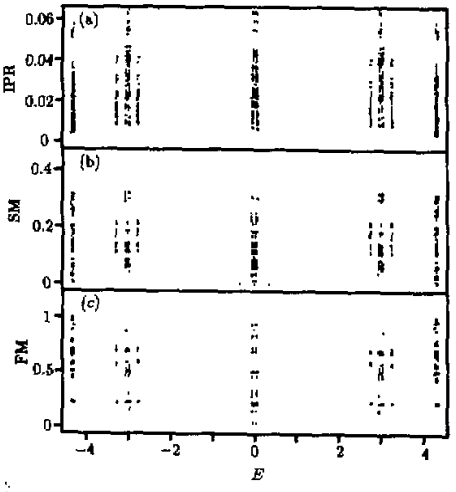

Fig. 3. The first moment (FM), second moment (SM), and inverse participation ratio (IPR) versus energy E for 10th generation of IS with 2378 atoms. The main five subbands are clearly shown: (a) and (b) show that the localization of wave functions are very different from each other; (c) shows that the average position of the wave functions spreads extensively.

Figure 3 shows the numerical results of IPR, SM, and FM versus eigenenergy for the 10th generation of the IS model with site number N=2378, where we can see the five-main-subband global structure. At the same time, Fig.3(a), which shows the IPR varying from 0.0006 to 0.06, suggests the coexistence of the three kinds of wave functions: extented, localized, and intermediate. Same conclusion can be drawn from Fig.3(b), which shows the SM extending from 0.0001 to 0.32. In Fig.3(c) we can see the average position of wave functions varies from 0.02 to 0.98, but the majority are between 0.4 and 0.7. More solid

evidence of the coexistence of different localizations is the behavior of the wave functions themselves. In Fig.4 we show the extended, intermediate, localized, and surface states, which also displays some kind of quasiperiodicity.

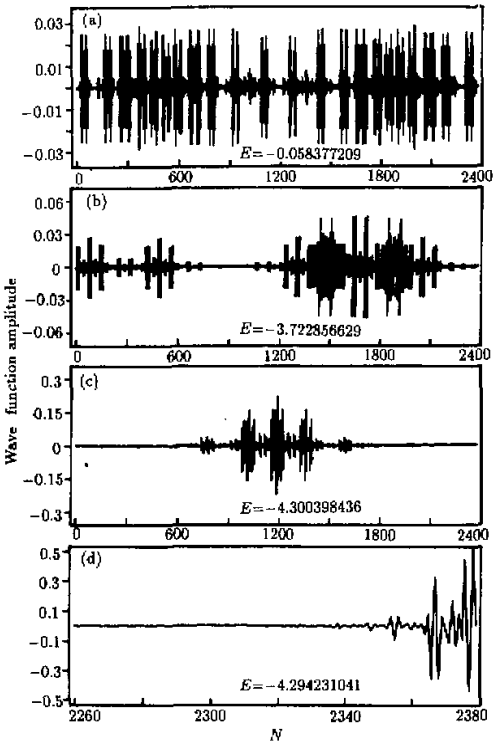

Fig. 4. Wave function with different localization for 10th generation of IS chain (N=2378), hopping integral $T_A = 0.5$, $T_B = 3$. (a) is an extended state, (b) is an intermediate state, (c) is a localized state, and (d) is a surface state.

IV. BRIEF SUMMARY

We have studied the transer model for a new class 1D two-tile quasiperiodic lattices, the Intergrowth Sequence (IS), in several aspects. The KKT method is used to study the electronic properties of the IS quasilattices. The numerical simulation shows that the energy spectra of the IS quasilattices are Cantor-like (see Fig.2), but possesses a different self-similarity from that of the Fibonacci quasicrystals[9]. The question of localization has been addressed from several approaches: the first and the second moment, the inverse participation ratio, the spatial distribution of the wave function. All these approaches

conclude the coexistence of the eigenstates with different localizations, extended, localized, and intermediate states. These display the perfect quasiperiodicity of the model studied. These peculiar physical properties of the studied model enhances our understanding for quasicrystalline systems.

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