Trace map and eigenstates of a Thue-Morse chain in a general model

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By the standard method proposed by Kolar and Nori [Phys. Rev. B **42**, 1062 (1990)], a rigorous eight-dimensional (8D) trace map for a general model of Thue-Morse (TM) sequences is obtained. Using this trace map, the characteristics of electronic eigenstates in TM lattices are explored in a very broad way. Simultaneously, a constraint condition for energy parameters, under which the complex 8D trace map can be simplified into the ordinary form, is found. It is also proved analytically that all eigenstates of TM lattices are extended when this constraint conditon is fulfilled. Furthermore, the properties of eigenstates beyond this constraint are investigated and some wave functions with critical features are discovered by the multifractal analysis. Our results support the previous viewpoint that a TM lattice is an intermediate stage between periodic and Fibonacci structures.

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I. INTRODUCTION

Since the discovery of a quasicrystalline phase in rapidly quenched Al-Mn alloys,[1] many efforts have been devoted to the research of quasiperiodic structures.[2–5] As we know currently, the physical properties of these systems are very intriguing and they have provided us with an approach to understand the intermediate phases between periodic and disordered structures. For simplicity, most of the research has been done with one-dimensional lattices and focused on characteristics of electrons and acoustic phonons. As a representative structure, the Fibonacci chain has been studied for many years and many authors have reported meaningful results.[5–8] Meanwhile, investigative interest has also turned to other aperiodic but yet deterministic structures, one of which is the so-called Thue-Morse (TM) sequence. Some early papers started the study on the physical properties for the TM sequence and its special features in comparison, for instance, to the well-known Fibonacci sequence.[9–12] After several years, it has been made clear that there exist extended states in TM lattices,[13] that the energy spectra are similar to Cantor sets,[14] and that the Fourier transformation of TM lattices is singular continuous.[15]

To analyze the physical behavior in deterministic aperiodic systems, many techniques have been developed, including transfer matrix, dynamic map, and renormalization group. Among these methods, the first two, which will be used mainly in this paper, are simple and very suitable for calculating the eigenenergies and for studying the features of relevant eigenstates. In general, the first step used to solve the problem is finding out the trace maps, because most sequences can be created by the so-called inflation or iteration method, i.e., the higher generations of sequences can be constructed through a rule by lower generations. For the TM sequence, the trace map in the on-site model has been revealed for many years,[16] and recently the trace maps for the transfer, the mixed, and even more general models were obtained by Ghosh and Karmakar using a real-space renormalization group (RSRG) technique.[17,18] But the RSRG method depends on the concrete form of basic transfer matrices, so there is doubt whether their conclusion can be proved or generalized by rigorous deduction. In fact, to seek the trace map of an aperiodic sequence, a useful approach based on the matrix operation was proposed by Kolar and Nori more than ten years ago.[19] This approach requires that all matrices entering iterations are unimodular. For the TM sequence in the general model there are four basic transfer matrices; however, two of them are not unimodular (see Sec. III). Thus it seems intuitively that the matrix operation method is inapplicable in this situation. Luckily, we eventually find a way to bypass this difficulty by adopting matrix combinations and finally attest that there exists an eight-dimensional (8D) trace map. Under a constraint condition for the energy parameters, this trace map can be simplified to the ordinary form and more surprisingly in this case all eigenstates are rigorously extended. Further, based on the 8D trace map, we also investigate other eigenstates of TM chains beyond this constraint and some new results are obtained.

The paper is organized as follows. In the next section the general model for TM sequences is given. Then the trace map in this model and its simplified form are derived in Sec. III. In Secs. IV and V, we use this trace map to calculate the eigenenergies and then to discuss the properties of eigenstates in the general model of TM chains. Finally, a brief conclusion is presented.

II. THE MODEL AND FORMULATION

With two building blocks denoted by L and S, a TM sequence can be constructed by the successive substitutions $L \rightarrow LS$ and $S \rightarrow SL$. Choosing L as the starting block, this process will give $L \rightarrow LS \rightarrow LSSL \rightarrow LSSLSLLS \rightarrow LSSLSLLSSLLSLSSL \rightarrow \cdots$. On the other hand, we can also begin with S; then the growing sequences will be $S \rightarrow SL \rightarrow SLLS \rightarrow SLLSLSSL \rightarrow SLLSLSSLLSSLSLLS \rightarrow \cdots$. To explore the physical properties of the TM structures, the transfer matrix method is widely used, so hereafter we use M_j to denote the global transfer matrix (defined later) of the former sequence and $\bar{M}_j$ to denote that of the latter one, where $j = 0,1,2,3,\ldots$ denote the generation number of the

TM sequences. Replacing $L(S)$ in M_j by $S(L)$, $\bar{M}_j$ will be obtained; so in this regard we say $\bar{M}_j$ is the complement to M_j.

Under the tight-binding approximation, an electron in a TM chain can be described by the equation

$$t_{n,n-1}\psi_{n-1}+t_{n,n+1}\psi_{n+1}+\epsilon_n\psi_n=E\psi_n, \tag{1}$$

where t's are the nearest-neighbor hopping integrals, ϵ's are the on-site potentials, ψ's are the electronic amplitudes, E is the electronic energy, and n is the site index. Now there are two kinds of bonds, one of which is denoted by L and the other by S. The bond L has a hopping integral t_L and the bond S has t_S. The bonds are arranged according to the TM sequence. Thus there are four types of sites characterized by the bond pairs LL, LS, SL, and SS, respectively. Here we use α, β, γ, and δ to represent these four types of sites and ϵ_α, ϵ_β, ϵ_γ, and ϵ_δ to denote the corresponding on-site potentials. Thus we get the general model for a TM chain with six energy parameters, and the conventional on-site and transfer models are just its simplified forms. In the general case there exist four basic transfer matrices as follows:

$$ll=\begin{pmatrix}(E-\epsilon_\alpha)/t_L & -1\\ 1 & 0\end{pmatrix},\quad sl=\begin{pmatrix}(E-\epsilon_\beta)/t_S & -t_L/t_S\\ 1 & 0\end{pmatrix},$$

$$ls=\begin{pmatrix}(E-\epsilon_\gamma)/t_L & -t_S/t_L\\ 1 & 0\end{pmatrix},\quad ss=\begin{pmatrix}(E-\epsilon_\delta)/t_S & -1\\ 1 & 0\end{pmatrix}. \tag{2}$$

We can also treat the classical elastic vibrations[20] in TM structures in a similar way.

We now take the basic transfer matrices for electrons in Eq. (2) for further study. Under Born–von Kármán boundary conditions, the global transfer matrix M_j can be obtained by the recursion relations

$$M_{j+1}=N_j\bar{N}_j,\quad \bar{M}_{j+1}=\bar{N}_jN_j,$$

$$N_{j+1}=M_jN_j,\quad \bar{N}_{j+1}=\bar{M}_j\bar{N}_j, \tag{3}$$

for $j\geqslant 0$ and with $M_0=ll$, $\bar{M}_0=ss$, $N_0=ls$ and $\bar{N}_0=sl$. A few initial global transfer matrices are $M_1=ls\cdot sl$, $M_2=ll\cdot ls\cdot ss\cdot sl$, and $M_3=ls\cdot sl\cdot ll\cdot ls\cdot sl\cdot ls\cdot ss\cdot sl$. It is important to note that the above recursion relations are equivalent to the following matrix transformations:

$$ll\rightarrow ls\cdot sl;\quad ss\rightarrow sl\cdot ls;$$

$$ls\rightarrow ll\cdot ls;\quad sl\rightarrow ss\cdot sl. \tag{4}$$

III. THE GENERAL TRACE MAP AND ITS SIMPLIFICATION

Although M_j and $\bar{M}_j$ can be confirmed as unimodular matrices, it is impossible to get the trace map from the recursion relations (3) or (4) by the Kolar-Nori standard method[19] because of the nonunimodularity of N_j and $\bar{N}_j$. But we find a way to evade this trouble. Defining $P_1=ll$ and $O_1=ls\cdot ss\cdot sl$ in addition to $M_1=ls\cdot sl$, now the recursion relation (4) is turned into

$$M_{j+1}=P_jO_j,$$

$$P_{j+1}=M_j,$$

$$O_{j+1}=P_jM_jO_j, \tag{5}$$

for $j\geqslant 1$. Evidently M_j, P_j, and O_j are all unimodular, implying that the standard method can be applied now. This is a three-letter dynamic map problem. To find the trace map, it needs eight coordinates:

$$x_1^j=\mathrm{Tr}M_j,\quad x_2^j=\mathrm{Tr}O_j,\quad x_3^j=\mathrm{Tr}P_j,\quad x_4^j=\mathrm{Tr}M_jO_j,$$

$$x_5^j=\mathrm{Tr}M_jP_j, x_6^j=\mathrm{Tr}O_jP_j,\quad x_7^j=\mathrm{Tr}M_jO_jP_j, x_8^j=\mathrm{Tr}M_jP_jO_j. \tag{6}$$

Then from Eq. (6) we have obtained an 8D trace map as follows

$$x_1^{j+1}=x_6^j,\quad x_2^{j+1}=x_7^j,\quad x_3^{j+1}=x_1^j,\quad x_4^{j+1}=x_6^jx_7^j-x_1^j,$$

$$x_5^{j+1}=x_8^j,\quad x_6^{j+1}=x_4^jx_5^j+x_6^j-x_2^jx_3^j,$$

$$x_7^{j+1}=x_7^jx_8^j-(x_1^j)^2-(x_3^j)^2-(x_5^j)^2+x_1^jx_3^jx_5^j+2,$$

$$x_8^{j+1}=x_7^jx_8^j-(x_1^j)^2-(x_2^j)^2-(x_4^j)^2+x_1^jx_2^jx_4^j+2. \tag{7}$$

This is the exact trace map of TM sequences in the general model. With its use, one can calculate the eigenenergies very effectively and accurately. Also from this 8D trace map, we find that for the general model there exists an invariant

$$I=x_6^{j+2}-x_6^j(x_7^{j+1}+x_8^{j+1})+x_6^{j+1}(x_6^j)^2. \tag{8}$$

Interestingly, it can be found that I always equals 2 exactly from the basic transfer matrices defined in Eq. (2).

The above 8D trace map is very complex. Fortunately, we have found a way to simplify it. Our algebraic operations strictly show that if and only if the constraint condition

$$\epsilon_\alpha+\epsilon_\delta=\epsilon_\beta+\epsilon_\gamma \tag{9}$$

for the on-site potentials is satisfied, the following five equations,

$$x_7^j-x_8^j=0,$$

$$x_7^jx_8^j-x_6^j(x_6^{j+1}-2)-(x_1^j)^2=0,$$

$$x_7^j+x_8^j-2x_1^j(x_6^j-1)=0,$$

$$x_6^j+(x_4^j)^2+(x_2^j)^2-x_1^jx_2^jx_4^j-2=0,$$

$$x_6^j+(x_5^j)^2+(x_3^j)^2-x_1^jx_3^jx_5^j-2=0, \tag{10}$$

hold for $j\geqslant 1$. In this case one can simplify the 8D trace map to the well-known form as[21]

$$x_6^{j+2}=(x_6^j)^2(x_6^{j+1}-2)+2. \tag{11}$$

If we note that $x_6^{j-1}=x_1^j=\mathrm{Tr}M_j$ and define $\chi_j=\frac{1}{2}\mathrm{Tr}M_j$, then the trace map can be rewritten in the ordinary form

$$\chi_{j+1}=4\chi_{j-1}^2(\chi_j-1)+1. \tag{12}$$

Recalling the energy parameters for the conventional on-site model, $\epsilon_\alpha=\epsilon_\beta\neq\epsilon_\gamma=\epsilon_\delta$ and $t_L=t_S$, for the transfer model, $\epsilon_\alpha=\epsilon_\beta=\epsilon_\gamma=\epsilon_\delta$ and $t_L\neq t_S$, and for the mixed model, $\epsilon_\alpha=\epsilon_\beta\neq\epsilon_\gamma=\epsilon_\delta$ and $t_L\neq t_S$. In all these cases the constraint condition (9) is met, so naturally the trace maps for these three special models is just formula (12), which was also found in Ref. 17 using the RSRG scheme.

Furthermore we have also studied the classical vibrating problem[18,20] of a TM atomic chain in the general model and found that it has one-to-one correspondence with the electronic case. If we define m_α, m_β, m_γ, and m_δ to denote the four kinds of atomic masses, and k_L and k_S to denote two kinds of different stiffness constants. A similar constraint condition for the classical vibrations to simplify the trace map into the ordinary form is $m_\alpha+m_\delta=m_\beta+m_\gamma$, which completely resembles Eq. (9) here.

IV. EXTENDED EIGENSTATES UNDER THE CONSTRAINT

Under the Born–von Kármán boundary conditions, the eigenvalues of a jth generation TM chain can be calculated by the equation

$$\chi_j=1. \tag{13}$$

Combining it with Eq. (12), i.e., under the constraint, we can find two obvious facts: (1) The solutions of Eq. (13) are just equivalent to the solutions of the following equations:

$$\chi_{j-2}=\chi_{j-3}=\cdots=\chi_1=0 \tag{14}$$

and

$$\chi_2=1. \tag{15}$$

(2) The eigenvalues of lower generations of TM sequences are preserved in higher generations. The reason is that $\chi_j=1$ gives

$$\chi_{j+1}=\chi_{j+2}=\cdots=1. \tag{16}$$

To prove analytically that all the eigenvalues from Eq. (14) give *extended* wave functions, we should invoke the three Pauli matrices $\sigma_x,\sigma_y,\sigma_z$ and the 2×2 identity matrix σ_I to resolve the matrices M_k, $\overline{M}_k$, N_k, and $\overline{N}_k$.[17,22,23] Then after a great deal of algebra, one can find that the eigenenergies from equation $\chi_{k-2}=0$ strictly render $M_k=\overline{M}_k=\sigma_I$ and simultaneously lead to the finding that the fourth matrix elements of N_k and $\overline{N}_k$ are zero. It should be emphasized that the unique requirement to obtain these results is Eq. (9) and the on-site, transfer, and mixed models are only its special examples.

When $M_k=\overline{M}_k=\sigma_I$, combining the recursion relations (3) and (4), it is easy to see that the global transfer matrix for a higher generation ($\geqslant k$) of TM sequences is a periodiclike $N_k\overline{N}_k$ array mixed with the identity matrix σ_I. This result is true even for a infinite TM chain. For example, $M_{k+1}=N_k\overline{N}_k$, $M_{k+2}=\sigma_I N_k\sigma_I\overline{N}_k$, and $M_{k+3}=N_k\overline{N}_k\sigma_I N_k\overline{N}_k N_k\sigma_I\overline{N}_k$, etc. In this way the aperiodic TM chain turns into a periodiclike chain by neglecting the clusters giving the identity matrix. So, naturally, the eigenstates given by Eq. (14) are all extended. A numerical example is illustrated in Fig. 1, which shows an extended eigenstate as expected. Besides being extended, the eigenstate is also *latticelike*, which means that the distribution of the electronic amplitudes forms a TM arrangement. Our further analysis shows that it originates from the fact that when $\chi_{k-2}=0$ the fourth matrix elements of N_k and $\overline{N}_k$ equal zero, which leads to $\psi_1=\psi_{2^k+1}=\psi_{2\times2^k+1}=\psi_{3\times2^k+1}=\cdots$. These relations are thoroughly proved by our numerical computations and can also be discerned from Fig. 1, where $k=6$.

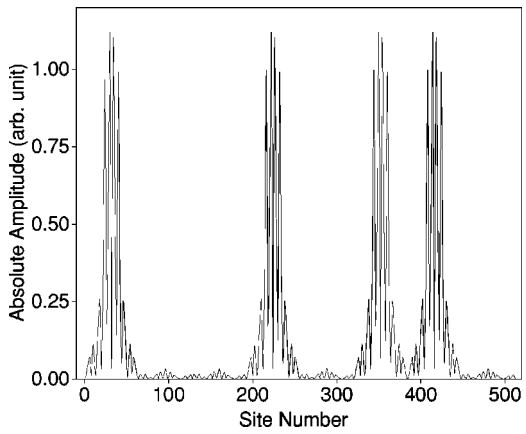

FIG. 1. Electronic wave function with $E=-4.284\,827\,042\,441$ from $\chi_4=0$, where $\epsilon_\alpha=0$, $\epsilon_\beta=0.4$, $\epsilon_\gamma=0.8$, $\epsilon_\delta=1.2$, $t_L=3.0$, and $t_S=2.0$.

On the other hand, except for the eigenvalues above that support delocalized eigenstates, the remaining four eigenvalues coming from Eq. (15) do not lead to M_j and $\overline{M}_j$ being the unit matrix and they actually correspond to eigenstates with linear growing amplitudes as the chain length increases.[22] The numerical calculations further show that these four eigenvalues determine the global wave functions at band edges. By the way, we have also investigated the eigenmode features of classical vibrations in TM lattices and found that they are very similar to those of electronic wave functions.

V. FURTHER DISCUSSIONS BEYOND THE CONSTRAINT

A. A rigorous latticelike wave function

We have proved that all the eigenstates of a TM chain, under the constraint condition $\epsilon_\alpha+\epsilon_\delta=\epsilon_\beta+\epsilon_\gamma$ in the well-studied on-site, transfer, or mixed models, are extended. We would like to ask about beyond the constraint condition, or if there are localized or critical states in TM chains; thus we return to the general model. A natural extension of the topic is to investigate the eigenstates for which Eq. (9) is not satisfied. So far it is difficult for us to solve the problem thor-

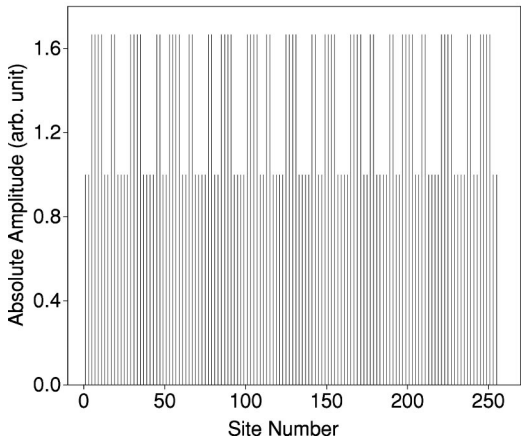

FIG. 2. Electronic wave function with $E=0.6$, where $\epsilon_\alpha=1.2$, $\epsilon_\beta=0.6$, $\epsilon_\gamma=0.6$, $\epsilon_\delta=0.9$, $t_L=5.0$, and $t_S=3.0$.

oughly because of the complexity of the original 8D trace map. As a special example, it is assumed that two of the four on-site potentials satisfy an equality $\epsilon_\beta=\epsilon_\gamma$. Defining $(\epsilon_\alpha-\epsilon_\beta)/t_S=p$, $(\epsilon_\delta-\epsilon_\beta)/t_S=q$, and $t_L/t_S=R$, we have found that for a special energy $E=\epsilon_\beta$ the four basic transfer matrices are

$$ll=\begin{pmatrix}-p/R & -1\\ 1 & 0\end{pmatrix},\quad sl=\begin{pmatrix}0 & -R\\ 1 & 0\end{pmatrix},$$

$$ls=\begin{pmatrix}0 & -1/R\\ 1 & 0\end{pmatrix},\quad ss=\begin{pmatrix}-q & -1\\ 1 & 0\end{pmatrix}. \tag{17}$$

Then it can be proved that the global transfer matrices are

$$M_1=\begin{pmatrix}-1/R & 0\\ 0 & -R\end{pmatrix},\quad M_2=\begin{pmatrix}1 & -(qR^2+p)/R\\ 0 & 1\end{pmatrix},$$

$$M_j=\begin{pmatrix}1 & -[A_j(p+qR^4)+B_j(p+q)R^2]/R^3\\ 0 & 1\end{pmatrix} \tag{18}$$

for $j\geqslant 3$. The coefficients $A_j=2^{j-3}$ and B_j $(j\geqslant 3)$ are determined by the recursion equation

$$B_{j+1}=\begin{cases}2B_j-1, & \text{if } j \text{ is even}\\ 2B_j+1, & \text{if } j \text{ is odd},\end{cases} \tag{19}$$

with $B_3=0$. In this case the energy ϵ_β is always the eigenvalue of any generations $(\geqslant 3)$ of TM sequences, and a corresponding eigenstate for the twelfth order is shown in Fig. 2. It is also an extended and latticelike eigenstate, just like those (see Fig. 1) under the constraint condition, although there are differences between them in the details.

A further analysis reveals that the eletronic amplitudes in Fig. 2 are arranged strictly according to the TM sequence. The possible origin of this rigorous latticelike wave function is that for the energy ϵ_β the cluster-type correlation appears in TM sequences, and transfer matrices for these clusters equal identity. Their contributions to the global transfer matrix can be neglected and the remaining host lattice become a periodic one. Naturally the relevant state is extended. In fact delocalized eigenstates in aperiodic structures were found in many situations with correlated disorder.[24] However, except for the special energy ϵ_β above, other eigenenergies will lead to eigenstates with a more chaotic nature, according to our numerical computations.

B. Critical states and multifractal analysis

By a minor analytic treatment, we consider another special case, where $\epsilon_\alpha=\epsilon_\delta\neq\epsilon_\beta=\epsilon_\gamma$ and $t_L=t_S=t$. Thus $ll=ss$ and $ls=sl$, so the recursion relation (3) can be written as

$$M_{j+1}=N_jN_j,\quad N_{j+1}=M_jN_j. \tag{20}$$

Defining

$$X_j=\mathrm{Tr}M_j,\quad Y_j=\mathrm{Tr}N_j,\quad Z_j=\mathrm{Tr}M_jN_j, \tag{21}$$

we have a simplified three-dimensional trace map

$$X_{j+1}=Y_j^2-2,\quad Y_{j+1}=Z_j,\quad Z_{j+1}=Y_j^2Z_j-Z_j-X_jY_j. \tag{22}$$

The invariant for this map is

$$I=X_jY_j-Z_j, \tag{23}$$

which is also equal to 2. Thus Eq. (22) turns into

$$X_{j+1}=Y_j^2-2,\quad Y_{j+1}=X_jY_j-2, \tag{24}$$

with initial conditions $X_0=(E-\epsilon_\alpha)/t$ and $Y_0=(E-\epsilon_\beta)/t$.

Using Eq. (24) one can calculate the eigenvalues, and in this case $X_j=2$ can lead to three independent equations

$$Y_{j-2}=Y_{j-3}=\cdots=Y_0=0, \tag{25}$$

$$X_{j-2}=0, \tag{26}$$

$$X_{j-2}Y_{j-2}=4\quad (X_{j-2}\neq Y_{j-2}). \tag{27}$$

It can be seen that the roots coming from Eq. (25) preserve the eigenvalues of higher generations $(>j)$ of TM sequences, and the remainder coming from the other two equations does not have this character. This difference may be observed in their distinguishing eigenstates.

We can prove that the eigenvalues extracted from Eq. (25) also lead to $M_j=\overline{M}_j=\sigma_I$, so the correponding eigenstates are strictly extended too. The numerical result for a twelfth-order TM chain is given in Fig. 3, with eigenenergy satisfying $Y_3=0$ and $X_{12}=2$. It is also a latticelike amplitude profile with obvious extended nature. Our multifractal analysis of the wave function confirms this conclusion, namely in the multifractal spectrum $[f(\alpha)\sim\alpha]$ there is only one multifractal point: $f(\alpha=1)=1$. We calculate the multifractal spectra with the prescription proposed by Kohmoto and co-workers and Halsey *et al.*[25] Since the finite size effect has been removed by extrapolation, we believe the results are convincing.

On the other hand, the eigenenergies determined by Eqs. (26) and (27) may lead to eigenstates with a *critical* nature. Two illustrating wave functions are shown in Figs. 4(a) and

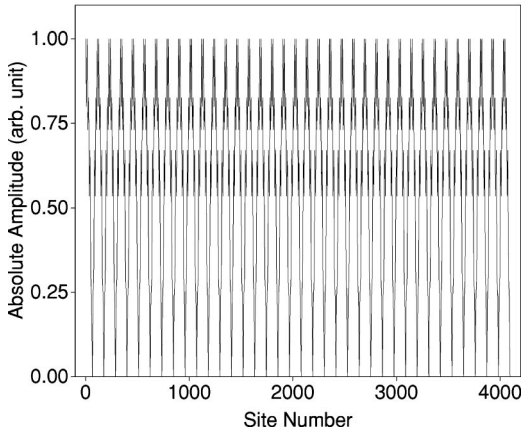

FIG. 3. Electronic wave function with $E=0.007\,342\,808\,757$ from $Y_3=0$, where the energy parameters are $\epsilon_\alpha=0.6$, $\epsilon_\beta=0.3$, $\epsilon_\gamma=0.3$, $\epsilon_\delta=0.6$, and $t_L=t_S=1.0$.

4(b). The corresponding eigenenergies satisfy $X_{10}=0$ and $X_{10}Y_{10}=4$ $(X_{10}\neq Y_{10})$, respectively. To understand the characteristics of these eigenstates, we perform a multifractal analysis. In this case we find the extrapolation is necessary to obtain reliable results, which are shown in Fig. 5. They are all clearly smooth curves, which reveal the critical feature of the eigenstates. For the electronic amplitude distributions in Figs. 4(a) and 4(b), the numerical result gives for the former $\alpha_{\min}=0.75$, $\alpha_{\max}=3.04$, $f_{\max}(\alpha)=1.0$ at $\alpha=1.05$ and for the latter $\alpha_{\max}=4.07$, $f_{\max}(\alpha)=1.0$ at $\alpha=1.24$. Due to the fact that the numerical convergence is not very good, we cannot get the accurate values of $\alpha_{\min}$ for the wave function in Fig. 4(b).

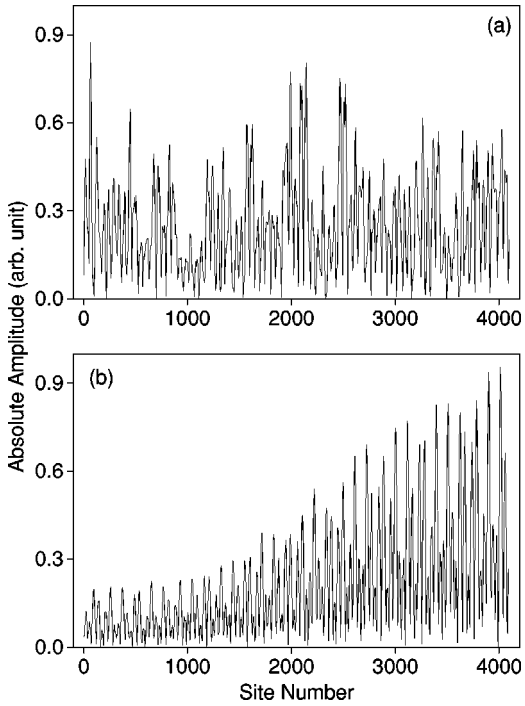

FIG. 4. Electronic wave function with (a) $E=-1.351\,634\,360\,223$ from $X_{10}=0$ and (b) $E=-1.486\,066\,084\,521$ from $X_{10}Y_{10}=4$ $(Y_{10}\neq 2)$, where the energy parameters are the same as in Fig. 3.

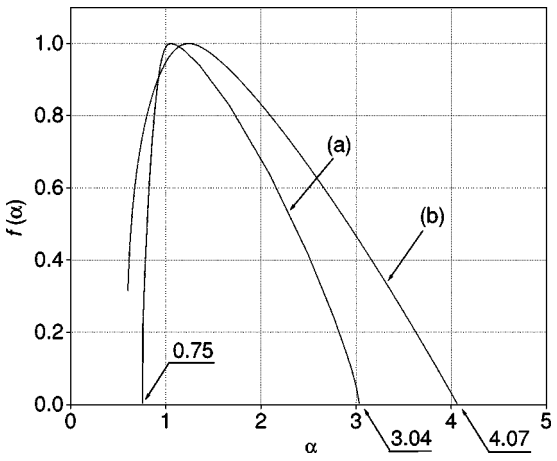

FIG. 5. Multifractal spectra for the wave functions in Figs. 4(a) and 4(b).

We have examined all the eigenstates for $j=7$ and found that the eigenvalues determined by Eq. (25) support the wave functions with the character shown in Fig. 3 and those determined by Eqs. (26) and (27) lead to the eigenstates with more disordered and chaotic features as in Fig. 4. But we also find some exceptions in the latter case, which is illustrated in Fig. 6. The eigenstates in Figs. 6(a) and 6(b) correspond to the eigenenergies satisfying $X_5=0$ and $X_5Y_5=4$ $(X_5\neq Y_5)$, respectively. They all resemble the *Bloch waves* and can be considered as extended eigenstates, which are also confirmed by our multifractal spectrum calculations.

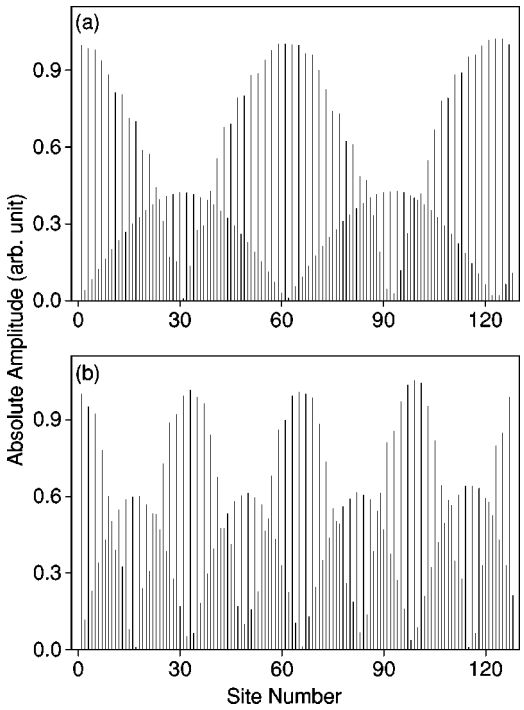

FIG. 6. Electronic wave function with (a) $E=0.258\,099\,418\,891$ from $X_5=0$ and (b) $E=0.181\,843\,863\,681$ from $X_5Y_5=4$ $(Y_5\neq 2)$, where the energy parameters are the same as in Fig. 3.

VI. SUMMARY

By the transfer matrix approach and Pauli matrix resovling technique, we have studied the trace map and the electronic eigenstates of a TM chain in the general model. We have found an 8D trace map, from which eigenenergies can be obtained. There is a constraint condition $\epsilon_\alpha+\epsilon_\delta=\epsilon_\beta+\epsilon_\gamma$ for the on-site potentials. When it is satisfied the complex 8D trace map can be simplified into an ordinary form, which is applicable to all well-studied cases, such as the on-site, transfer, and mixed models. It is justified that in this case that all the electronic eigenstates, except four whose eigenenergies are located at band edges, have a rigorously *extended* and *latticelike* nature. It is also found that if an eigenvalue of lower-order TM sequence is preserved to that of a higher-order sequence, it gives rise to the obvious delocalized eigenstates. Moreover, beyond the constraint, i.e., when the trace map does not take the ordinary form, the *extended* and *critical* eigenstates can coexist in the general model of TM sequences, according to our numerical computations and multifractal analysis. Note that there are only *Bloch waves* in periodic structures and *critical* eigenstates in the Fibonacci sequence. Our investigation indicates that the TM sequence is the intermediate stage linking the perfect periodic and Fibonacci structures. Our results also indicate that the classical vibrations are completely correspondent to electrons in TM structures.

Finally, it should be noted that, recently, a similar conclusion about the constraint condition for extended states was obtained by Chattopadhyay and Chakrabarti using the renormalization group approach.[26] However, the relation between the constraint condition and the trace map is elucidated here. Furthermore, we have used an alternative way to confirm the existence of delocalized eigenstates under the constraint and also reported some analytic and numerical results beyond this constraint.

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