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## Extended states in aperiodic systems

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**Abstract.** The existence of electronic states in aperiodic chains—both the generalized Fibonacci (GF) chain with the inflation rule ( $A \rightarrow A^m B^n, B \rightarrow A$ ) and the generalized Thue–Morse (GTM) ( $A \rightarrow A^m B^n, B \rightarrow B^n A^m$ ) chain—is proved analytically. There might be a critical value  $\lambda_c$  for the GF chain. If the ratio  $V_A/V_B$  is greater than  $\lambda_c$  where  $V_A$  and  $V_B$  are the potentials in the GF hopping Hamiltonian, our numerical calculation seems to show that the extended state will vanish.

Quasi-periodic and aperiodic chains have been the subject of great interest since the experimental discover of the quasicrystal (Schechtman *et al* 1984) and the recent advent of new experimental techniques in the fabrication of high-quality superlattices including quasi-periodic ones (Merlin *et al* 1985, Karkut *et al* 1986). The quasi-periodic Fibonacci (QF) chain has been studied in great detail. It is constructed using the following inflation rule:

$$A \rightarrow AB \quad B \rightarrow A$$

where  $A$  or  $B$  is a symbol such as the atom or distance etc. According to this inflation rule, the Fibonacci chain can be generated as follows.

$$1 : S_1 = B$$

$$2 : S_2 = A$$

$$3 : S_3 = AB = S_2 S_1$$

$$4 : S_4 = ABA = S_3 S_2$$

$$5 : S_5 = ABAAB = S_4 S_3$$

$$6 : S_6 = ABAABABA = S_5 S_4$$

$\vdots$

$$k : S_k = S_{k-1} S_{k-2}$$

$\vdots$

(1)

Some generalized Fibonacci (GF) chains have also been introduced in many studies using the inflation rule

$$A \rightarrow A^m B^n \quad B \rightarrow A. \tag{2}$$

This can also be written as

$$S_{k+1} = S_k^m \cdot S_{k-1}^n \quad k \geq 2 \quad S_1 = B, S_2 = A. \tag{3}$$

The specific names of some GF chains are defined as follows.

- $n = 1, m = 1$  : Golden mean or Fibonacci chain
- $n = 1, m = 2$  : Silver mean
- $n = 1, m = 3$  : Bronze mean
- $n = 2, m = 1$  : Copper mean
- $n = 3, m = 1$  : Nickel mean.

The total number of symbols ( $A$  and  $B$ ) in the  $k$ th level of the GF chain is denoted by a GF number  $F_k$ . This must satisfy the following equation:

$$F_{k+1} = mF_k + nF_{k-1} \quad F_1 = 1, F_2 = 1. \tag{4}$$

The ratio  $\sigma = \lim_{k \rightarrow \infty} F_{k+1}/F_k$  can be found from the following equation:

$$\sigma = \frac{1}{2}[m + \sqrt{m^2 + 4n}]. \tag{5}$$

For example:  $\sigma_g = 1/2[1 + \sqrt{5}]$  for the golden mean and  $\sigma_s = 1 + \sqrt{2}$  for the silver mean. It is known that GF chains with  $n = 1$  are quasi-periodic and that those with  $n \geq 2$  will be aperiodic.

Another type of aperiodic chain is the Thue-Morse (TM) chain and its extensions—the generalized TM (GTM) chain—have also been studied with much interest. Its inflation rule is

$$A \rightarrow A^m B^n \quad B \rightarrow B^n A^m. \tag{6}$$

When  $n = 1$  and  $m = 1$ , the chain is simply called the TM chain and it is given by

$$\begin{aligned} S_1 &= A \\ S_2 &= AB \\ S_3 &= ABBA \\ S_4 &= ABBABAAB \\ S_5 &= ABBABAABBAABABBA \\ &\vdots \end{aligned} \tag{7}$$

Let us define  $\tilde{S}_1 = B$ . Starting from  $\tilde{S}_1$  and the inflation rule ( $A \rightarrow AB$  and  $B \rightarrow BA$ ), we can also construct the following sequence:

$$\begin{aligned} \tilde{S}_2 &= BA \\ \tilde{S}_3 &= BA \cdot AB = \tilde{S}_2 \cdot S_2 \\ \tilde{S}_4 &= BAAB \cdot ABBA = \tilde{S}_3 \cdot S_3 \\ &\vdots \\ \tilde{S}_k &= \tilde{S}_{k-1} S_{k-1}. \end{aligned} \tag{8}$$

Obviously, the  $\tilde{S}_k$  can be obtained from the  $S_k$  by changing  $A$  to  $B$  and  $B$  to  $A$  and the TM sequence can be written simply as

$$S_k = S_{k-1} \tilde{S}_{k-1} \quad (k \geq 2).$$

Similarly, the GTM chain can be constructed without any difficulty. The number of symbols in the GTM chain is  $F_k = (m + n)^k$  and the ratio  $\sigma = m + n$ .

The physical properties of one-dimensional quasi-periodic and aperiodic systems are very different from periodic as well as disordered systems. They also appear to be in the intermediate level between them. For example, the electronic spectrum of a periodic system consists of absolutely continuous bands and the wavefunctions are all periodic (a special type of extended states). A one-dimensional disorder system has a pure point spectrum and exclusively exponentially localized states. However, the Fibonacci lattice has a Cantor set spectrum with zero Lebesgue measure and exclusively critical states (CS) which are neither localized (LS) nor extended (ES) in the ordinary sense (Kohmoto *et al* 1987). Numerical calculation indicated the existence of LS, CS and ES in the nickel GF chain with ( $m = 1, n = 3$ ) (Severin and Riklund 1989) and an analytical proof showed that the existence of LS and even periodic states in the GF chain with the inflation rule  $S_{L+1} = S_{L-1}^2 S_L$  (Everin *et al* 1989). Numerical results showed that the LS can exist in the chain with copper mean ( $m = 1, n = 2$ ) and CS in chains with golden and silver means ( $m = 2, n = 1$ ) (Gumbs and Ali 1988). TM chains show crystal-like hopping conduction (Aldea and Dulea 1988) and extended electronic states (Riklund *et al* 1987). The existence of ES in the TM chain ( $m = 1, n = 1$ ) was proved analytically and the low bound of the fraction of the ES is at least  $\frac{1}{2}$  (Lin *et al* 1991).

In this paper, we would extend the proof of the existence of ES to more general cases for the GF ( $n \geq 2$ ) and GTM chains. The model of the electronic Hamiltonian is

$$\psi_{n+1} + \psi_{n-1} + V_n \psi_n = E \psi_n. \tag{9}$$

If we define

$$\psi_n = \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}$$

equation (1) will become

$$\psi_{n+1} = M(n) \psi_n \tag{10}$$

where  $M(n)$  is defined by

$$M(n) = \begin{pmatrix} E - V_n & -1 \\ 1 & 0 \end{pmatrix}$$

and  $\det(M) = 1$ . The elements of matrix  $M(n)$  are  $M_{11} = E - V_n$ ,  $M_{12} = -1$ ,  $M_{21} = 1$  and  $M_{22} = 0$ . In the vibration problem, instead of  $E - V_n$ , the  $M_{11}$  will be  $(2 - \mu_n \Omega^2 - 1)$ . Let us denote the total transfer matrix for the  $l$ th-level  $S_l$  as  $M_l$ . Any two-dimensional matrix  $a$  with  $\det(a) = 1$  must have following equations:

$$\begin{aligned} a^2 &= xa - I \\ a^k &= d_k(x)a - d_{k-1}(x)I \\ x &= \text{Tr}\{a\} \end{aligned} \quad (11)$$

where  $d_k$  is a second kind of Chebyshev's polynomial and satisfies the following recursion relations (Kolar and Ali 1990, Kolar *et al* 1991):

$$\begin{aligned} d_{k+1}(x) &= xd_k(x) - d_{k-1}(x) \\ d_0(x) &= 0 \quad d_1(x) = 1 \quad d_2(x) = x \quad d_3(x) = x^2 - 1 \\ d_4(x) &= x^3 - 2x, \dots \quad d_{2k}(x) = 0 \quad d_{2k+1}(x) = (-1)^k. \end{aligned} \quad (12)$$

### 1. GF chain

Since the inflation rule is  $S_{k+1} = S_k^m S_{k-1}^n$  for a GF chain where  $S_k$  is the  $k$ th-level GF chain, the recursion relation of the transfer matrix is

$$M_{k+1} = M_{k-1}^n M_k^m \quad k \geq 2. \quad (13)$$

In general, the higher level transfer matrix of the GF chain must be constructed from two lower level matrices  $M_{k-1}$  and  $M_k$ :

$$M_N = M_N(M_{k-1}, M_k) \quad N \geq k + 1. \quad (14)$$

Sometimes, the aperiodic property in an infinite chain might be changed sensitively by introducing the approximation of a periodic boundary condition. Therefore, we will work carefully without introducing a periodic approximation. In the case of  $n \geq 2$ , if there is energy  $E$  (or  $\Omega$  in a vibrating system) to give  $d_n(x_k) = 0$ , we must have  $d_{n-1}(x_k)^2 = 1$  and  $d_{n-1}(x_k) = \pm 1$  by means of the following relation for Chebyshev's polynomial (Kolar and Ali 1990):

$$d_{q+1}^2 + d_q^2 = d_l^2 + d_q d_{q+l}(d_{l+1} - d_{l-1}). \quad (15)$$

Then

$$\begin{aligned} M_k^n &= d_n(x_k)M_k - d_{n-1}(x_k)I = \pm I \\ M_{k+2} &= [M_k]^n [M_{k+1}]^m = \pm [M_{k+1}]^m \\ M_N &= f(M_k, M_{k+1}) = f(I, M_{k+1}) = f(M_{k+1}) \\ &= \pm M_{k+1}^Q \quad N \geq k + 1. \end{aligned} \quad (16)$$

(17)

Table 1. Percentage of ESS.

$n = 2, m = 1, V_1 = 1.0, V_2 = 2.0$			
$k$	$R(k)$	Number of ES	ES%
3	3	2	66.7
4	8	5	62.5
5	19	12	63.15
6	40	25	62.50
7	83	52	62.65
8	168	105	62.50
9	339	212	62.54

where  $Q_p$  is an integer number. There are  $F_{N-k+1}$  matrices including both the  $M_k (= \pm I)$  and  $M_{k+1}$ . An infinite aperiodic system means  $N \rightarrow \infty$ . Since  $\det M_{k+1} = 1$ , the eigenvalues  $\eta$  of  $M_{k+1}$  can be found from

$$\eta^2 - x_{k+1}\eta + 1 = 0$$

$$\eta_{\pm} = 1/2\{x_{k+1} \pm \sqrt{(x_{k+1}^2 - 4)}\}. \tag{18}$$

After transforming the basis, the transfer matrix  $M_N$  becomes

$$M_N = \begin{pmatrix} \eta_+^{Q_p} & 0 \\ 0 & \eta_-^{Q_p} \end{pmatrix}$$

If  $|x_{k+1}| \leq 2$ , we will have

$$\eta_{\pm} = \exp\{\pm i\theta\}.$$

Therefore,

$$M_N = \begin{pmatrix} e^{iQ_p\theta} & 0 \\ 0 & e^{-iQ_p\theta} \end{pmatrix}.$$

This means that the modulus of the wavefunction will not vanish at  $F_{N-k+1}$  points aperiodically distributed along the whole chain and the ratio of the points in the chain is  $\eta = F_{N-k+1}/F_N = \sigma^{-k+1}$ . Thus such states must be extended. If  $|x_{k+1}(E_i)| > 2$ , we will have two real roots:  $\lambda_+ > 1$  and another at  $\lambda_- < 1$ . In this case, the states appear localized. So, the roots  $\{E_i\}$  of  $d_n(x_k) = 0$  will yield some energies of states in which some will be extended if  $|x_{k+1}(E_i)| \leq 2$  and some might be localized if  $|x_{k+1}(E_i)| > 2$ . As an example, we have done the calculations for the case  $n = 2, m = 1$ . Since  $d_2(x) = x, x_k = 0$  yields the condition  $d_2(x_k) = 0$ . The solutions of the equation  $\{E_i\}$  have been solved numerically for many different values of  $k$  and  $V_2$  where  $V_1$  is fixed at one. For example, in the case of  $V_2 = 2.5, x_3(E) = 0$  gives three roots:  $E_1 = -0.402\ 255\ 8, E_2 = 1.433\ 254\ 0$  and  $E_3 = 3.469\ 001\ 8$ . They yield  $x_4(E_1) = -0.097\ 744\ 2, x_4(E_2) = -1.933\ 254\ 0$  and  $x_4(E_3) = -3.969\ 001\ 8$ . This means that the state with energy  $E_1$  or  $E_2$  must be extended. We have solved the higher-level equations  $x_k(E) = 0$  up to  $k = 9$  where the number of solutions of  $x_k(E) = 0$  is 5 for  $k = 4, 11$  for  $k = 5, 21$  for  $k = 6, 43$  for  $k = 7, 85$  for  $k = 8$  and 171 for  $k = 9$ . The total number of roots is 339 and denoted by  $R(k = 9)$ . Then we check the value of  $x_{k+1}(E_i)$  for each root of  $x_k(E_i) = 0$  so that we can judge whether it is extended and estimate the percentage of extended states (ES%) in the total number of roots. Table 1 gives the results from our numerical calculations. We have found that ES% is about 62.5% and the convergence of ES% seems very fast.

Figures 1–3 show the relations of  $x_{k+1}(E) \sim E$  where the  $E$  is one of the roots from equation  $x_k(E) = 0$ , figure 4 the density of states for 339 roots in the case of  $n = 2, m = 1, V_1 = 1.0, V_2 = 2.0$  and figure 5 the  $ES\% \sim V_2$ . From figures 1–4, we can see that there are some gaps in the energy states and a mobility edge which seems to be at the boundary of a gap.  $ES\%$  decreases and the gap, as well as the number of gaps, increase with increasing  $V_2$ . The critical value of  $V_2$  is near 4.403 so that there might be no ES when  $V_2 \geq 4.403$ . Thus, the existence of ES in some aperiodic GF chains ( $n \geq 2$ , any  $m$ ) has been proved when  $V_2/V_1$  does not exceed some critical value. The case  $V_1 > V_2$  is similar. Meanwhile, we have also checked the case of the periodic chain ( $V_1 = V_2$ ) by means of the above method. The calculations always show that all states are exactly extended in any case.

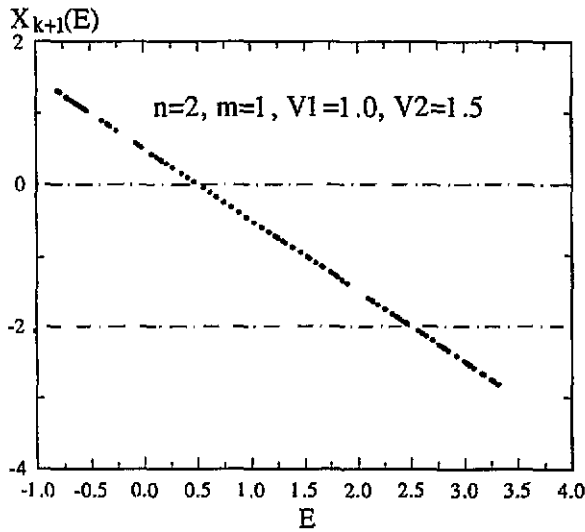


Figure 1. The relation between  $x(E)$  and  $E$  for the case of  $n = 2, m = 1, V_1 = 1.0$  and  $V_2 = 1.5$ .

**2. GTM chain**

From the inflation rule for the GTM

$$A_{k+1} = [A_k]^m [B_k]^n \quad B_{k+1} = [B_k]^n [A_k]^m \quad (19)$$

the recursion equation of the transfer matrix must be

$$M_{k+1} = [\tilde{M}_k]^n [M_k]^m \quad \tilde{M}_{k+1} = [M_k]^m [\tilde{M}_k]^n \quad k \geq 1 \quad (20)$$

where  $\tilde{M}_1 = M(1), M_1 = M(2)$ . Obviously, we have

$$\text{Tr}(M_k) = \text{Tr}(\tilde{M}_k) \quad k \geq 2 \quad (21)$$

$$x_k = \text{Tr}(M_k) \quad \bar{x}_k = \text{Tr}(\tilde{M}_k). \quad (22)$$

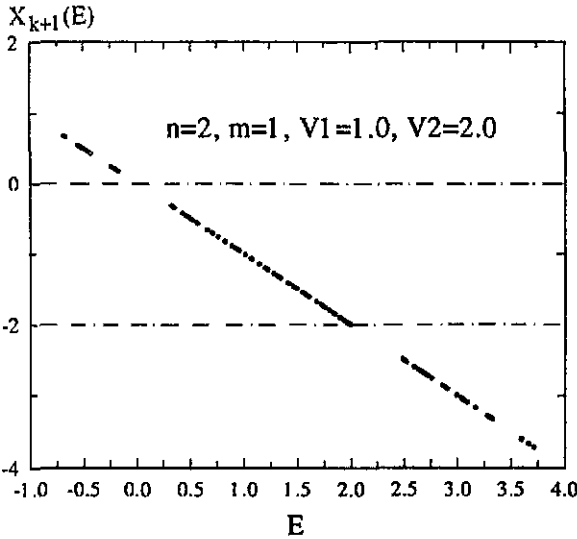


Figure 2. The relation between  $x(E)$  and  $E$  for the case of  $n = 2, m = 1, V_1 = 1.0$  and  $V_2 = 2.0$ .

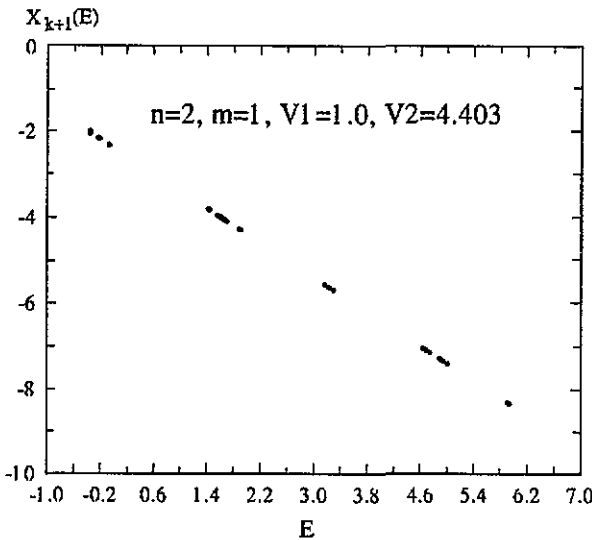


Figure 3. The relation between  $x(E)$  and  $E$  for the case of  $n = 2, m = 1, V_1 = 1.0$  and  $V_2 = 4.403$ .

In the case of  $m = 1, n = 1$ , we have proved the lower bound of the existence of ESS (Lin *et al* 1991). The more general case will be discussed in this paper. The  $N$ th-level transfer matrix  $M_N$  of the GTM chain can be expressed by any two lower level ones:  $M_k$  and  $\tilde{M}_k$ . If we set  $|\tilde{x}_k| = 2$ , the  $|x_k|$  will also be 2 due to equation (21). Matrices  $\tilde{M}_k$  and  $M_k$  can be transformed to  $\pm I$  by a unitary transformation. From the equation  $\tilde{M}_k = 0$ , we can determine the energies  $\{E_i\}$ . For those  $\{E_i\}$ , we obtain

$$M_N = \pm I \cdot I \cdots \cdots I = \pm I. \tag{23}$$



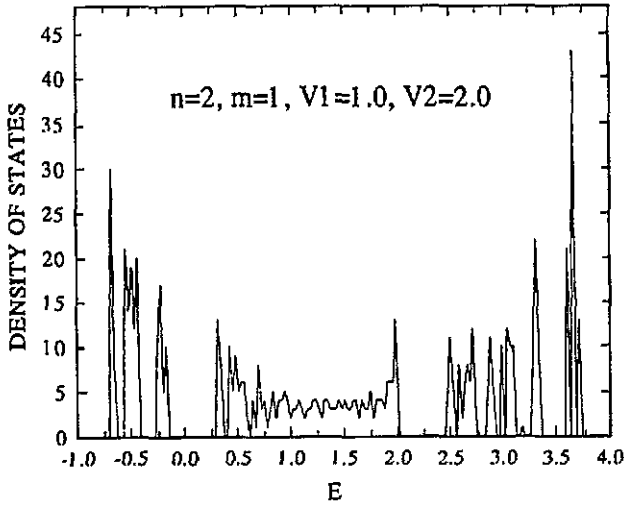


Figure 4. The distribution of density of states for the case of  $n = 2, m = 1, V_1 = 1.0$  and  $V_2 = 2.0$ .

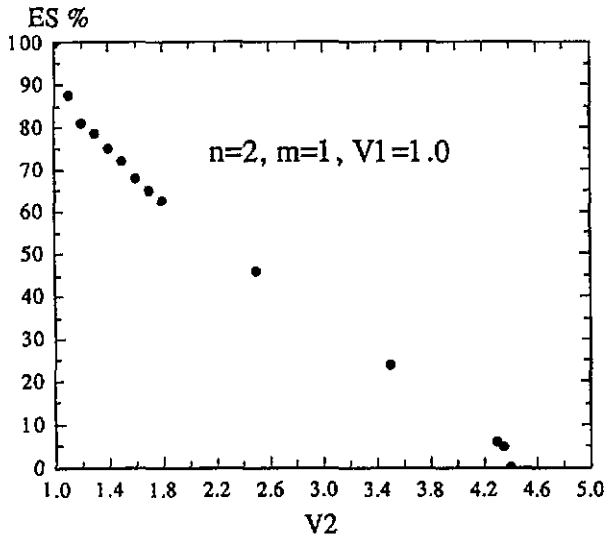


Figure 5. The percentage of extended states for different values of  $V_2$ , where  $V_1 = 1.0$ .

The number of  $I$ s in equation (23) must be  $F_{N-k} = (n + m)^{N-k}$  so that the wavefunction will have  $F_{N-k}$  locations periodically distributed in the chain without any decay. Therefore, the properties of the GTM chain are more similar to those of a periodic chain even though its structure is aperiodic which seems more similar to disorder than to a quasi-periodic chain. The existence of ES in the GTM chain has been proved.

In conclusion, we have proven the existence of ESS in the GF chain with  $n \geq 2$  and any GTM chain. Some evidence shows that there might be a critical value  $\lambda_c$ . If the value of the ratio  $V_2/V_1 \geq \lambda_c$ , there is no ES for the GF chain.

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