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## LETTER TO THE EDITOR

# Extended states in one-dimensional hierarchical lattices

Zhifang Lin<sup>†</sup> and Masaki Goda<sup>†‡</sup>

<sup>†</sup> Graduate School of Science and Technology, Niigata University, Niigata 950-21, Japan

<sup>‡</sup> Faculty of Engineering, Niigata University, Niigata 950-21, Japan<sup>§</sup>

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**Abstract.** An on-site tight-binding model in one dimension with a hierarchical distribution of site energies is studied. An infinite number of extended states are analytically shown to exist by using both the trace map for the transfer matrices technique and the real-space renormalization group approach. The energies corresponding to these extended states constitute a dense set in the energy spectrum. Unlike the extended states in the usual deterministic aperiodic and disordered systems, the existence of the extended states in the hierarchical chain is believed to be dependent on the property of the entire lattice rather than that of a certain finite cluster.

Recently, there has been much interest in the problem of extended electron states in various one-dimensional (1D) non-periodic systems ranging from disordered systems [1,2] to a variety of deterministic aperiodic systems [3–10]. In most cases, the extended states are identified by numerical calculation [1,3–7]. The analytical treatment is relatively limited. Up to very recently, Sil *et al* [10] discussed analytically the condition under which the 1D system can support the extended electron states [10]. They showed that if a certain finite cluster of atoms is distributed in some manner on a periodic host chain to make the resultant chain aperiodic, for some special discrete energy values, it is possible that these doping clusters will make identity contributions to the total transfer matrix [11] and, therefore, at these special energies, one may disregard the presence of the doping clusters and the remaining chain will still be periodic, which will evidently support the extended states. A good example presented by them is the so-called copper-mean aperiodic chain, which is shown to have an infinite number of extended states forming fragmented minibands. Clearly, this type of extended electron states is due to the property of the doping clusters on the periodic host chain. For this type of extended state, one can further take into account the correlation effects of the clusters at larger and larger length scales by using the real-space renormalization group approach, and finally obtaining the entire spectrum of extended states [10]. In this letter, we present an example in which the existence of the extended states seems to be dependent on the property of the entire lattice. They cannot be treated using the idea of a certain type of doping cluster on a periodic host chain, and therefore we believe that they result from different physical fundamentals.

The model considered here is the 1D on-site tight-binding Schrödinger equation on a spatially periodic lattice with a hierarchical distribution of site energies. The hierarchy of the site energies is defined by the inflation scheme

$$S_{N+1} = (S_N A_N)^{m_N - 1} S_N \quad (1)$$

<sup>§</sup> Mailing address.

where  $S_1 = A_0^{m_0-1}$ ,  $A_i$  are an infinite set of constituent elements and  $m_i \geq 2$  are a set of integers defining the hierarchy. Let  $\bar{S}_N = S_N A_{N+1}$  be the  $N$ th-order hierarchical system with length  $L_N = \prod_{i=0}^{N-1} m_i$ ; the real hierarchical chain corresponds to the limit of  $\bar{S}_N$  as  $N \rightarrow \infty$ . Note that if we put  $m_i \equiv 2$ , inflation scheme (1) generates the usual regular uniform bifurcating hierarchical structure, which has received considerable interest in recent years (see [12] for a review). The motion of the electron on this on-site tight-binding model is governed by

$$\phi(n+1) + \phi(n-1) + (V_n - E)\phi(n) = 0 \tag{2}$$

where  $\phi(n)$  and  $V_n$  denote, respectively, the amplitude of the wavefunction and the site energy at site  $n$ , and  $E$  is the eigen-energy of the electron. The diagonal elements  $V_n$  are given by  $u_k$  if  $n$  is a site of type  $A_k$ , with  $k = 0, 1, 2, \dots$ . The nearest-neighbour hopping matrix element is set equal to unity. Here we show analytically that the on-site tight-binding hierarchical model possesses infinitely many extended states. The existence of the extended states cannot be understood by the property of certain finite doping cluster on a periodic chain. On the contrary, they depend on the lattice as a whole.

To proceed, we rewrite equation (2) in transfer matrix form [11]:

$$\begin{pmatrix} \phi(n+1) \\ \phi(n) \end{pmatrix} = T(n) \begin{pmatrix} \phi(n) \\ \phi(n-1) \end{pmatrix} \quad T(n) = \begin{pmatrix} E - V_n & -1 \\ 1 & 0 \end{pmatrix}. \tag{3}$$

Note that one important property for the hierarchical system is that

$$T(n) = T(n + L_k) \quad n \neq p \times L_k \tag{4}$$

where  $p$  and  $k$  are arbitrary positive integers. The total transfer matrix of the  $N$ th-order chain  $\bar{S}_N$  with length  $L_N$  is defined as

$$T_N = T(L_N)T(L_N - 1) \cdots T(2)T(1). \tag{5}$$

The energy spectrum for the  $N$ -order periodic approximation of the infinite hierarchical chain is now taken to be the set [11]  $\{E \mid |x_N(E)| \leq 1\}$  with  $x_N(E) = \text{Tr}[T_N(E)]/2$ . By noting the fact that an  $(N + 1)$ th-order chain is equal to  $m_N$  successive  $N$ th-order chains except for the last site energy, it is easy to derive

$$T_{N+1} = (I + \Lambda_N I_0)(T_N)^{m_N} \tag{6}$$

where  $\Lambda_N = u_N - u_{N+1}$ ,  $I$  is the  $2 \times 2$  unit matrix and

$$I_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{7}$$

With the use of the relation

$$A^l = \frac{C'_l(a)}{l} A - \frac{C'_{l-1}(a)}{l-1} I \quad a = \frac{1}{2} \text{Tr}(A) \tag{8}$$

for any unimodular matrix  $A$ , equation (6) leads to the following trace map

$$\begin{aligned} x_{N+1} &= C_{m_N}(x_N) + C'_{m_N}(x_N)\Lambda_N y_N / m_N \\ y_{N+1} &= C'_{m_N}(x_N)y_N / m_N \end{aligned} \tag{9}$$

where  $x_N = \text{Tr}(T_N)/2$ ,  $y_N = \text{Tr}(I_0 T_N)/2$ , and  $C_l(x)$  is the  $l$ th Chebyshev polynomial with the recursion relation

$$C_l(x) = 2xC_{l-1}(x) - C_{l-2}(x)$$

and the initial conditions  $C_0(x) = 1$  and  $C_1(x) = x$ , whereas  $C'_l(x) = dC_l(x)/dx$ . The initial conditions for the trace map are given by

$$x_0' = (E - U_0)/2 \quad y_0 = 1/2. \quad (10)$$

By using the property of Chebyshev polynomials, it is not difficult to find that the above trace map has the non-escaping orbits:  $C'_{m_K}(x_K) = 0$ ,  $|x_{K+l}| = 1$  and  $y_{K+l} = 0$  with  $l \geq 1$  and  $K \geq 0$ . The energy values giving rise to these orbits are apparently the allowed energies, i.e. in the spectrum [11] for the infinite hierarchical chain since  $\lim_{N \rightarrow \infty} |x_N(E)| = 1$ . In the following, we will show that these eigen-energies correspond to extended states.

For a particular energy  $E^*$  which leads to  $C'_{m_K}(x_K) = 0$ , it follows from  $|x_{K+l}| = 1$  and  $y_{K+l} = 0$  that

$$T_{K+l} = \pm(I + \alpha_{K,l}I_0) \quad (11)$$

with  $l \geq 1$  and  $\alpha_{K,l}$  a non-vanishing parameter dependent on  $K$  and  $l$ . Therefore, for an  $N$ th-order chain of length  $L_N$  with  $N > K$ ,

$$\begin{pmatrix} \phi(L_N + 1) \\ \phi(L_N) \end{pmatrix} = T_N \begin{pmatrix} \phi(1) \\ \phi(0) \end{pmatrix} = \pm \begin{pmatrix} \phi(1) + \alpha_{K,N-K}\phi(0) \\ \phi(0) \end{pmatrix} \quad (N > K). \quad (12)$$

With appropriate (periodic or antiperiodic) boundary conditions, the above formula implies  $\phi(0) = 0$ . Then equation (11) suggests

$$\phi(q \times L_{K+1}) = \pm\phi(0) = 0 \quad \phi(q \times L_{K+1} + 1) = \pm\phi(1) \quad (13)$$

where  $q = 1, 2, \dots, L_N/L_{K+1}$ . Taking into account equations (4) and (13) with  $q = 1$ , we have, for  $n \neq p \times L_{K+1}$ ,

$$\begin{aligned} \begin{pmatrix} \phi(L_{K+1} + n + 1) \\ \phi(L_{K+1} + n) \end{pmatrix} &= T(L_{K+1} + n)T(L_{K+1} + n - 1) \cdots T(L_{K+1} + 1) \begin{pmatrix} \phi(L_{K+1} + 1) \\ \phi(L_{K+1}) \end{pmatrix} \\ &= \pm T(n)T(n - 1) \cdots T(1) \begin{pmatrix} \phi(1) \\ \phi(0) \end{pmatrix} = \pm \begin{pmatrix} \phi(n + 1) \\ \phi(n) \end{pmatrix}. \end{aligned} \quad (14)$$

Combination of (13) and (14) gives

$$\phi(n + L_{K+1}) = \pm\phi(n) \quad (15)$$

where  $n$  can be any positive integer. Therefore, the eigenstate corresponding to energy  $E^*$  is extended and periodic (with period  $L_{K+1}$  or  $2L_{K+1}$ ). In fact, the extendedness of the wavefunctions arises from the fact that  $\phi(q \times L_{K+1}) = 0$ . Since the wavefunction vanishes on these  $q \times L_{K+1}$  sites, it is not affected by the hierarchy introduced on these sites. The electron effectively 'feels' a periodic potential with period  $p = L_{K+1}$ , which gives rise to the extended wavefunction in the whole hierarchical system. Clearly, as the system consists of an infinite number of site energies ( $u_k$  with  $k = 0, 1, 2, \dots$ ), disregarding any finite types

of clusters will still leave us with an aperiodic system. As a matter of fact, no product of any finite number of consecutive transfer matrices  $T(n)$  offers identity contribution to the total transfer matrix, so we believe that the existence of the extended states is due to the property of the whole lattice rather than that of certain finite doping clusters on the periodic host chain. This is rather different from the extended states appearing in the usual deterministic aperiodic and disordered cases [10].

As the problem involves a hierarchical distribution of site energies and possesses self-similarity, one may expect an understanding within the real-space renormalization group context. To this end, we may implement an exact decimation method, which will preserve the hierarchical structure. After decimating all  $A_0$  sites and relabelling the remaining ones, we are left with a new set of equations, which can be cast in the same form as the original one (2), except that the original parameters  $E$  and  $u_k$  are renormalized as follows

$$E' = \frac{EC'_{m_0}(\epsilon)}{m_0} - \frac{2C'_{m_0-1}(\epsilon)}{m_0 - 1} \quad (16)$$

$$u'_{k-1} = \frac{u_k C'_{m_0}(\epsilon)}{m_0} \quad k = 1, 2, \dots$$

where  $\epsilon = (E - u_0)/2$ . If for some particular energy values  $C'_{m_0}(\epsilon) = 0$ , then at these energies,  $u'_k \equiv 0$ , the renormalized chain effectively consists only of one type of site with vanishing site energy and, therefore, there will be extended states for the whole system at these energies provided that these energies are allowed ones (see below). To determine the other extended states, one can consider the successive renormalized versions of the original chain. The hierarchical structure of the original lattice implies that one can apply the decimation procedure to every renormalized version (but with different rescaling factor  $m_l$ ). At any  $(k+1)$ th stage of renormalization, a new set of energy values for which the eigenstates are extended can be found from  $C'_{m_k}(\epsilon^{(k)}) = 0$ , where  $\epsilon^{(k)} = (E^{(k)} - u_0^{(k)})/2$  with  $E^{(k)}$  and  $u_0^{(k)}$  denoting, respectively, the value of  $E$  and  $u_0$  after  $k$  times of decimation. The expression of  $E^{(k)}$  and  $u_0^{(k)}$  can be obtained by successive iterations of the recursion relations similar to (16) with  $m_0$  replaced by different  $m_l$  at different consecutive decimation stage  $l$ . As is shown below, the number of allowed energy values which satisfy  $C'_{m_k}(\epsilon^{(k)}) = 0$  and correspond to extended states increases with the progress of renormalization and finally, the totality of all these energies constitutes a dense energy set in the energy spectrum.

There are still two questions. The first one is whether  $C'_{m_k}(\epsilon^{(k)}) = 0$  which leads to vanishing site energy at each site and  $C'_{m_k}(x_k) = 0$  which gives rise to the non-escaping orbit  $\lim_{l \rightarrow \infty} |x_l(E)| = 1$  in the dynamic trace map will be fulfilled at the same energy set. The second question is whether there are real energy values for which  $C'_{m_k}(\epsilon^{(k)}) = 0$  or  $C'_{m_k}(x_k) = 0$  holds. Let us first focus on the first question. After  $K$  times of renormalization, one has the following equation of motion

$$\phi[(n+1)L_K] + \phi[(n-1)L_K] + (V_n^{(K)} - E^{(K)})\phi(nL_K) = 0. \quad (17)$$

For  $n = 1$ , the above equation reads

$$\phi(2L_K) + \phi(0) + (u_0^{(K)} - E^{(K)})\phi(L_K) = 0. \quad (18)$$

After some algebra, it is possible to have

$$\phi(L_{K+1}) = \frac{C'_{m_K}(\epsilon^{(K)})}{m_K} \phi(L_K) - \frac{C'_{m_K-1}(\epsilon^{(K)})}{m_K - 1} \phi(0). \quad (19)$$

On the other hand, equations (6) and (8) imply

$$T_{K+1} = (I + \Lambda_K I_0) \left[ \frac{C'_{m_K}(x_K)}{m_K} T_K - \frac{C'_{m_K-1}(x_K)}{m_K - 1} I \right]. \quad (20)$$

By applying the above equation to  $\begin{pmatrix} \phi_1 \\ \phi_0 \end{pmatrix}$ , it is straightforward to find

$$\phi(L_{K+1}) = \frac{C'_{m_K}(x_K)}{m_K} \phi(L_K) - \frac{C'_{m_K-1}(x_K)}{m_K - 1} \phi(0). \quad (21)$$

Comparison of (19) and (21) yields

$$C'_{m_K}(\epsilon^{(K)}) = C'_{m_K}(x_K). \quad (22)$$

So, any energy value satisfying  $C'_{m_K}(\epsilon^{(K)}) = 0$  and giving rise to vanishing site energies will be an allowed energy since it also leads to a non-escaping orbit [11].

Now we turn to the second question. For simplicity, we discuss the case with  $m_i \equiv 2$ , for other cases the generalization is straightforward. From the trace map (9) and its initial conditions (10), one sees that  $x_l \rightarrow +\infty$  as  $E \rightarrow \pm\infty$  with  $l \geq 1$ . Again, from (10) it happens that  $C'_2(x_0(E)) = 4x_0(E) = 0$  has one real root, denoted by  $E_{0,1}$ . With  $x_1(E_{0,1}) = -1$  and  $\lim_{E \rightarrow \pm\infty} x_1(E) = +\infty$ , it follows that  $x_1(E) = 0$  should have two distinct real roots,  $E_{1,1} < E_{0,1} < E_{1,2}$ . Similarly,  $\lim_{E \rightarrow \pm\infty} x_2(E) = +\infty$ , together with  $x_2(E_{0,1}) = 1$  and  $x_2(E_{1,1}) = x_2(E_{1,2}) = -1$  implies that  $x_2(E) = 0$  should have four distinct real roots:  $E_{2,1} < E_{1,1} < E_{2,2} < E_{0,1} < E_{2,3} < E_{1,2} < E_{2,4}$ . By induction, it is easy to show that  $x_K(E) = 0$  has  $2^K$  distinct real roots. For the general case, by exploiting the property of the Chebyshev polynomial, a similar discussion leads to the conclusion that  $C'_{m_K}(x_K) = 0$  has

$$r_K = (m_K - 1) \left( 1 + \sum_{i=0}^{K-1} r_i \right) \quad \text{with} \quad r_0 = m_0 - 1 \quad (23)$$

distinct real roots. Therefore, for the real hierarchical chain corresponding to the limit of  $\bar{S}_N$  as  $N \rightarrow \infty$ , there are, in fact, an infinite number of extended eigenstates, the totality of which constitutes a dense set in the allowed energy spectrum.

To summarize, we have analytically shown the existence of infinitely many extended and periodic states which forms a dense energy set in the energy spectrum of 1D hierarchical on-site tight-binding model. As the hierarchical system is composed of an infinite number of constituents, we believe that these extended states are not a result of the property of certain finite clusters [10], they are seemingly due to the property of the whole lattice. For this type of extended states, the way in which to find the entire spectrum of the extended states has yet to be studied.

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