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The exact Green function of a one-dimensional Thue–Morse lattice

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Abstract. A real-space renormalization-group approach for calculating the exact electronic Green function of an infinite Thue–Morse chain is presented. This approach is based on a renormalization transformation introduced according to the self-similar structure of the chain and the recursion relations for the matrix elements of the Green function. Numerical results for the local density of states for the off-diagonal model show the existence of the extended states.

1. Introduction

Since the remarkable discovery of quasicrystals, there has been considerable interest in the theoretical study of one-dimensional (1D) quasiperiodic systems. As a 1D analogue of the Penrose lattice, the 1D Fibonacci lattice has been investigated in great detail. It is clear now that the electronic energy spectra of Fibonacci lattices for diagonal and off-diagonal models in the tight-binding Hamiltonian framework have a Cantor-set structure [1–6].

In recent years, other 1D quasiperiodic and aperiodic systems [7–20], and in particular the generalized Fibonacci lattices [9–13] and the Thue–Morse lattice [14–20], have attracted much attention due to their rich physical properties and the possibility of experimental realization of the related superlattices [21–22]. The dynamical-trace-map scheme proposed by Kohmoto *et al* [1, 3], and independently by Ostlund *et al* [2], for the Fibonacci lattice was successfully extended to study the electronic properties of the generalized Fibonacci lattices for diagonal and off-diagonal models [9–12]. As for the electronic properties of the Thue–Morse lattice, works were mainly devoted to the diagonal model [14–19]. Axel and co-workers first derived the trace map [14]. Riklund *et al* [15] numerically calculated the energy spectrum and the wavefunctions; they found that the spectrum consists of six main clusters and that the wavefunctions at the lowest and the highest energies are extended. The energy spectra for both weak and strong potentials were discussed by Cheng *et al* [16]. Kolář *et al* [17] studied the dynamical behaviour of the trace map. The gap sizes of the spectrum were

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determined analytically by Bellissard [18] and Kolář *et al* [17]. For the off-diagonal model, Qin *et al* [20] analysed the structure of the energy spectrum based on the renormalization-group (RG) scheme developed by Niu and Nori [5]. Their analysis showed the complexity of the self-similarity in the spectrum and it is for this reason that the calculations for the energy spectrum to greater than second order become very difficult.

Recently, Ashraff and Stinchcombe [23, 24] proposed a real-space renormalization-group (RSRG) approach to calculate the Green function of a 1D Fibonacci lattice. Since their work, there has lately been an increasing interest in calculating the exact Green functions of 1D Fibonacci and generalized Fibonacci lattices [25–30]. So far, however, less attention has been paid to the determination of the Green function of the 1D Thue–Morse lattice. In addition, due to the difference in the construction rules for those lattices, it seems difficult to apply the RSRG scheme for the Fibonacci and generalized Fibonacci lattices, which are characterized by the splitting of the original chain into finite new chains, to the Thue–Morse case. To calculate the Green function of the Thue–Morse chain, in this paper we give a new RSRG approach which is based on the recursion relations for the matrix elements of the Green function obtained by Wu and co-workers [31, 32] for a 1D disordered system.

2. RSRG scheme

We use the following 1D tight-binding Hamiltonian

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{ij} V_{ij} |i\rangle\langle j| \tag{1}$$

where ϵ_i is the site energy of site i and V_{ij} is the nearest-neighbour hopping integral. The Green function $G(Z)$ is defined by

$$G(Z) = 1/(Z - H) \tag{2}$$

where $Z = E + i0^+$ and E is the energy. The matrix elements of the Green function $G_{ij} = \langle i|G(Z)|j\rangle$ satisfy the following equation

$$(Z - \epsilon_i)G_{ij} = \delta_{ij} + \sum_k V_{ik} G_{kj}. \tag{3}$$

From (3), Wu and co-workers [31, 32] obtained the recursion relations for G_{ij} as follows

$$G_{ii} = (Z - \epsilon_i - V_{i,i+1}\Delta_{i+1}^{+} V_{i+1,i} - V_{i,i-1}\Delta_{i-1}^{-} V_{i-1,i})^{-1} \tag{4}$$

$$\Delta_i^{\pm} = (Z - \epsilon_i - V_{i,i\pm1}\Delta_{i\pm1}^{\pm} V_{i\pm1,i})^{-1} \tag{5}$$

$$G_{ij} = G_{ii} V_{i,i\pm1}\Delta_{i\pm1}^{\pm} V_{i\pm1,i\pm2}\Delta_{i\pm2}^{\pm} \cdots V_{j\mp1,j}\Delta_j^{\pm} \qquad (j \gtrless i). \tag{6}$$

In our model for the Thue–Morse chain, the nearest-neighbour hopping integrals V_{ij} take two kinds of values V_A and V_B arranged in the Thue–Morse sequence. The Thue–Morse sequence S_∞ is given by the recursion relation $\{S_{l+1}\} = \{S_l, \tilde{S}_l\}$

for $l \geqslant 1$ with $S_1 = \{AB\}$, in which $\bar{S}_l$ is the complement of S_l obtained by interchanging A and B in S_l, or by the inflation rule (A, B)→(AB, BA) starting with AB. The site energy ϵ_i takes one of the following four values according to the local environment of site i

$$\epsilon_i = \begin{cases} \epsilon_\alpha & V_{i-1,i} = V_{i,i+1} = V_A \\ \epsilon_\beta & V_{i-1,i} = V_A \qquad V_{i,i+1} = V_B \\ \epsilon_\gamma & V_{i-1,i} = V_B \qquad V_{i,i+1} = V_A \\ \epsilon_\delta & V_{i-1,i} = V_{i,i+1} = V_B. \end{cases} \tag{7}$$

Obviously, this model is a general one. The diagonal and the off-diagonal models correspond to ($V_A = V_B, \epsilon_\alpha = \epsilon_\gamma \neq \epsilon_\beta = \epsilon_\delta$) and ($V_A \neq V_B, \epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = \epsilon_\delta$), respectively.

To obtain the exact Green function of an infinite Thue–Morse chain, we first introduce a basic renormalization transformation T. This basic transformation is a decimation for sites with site energies ϵ_β and ϵ_γ in the Thue–Morse chain and can be represented by (AB, BA)→(A′, B′). After applying it to a Thue–Morse chain, we can obtain a new Thue–Morse chain with six renormalized parameters $\{\epsilon'_\alpha, \epsilon'_\beta, \epsilon'_\gamma, \epsilon'_\delta, V'_A, V'_B\}$ which are given by the following RG equation

$$\begin{aligned} \epsilon'_\alpha &= \epsilon_\gamma + \frac{V_A^2 + V_B^2}{Z - \epsilon_\beta} \qquad \epsilon'_\beta = \epsilon_\delta + \frac{V_B^2}{Z - \epsilon_\beta} + \frac{V_B^2}{Z - \epsilon_\gamma} \\ \epsilon'_\gamma &= \epsilon_\alpha + \frac{V_A^2}{Z - \epsilon_\beta} + \frac{V_A^2}{Z - \epsilon_\gamma} \qquad \epsilon'_\delta = \epsilon_\beta + \frac{V_A^2}{Z - \epsilon_\gamma} + \frac{V_B^2}{Z - \epsilon_\gamma} \\ V'_A &= \frac{V_A V_B}{Z - \epsilon_\beta} \\ V'_B &= \frac{V_A V_B}{Z - \epsilon_\gamma}. \end{aligned} \tag{8}$$

Comparing the original Thue–Morse chain with the new one, which is obtained by two iterations of transformation T, we find that there is a special site in the original Thue–Morse chain which remains undecimated by T and its environment in the new chain, i.e. the arrangement of the renormalized hopping integrals and site energies around it is the same as that in the old one. This special site, which has the same properties as the key site of the Fibonacci chain [25–28], is called here the key site of the Thue–Morse chain. There are two types of key sites for the Thue–Morse chains of different generations, which are termed type S_β and S_δ according to their corresponding site energies ϵ_β and ϵ_δ respectively. Each chain has only one key site and Thue–Morse chains of successive generations have key sites of different types. We illustrate the basic transformation T in figure 1. From figures 1(*a*) and (*b*), one can clearly see the properties of the key site of the Thue–Morse chain.

According to the properties of the key site of the Thue–Morse chain, we can obtain the exact local Green function (LGF), G_{00}, at the key site by infinite iterations of transformation T. From (3), it follows that

$$(Z - \epsilon_0)G_{00} = 1 + V_{0-1}G_{-10} + V_{01}G_{10}. \tag{9}$$

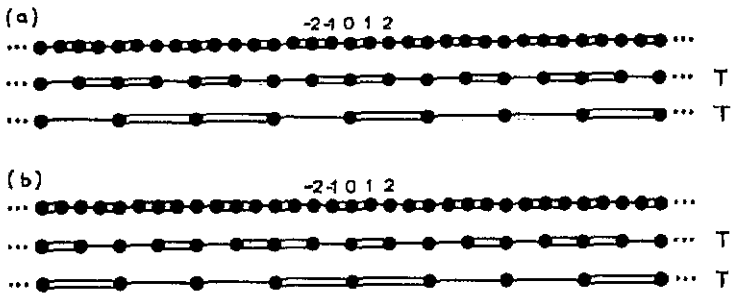

Figure 1. A schematic representation of the basic transformation T for the Thue–Morse chain. A Thue–Morse chain with key site (site 0) of (*a*) type S_β, (*b*) type S_δ.

After $2n$ iterations of the transformation T, we obtain a new Thue–Morse chain with renormalized parameters $\{\epsilon_\alpha^{(2n)}, \epsilon_\beta^{(2n)}, \epsilon_\gamma^{(2n)}, \epsilon_\delta^{(2n)}, V_A^{(2n)}, V_B^{(2n)}\}$. For this new chain, there is an equation for G_{00} similar to (9). Since there is the relation

$$\lim_{n\to\infty} V_A^{(2n)} = \lim_{n\to\infty} V_B^{(2n)} = 0 \tag{10}$$

the LGF, G_{00}, of the key site is then given by

$$G_{00} = 1/(Z - \epsilon_0^*) \tag{11}$$

where $\epsilon_0^* = \lim_{n\to\infty} \epsilon_\beta^{(2n)}$ if the key site is type S_β and $\epsilon_0^* = \lim_{n\to\infty} \epsilon_\delta^{(2n)}$ if it is type S_δ.

Now we turn to the calculation of the initial values Δ_1^+ and Δ_{-1}^- in the recursion relation (5) for $\Delta_i^\pm$. We apply transformation T only to the right part of the Thue–Morse chain to the key site, i.e. only decimate the sites to the right of site 0 in figure 1. Obviously, the RG equation for the renormalized parameters of the right half of the chain is the same as that in (8), while the parameters of the left half of the chain remain unchanged. As for the key site, the RG equation for its site energy is

$$\epsilon_{0R}' = \epsilon_0 + \frac{V_B^2}{Z - \epsilon_\gamma}. \tag{12}$$

Therefore, after $2n$ iterations of the RG equations (8) and (12), and using (9) and (10), one can obtain

$$G_{-10} = \frac{(Z - \epsilon_{0R}^*)}{V_{0-1}} G_{00} - \frac{1}{V_{0-1}} \qquad G_{10} = \frac{(\epsilon_{0R}^* - \epsilon_0)}{V_{01}} G_{00} \tag{13}$$

where $\epsilon_{0R}^* = \lim_{n\to\infty} \epsilon_{0R}^{(2n)}$.

It is easy to see from the definition of the Green function that $G_{ij} = G_{ji}$, since $H_{ij} = H_{ji}$. From (6), we have

$$G_{01} = G_{00} V_{01} \Delta_1^+ \qquad G_{0-1} = G_{00} V_{0-1} \Delta_{-1}^-. \tag{14}$$

So substitution of G_{-10} and G_{10} into (14) finally give Δ_1^+ and Δ_{-1}^-. Using recursion relation (5), one can easily obtain $\Delta_i^\pm$ for arbitrary i and then calculate all of the matrix elements of the Green function from (4) and (6).

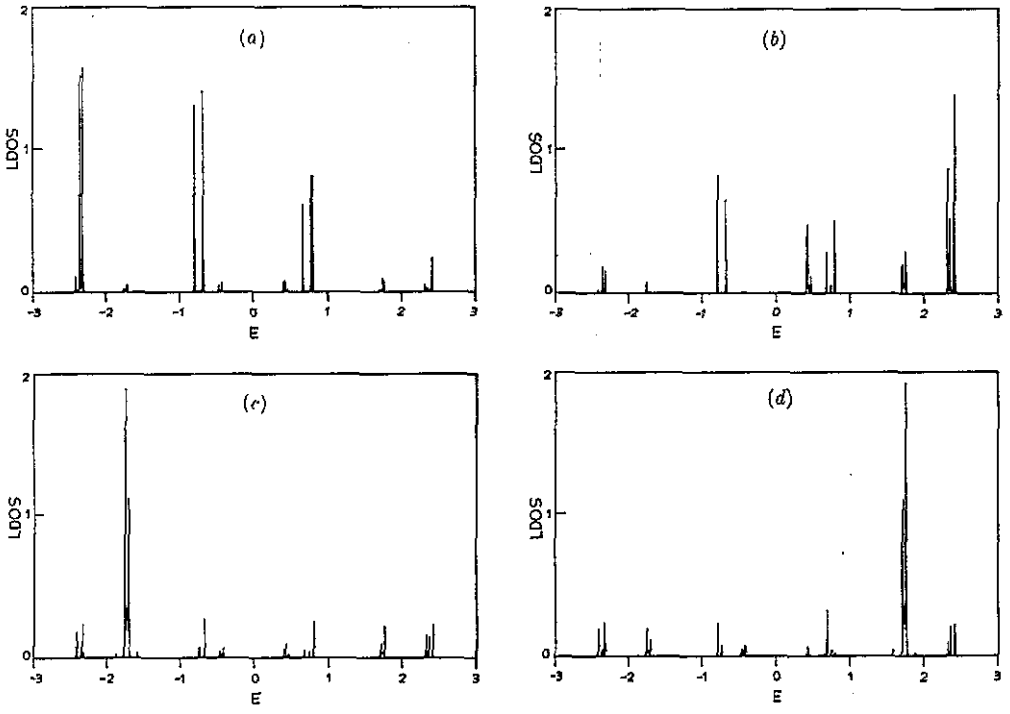

Figure 2. The LDOS (arbitrary units) at several sites of the Thue–Morse chain with the key site S_δ, in which $\epsilon_\alpha = -\epsilon_\beta = \epsilon_\gamma = -\epsilon_\delta = 1$ and $V_A = V_B = 1$: (*a*) site 0; (*b*) site 1; (*c*) site 3; (*d*) site 4.

3. Numerical results and discussions

The Green function can reveal a lot of physical properties of the system. For instance, the local density of states (LDOS) at site i is given by

$$\rho_i(E) = -(1/\pi)\,\mathrm{Im}\,G_{ii}(E + i0^+) \tag{15}$$

where Im denotes the imaginary part of a complex quantity. In this section, we give some numerical results for the LDOS of the Thue–Morse chain calculated by the RSRG scheme presented in section 2. In our calculation, site 0 of the Thue–Morse chain is the key site S_δ (see site 0 in figure 1(*b*)). Figures 2(*a*)–(*d*) are devoted to several sites of the Thue–Morse chain for the diagonal model, in which the site energies and hopping integrals are chosen to be $\epsilon_\alpha = -\epsilon_\beta = \epsilon_\gamma = -\epsilon_\delta = 1$ and $V_A = V_B = 1$. Each LDOS in figure 2 has six main clusters. The five main gap sizes of the LDOS in figure 2 show a good agreement with the numerical results of Riklund *et al* [15] and the analytical calculation by Bellissard [18] and Kolář *et al* [17]. It is interesting that the LDOS does not contain any smooth part, although the numerical results for the wavefunctions at some energies suggested the existence of extended states in the Thue–Morse chain for the diagonal model [15]. This observation, which is checked by a lot of calculations for various values of the site energies, is different from that in the LDOS of a family of generalized Fibonacci lattices, for which the extended state corresponds to a rather smooth part of the LDOS [7, 28, 29]. Such a correspondence occurs in figure 3 for the off-diagonal model; the LDOS exhibits a smooth behaviour

around energies $0, \pm 0.89$ and ± 1.80. It is known that the LGF is purely imaginary at the energy of the extended state [33]. Careful examination of the LGF for the Thue–Morse chain shows that the values of the real parts at the above-mentioned energies are zero, implying that the energies corresponding to the smoothness of the LDOS in figure 3 are those of the extended states appearing in the Thue–Morse chain for the off-diagonal model.

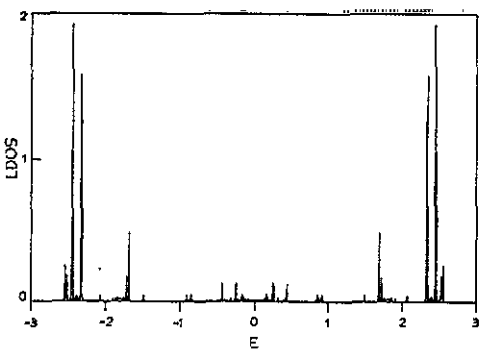

Figure 3. The LDOS (arbitrary units) at the key site S_δ of the Thue–Morse chain, in which $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = \epsilon_\delta = 0$, $V_A = 1$ and $V_B = 1.5$.

Finally, we would like to point out that the RSRG scheme presented in this paper is also suitable for the determination of the Green functions of the Fibonacci lattice and a family of the generalized Fibonacci lattices, because of the existence of the key sites for those lattices. In fact, we have calculated the LDOS of the Fibonacci chain by the method given here and compared it with those given in [26]. Results obtained by different RSRG approaches match each other very well.

Acknowledgments

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