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Electronic properties of quasiperiodic Fibonacci chain including second-neighbor hopping in the tight-binding model

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Abstract. We present an exact real-space renormalization group (RSRG) scheme for the electronic Green's functions of one-dimensional tight-binding systems having both nearest-neighbor and next-nearest-neighbor hopping integrals, and determine the electronic density of states for the quasiperiodic Fibonacci chain. This RSRG method also gives the Lyapunov exponents for the eigenstates. The Lyapunov exponents and the analysis of the flow pattern of hopping integrals under renormalization provide information about the nature of the eigenstates. Next we develop a 4×4 transfer matrix formalism for this generalized tight-binding system, which enables us to determine the wave function amplitudes. Interestingly, we observe that like the nearest-neighbor tight-binding Fibonacci chain, the present generalized tight-binding system also have critical eigenstates, Cantor-set energy spectrum and highly fragmented density of states. It indicates that these exotic physical properties are really the characteristics of the underlying quasiperiodic structure.

PACS. 71.23.Ft Quasicrystals – 61.44.-n Semi-periodic solids

1 Introduction

The discovery of isocahedral symmetry in AlMn based inter-metallic alloys by Shechtman *et al.* [1] stimulated wide interest in the physics of quasiperiodic systems, which are intermediate between periodic and random structures. An interesting problem in condensed matter physics is whether the quasiperiodic structure leads to new and unexpected physical properties. The notions like critical wavefunctions, Cantor-set energy spectrum, scaling behavior of the density of states etc. have evolved from the studies [2–7] of one-dimensional simple model systems. The electronic structures of one-dimensional Fibonacci [4], period-doubling [8], Thue-Morse [9] etc. quasiperiodic lattices are commonly studied using the nearest-neighbor tight-binding (TB) model Hamiltonian. The general wisdom is that the exotic physical properties are characteristics of quasiperiodic systems. Now from theoretical point of view, it is quite important and also relevant to see how susceptible are these exotic physical properties, characteristics of quasiperiodic structure, as one generalizes the model for the system.

In this paper we have addressed this problem, and studied the electronic properties of the well-known Fibonacci lattice within the tight-binding framework including both nearest-neighbor (first-neighbor) and next-nearest-neighbor (second-neighbor) electronic hopping among the atoms. An added interest in this model is due to the fact that we may regard this case as approximating better the real samples than the nearest-neighbor TB Hamiltonian. So far much less attention has been paid in the literature [10] for studying this class of systems with the above kind of generalization of the TB Hamiltonian. The increase in the level of complexity by this generalization is not readily amenable to analysis through real-space renormalization group [11,12] (RSRG) or trace-map [4,9] techniques, the standard theoretical tools available for studying quasiperiodic systems. Thus any analytical study of the properties of this systems is really a challenging task, and the most satisfying feature of the present work is that we have succeeded to develop an exact RSRG scheme for the electronic Green's function of the Fibonacci chain taking both the nearest-neighbor and second-neighbor hopping in the TB model. The basic idea here is to group the lattice points into smallest possible blocks such that the blocks virtually behave like pseudo-atoms with only nearest-neighbor hopping between them. One can easily generalize this scheme to include higher order hopping integrals in the TB Hamiltonian. This RSRG method enables us to determine the electronic density of states with arbitrary accuracy, and also gives the allowed spectrum very correctly. The analysis of the renormalized hopping integrals provides information about the localization behavior of the eigenstates. Apart from the RSRG scheme, we have also studied this system using transfer matrix method. For this purpose we have to formulate the transfer matrix method for the second-neighbor problem, the transfer matrices are now 4×4 matrices instead

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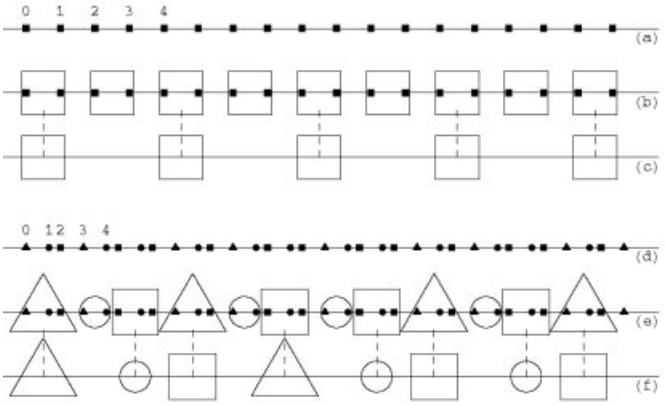

Fig. 1. (a) Section of an infinite periodic chain, (b) construction of blocks or pseudo-atoms in the periodic chain, (c) illustration of block decimation scheme in the periodic chain, (d) section of an infinite Fibonacci chain, (e) construction of blocks or pseudo-atoms in the Fibonacci chain, and (f) illustration of block decimation scheme in the Fibonacci chain.

of the usual 2×2 matrices. The eigenfunctions of the systems are obtained explicitly from the transfer matrix method. From our study it is apparent that the exotic features in the physical properties of the Fibonacci chain are characteristics of the quasiperiodic structure, and quite independent of the details of the TB model.

The organization of the paper is as follows. In Section 2 we describe the TB model for the Fibonacci chain taking both nearest-neighbor and second-neighbor electronic hopping among the atoms. We introduce in Section 3 our basic idea for finding the Green's functions of the above system using the RSRG procedure. This section also contains the calculations for the density of states and the Lyapunov exponent. The transfer matrix formalism for the second-neighbor TB system is developed in Section 4. We present the results of our calculations in Section 5, and then conclude in Section 6.

2 The model

One-dimensional quasiperiodic Fibonacci tiling can be obtained from a sequence of two elementary units, for example, L and S, which will be regarded as bonds on a lattice as shown in Figure 1. This sequence is generated from a seed, say S, applying the inflation rules $L \rightarrow LS$ and $S \rightarrow L$ recursively. Alternatively, the nth generation Fibonacci sequence S_n may be generated from the stacking rule $S_{n+1} = S_n S_{n-1}$ starting with $S_0 = S$ and $S_1 = L$. The sequence S_n contains F_n number of total symbols, where F_n is the nth order Fibonacci number obtained from the rule $F_{n+1} = F_n + F_{n-1}$ with $F_0 = 1 = F_1$. Thus S, L, LS, LSL, $LSLLS$ etc. are the first few generations of the Fibonacci sequence.

We describe the system by the tight-binding equation of motion

$$(E - \epsilon_i)\psi_i = t_{i,i+1}\psi_{i+1} + t_{i,i-1}\psi_{i-1} + t_{i,i+2}\psi_{i+2} + t_{i,i-2}\psi_{i-2} \qquad (1)$$

where ϵ_i's are the on-site potentials, $t_{i,i\pm1}$'s and $t_{i,i\pm2}$'s are respectively the nearest-neighbor and the second-neighbor hopping integrals, ψ_i's are the amplitudes, i being the site index. The on-site model of the Fibonacci chain for the second-neighbor problem is obtained when all $t_{i,i\pm1}$'s are equal to t_1 (say) and all $t_{i,i\pm2}$'s are equal to t_2 (say), while ϵ_i's are either $\epsilon_{\rm A}$ or $\epsilon_{\rm B}$ arranged in a Fibonacci sequence. Similarly, for the transfer model ϵ_i's are all equal, while $t_{i,i\pm1}$'s take two values t_L or t_S and $t_{i,i\pm2}$'s take values t_{LL}, t_{LS} or t_{SL} depending upon the decoration of the segment of Fibonacci lattice across which hopping takes place. In order to implement the RSRG scheme [9,11] we define a general model for the Fibonacci chain as follows. Depending upon the local environment we can identify α, β and γ sites in the Fibonacci chain corresponding to the lattice points flanked by LL, LS and SL bonds respectively. Now we describe the general model of the Fibonacci chain by three on-site potentials ϵ_α, ϵ_β and ϵ_γ corresponding to the α, β and γ sites respectively and by the nearest-neighbor hopping integrals as t_L and t_S and the second-neighbor hopping integrals as t_{LL}, t_{LS} and t_{SL}, where the labeling of the hopping integrals follows the same convention as that for the transfer model. This kind of labeling of the sites and the bonds is essential for implementing the RSRG decimation [9]. It turns out that the on-site and the transfer models are the special cases of the general model.

3 RSRG scheme for the Green's functions

To introduce the basic idea of our RSRG method for finding the single-particle electronic Green's functions for the second-neighbor TB system, let us first consider the simple case of a periodic chain and then we deal with the quasiperiodic Fibonacci lattice. The equations of motion for the single-particle electronic Green's functions are given by

$$(E - \epsilon_i)G_{ij} = \delta_{ij} + t_{i,i+1}G_{i+1j} + t_{i,i-1}G_{i-1j} + t_{i,i+2}G_{i+2j} + t_{i,i-2}G_{i-2j} \qquad (2)$$

where G_{ij} is the (ij)th matrix element of the Green's function in the Wannier representation, and E represents the complex energy $E + i0^+$.

(a) Periodic chain: In Figure 1a, we display a segment of the periodic chain and describe the system by the Hamiltonian parameters $\epsilon_i = \epsilon$, $t_{i,i\pm1} = t_1$ and $t_{i,i\pm2} = t_2$ for all i's. The equations of motion for the Green's functions now have the following explicit form

$$\begin{aligned}
&\vdots \\
(E-\epsilon)G_{-20} &= t_1(G_{-10} + G_{-30}) + t_2(G_{00} + G_{-40}) \\
(E-\epsilon)G_{-10} &= t_1(G_{00} + G_{-20}) + t_2(G_{10} + G_{-30}) \\
(E-\epsilon)G_{00} &= t_1(G_{10} + G_{-10}) + t_2(G_{20} + G_{-20}) + 1 \\
(E-\epsilon)G_{10} &= t_1(G_{20} + G_{00}) + t_2(G_{30} + G_{-10}) \\
(E-\epsilon)G_{20} &= t_1(G_{30} + G_{10}) + t_2(G_{40} + G_{00}) \\
(E-\epsilon)G_{30} &= t_1(G_{40} + G_{20}) + t_2(G_{50} + G_{10}) \\
&\vdots
\end{aligned} \qquad (3)$$

For convenience henceforth we suppress the second index "0" of the Green's function. Let us try to renormalize this periodic lattice by the usual procedure, *e.g.*, by decimating alternate sites of the lattice. If we decimate all the odd sites, then it is almost impossible to obtain a close set of the renormalized equations involving only even G_i's eliminating all odd G_i's from the coupled set of equation (3). Thus the implementation of the RSRG procedure is not straightforward even for a periodic system in the presence of second-neighbor hopping integrals.

We overcome this problem in the following way. We make the picture that the lattice is composed of identical blocks as shown in Figure 1b, where each block contains a pair of neighboring atoms. Now, the Wannier states associated with a given block is connected only with Wannier states of its neighboring blocks. Thus if we consider these blocks as pseudo-atoms, the second-neighbor TB periodic chain virtually behaves like a nearest-neighbor TB system with some effective hopping between the neighboring pseudo-atoms. In this picture, we can cast the original equation (3) for the Green's functions into the following nearest-neighbor TB form

$$\begin{aligned} &\vdots \\ (E\Pi_2 - \bar{\epsilon})g_{-1} &= Tg_0 + \tilde{T}g_{-2} \\ (E\Pi_2 - \bar{\epsilon})g_0 &= Tg_1 + \tilde{T}g_{-1} + C \\ (E\Pi_2 - \bar{\epsilon})g_1 &= Tg_2 + \tilde{T}g_0 \\ &\vdots \end{aligned} \tag{4}$$

where $\tilde{T}$ denotes the transpose of the matrix T and

$$\bar{\epsilon} = \begin{pmatrix} \epsilon & t_1 \\ t_1 & \epsilon \end{pmatrix}, \quad T = \begin{pmatrix} t_2 & t_1 \\ 0 & t_2 \end{pmatrix},$$

$$C = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{and} \quad g_i = \begin{pmatrix} G_{2i+1} \\ G_{2i} \end{pmatrix},$$

with $i = \pm 1, \pm 2$, etc., and Π_2 is a 2×2 identity matrix. The indices for g_i's correspond to those of the blocks and they are different from the site indices.

Now we can easily apply the renormalization scheme to the set of matrix equation (4). First we eliminate all odd g_i's and then rename the remaining g_i's appropriately. The resulting equations will be of the same form as that of the starting set of equation (4), provided we renormalize $\bar{\epsilon}$ and T as follows

$$\begin{aligned} \bar{\epsilon}^{'} &= \bar{\epsilon} - T[\bar{\epsilon}]^{-1}\tilde{T} - \tilde{T}[\bar{\epsilon}]^{-1}T, \\ T^{'} &= T[\bar{\epsilon}]^{-1}T. \end{aligned} \tag{5}$$

In this RSRG scheme we have actually decimated pseudo-atoms or blocks instead of sites of the original lattice, and this decimation scheme has been illustrated in Figure 1c. This is an exact RSRG procedure since no information of the original equation (3) is lost during renormalization. The successive renormalization of the system basically corresponds to the iteration of the recursion relations equation (5). The pseudo-atoms become far apart as we renormalize the system, which physically means that T flows to a null matrix and $\bar{\epsilon}$ goes to a fixed point value $\bar{\epsilon}^*$. In this limit we have $g_0 = (E\Pi_2 - \bar{\epsilon}^*)^{-1}C$ and it readily gives the site-diagonal Green's function $G_{00}(E)$. $G_{00}(E)$ can be calculated with arbitrary accuracy, the level of accuracy is determined by the smallness of the elements of T. Once the site-diagonal Green's functions $G_{00}(E)$ is known, we can compute the local electronic density of states from the relation

$$\rho(E) = -\frac{1}{\pi}\mathrm{Im}G_{00}(E). \tag{6}$$

For the periodic case, the density of states can also be obtained from the dispersion relation $\epsilon(k)$ using the formula

$$\rho(E) = \frac{a}{\pi} \quad \left(\frac{\mathrm{d}\epsilon(k)}{\mathrm{d}k}\right)^{-1},$$

where

$$\epsilon(k) = \epsilon + 2t_1\cos(ka) + 2t_2\cos(2ka),$$

a being the lattice constant.

We have calculated $\rho(E)$ both from the dispersion relation and also using the RSRG method, and this confirms that the present RSRG method works extremely well. This RSRG scheme provides a powerful method for computing the density of states since it essentially requires the iteration of certain recursion relations, and $\rho(E)$ can be determined with arbitrary accuracy. One can easily generalize this method to the case where higher neighbor hopping integrals are present in the TB Hamiltonian. For instance, if we include 3rd-neighbor hopping integrals in the Hamiltonian, then we simply have to start with blocks consisting of three neighboring atoms.

(b) Fibonacci chain: With the above background we now focus our attention on the quasiperiodic Fibonacci chain. A portion of the Fibonacci chain is shown in Figure 1d. We take the general model for the Fibonacci chain, which we have already described in the introduction. The Green's functions satisfy the following hierarchy of equations (see Fig. 1d)

$$\begin{aligned} &\vdots \\ (E-\epsilon_\alpha)G_3 &= t_L G_2 + t_L G_4 + t_{LS}G_1 + t_{LS}G_5 \\ (E-\epsilon_\beta)G_4 &= t_L G_3 + t_S G_5 + t_{LL}G_2 + t_{LS}G_6 \\ (E-\epsilon_\gamma)G_5 &= t_S G_4 + t_L G_6 + t_{LS}G_3 + t_{LS}G_7 \\ (E-\epsilon_\beta)G_6 &= t_L G_5 + t_S G_7 + t_{LS}G_4 + t_{LS}G_8 \\ (E-\epsilon_\gamma)G_7 &= t_S G_6 + t_L G_8 + t_{LS}G_5 + t_{LL}G_9 \\ &\vdots \end{aligned} \tag{7}$$

setting $t_{LS} = t_{SL}$. Here the second index of the Green's functions correspond to the zeroth site of the Fibonacci lattice as shown in Figure 1d, and we again suppress it for convenience. For the Fibonacci chain, the usual renormalization scheme is to decimate sites following the deflation rules $LS \to L$, $L \to S$ (see Refs. [11,12] for details).

But this scheme is not readily applicable to the present problem, since we can not renormalize the set of coupled equation (7) in a straightforward way preserving the Fibonacci symmetry. As in the periodic case, we therefore introduce the idea of elementary blocks or pseudo-atoms for implementing the RSRG scheme in the Fibonacci chain corresponding to the second-neighbor TB Hamiltonian. In the Fibonacci lattice, we have to consider α, β and γ type blocks as illustrated in Figure 1e such that Fibonacci order is maintained among the blocks. Now this lattice made of blocks essentially behaves like a nearest-neighbor TB Fibonacci chain with some effective hopping among the pseudo-atoms. So we can express the set of equation (7) into an equivalent nearest-neighbor tight-binding form, which are given by

$$\begin{aligned}
&\vdots \\
(E\Pi_2 - \bar{\epsilon}_\beta)g_1 &= T_S g_2 + \tilde{T}_{\alpha\beta} g_0 \\
(E\Pi_3 - \bar{\epsilon}_\gamma)g_2 &= T_{\gamma\alpha} g_3 + \tilde{T}_S g_1 \\
(E\Pi_3 - \bar{\epsilon}_\alpha)g_3 &= T_{\alpha\beta} g_4 + \tilde{T}_{\gamma\alpha} g_2 \\
(E\Pi_2 - \bar{\epsilon}_\beta)g_4 &= T_S g_5 + \tilde{T}_{\alpha\beta} g_3 \\
(E\Pi_3 - \bar{\epsilon}_\gamma)g_5 &= T_{\gamma\beta} g_6 + \tilde{T}_S g_4 \\
&\vdots
\end{aligned} \tag{8}$$

where

$$\bar{\epsilon}_{\alpha(\gamma)} = \begin{pmatrix} \epsilon_\gamma & t_S & t_{LS} \\ t_S & \epsilon_\beta & t_L \\ t_{LS} & t_L & \epsilon_{\alpha(\gamma)} \end{pmatrix}, \quad \bar{\epsilon}_\beta = \begin{pmatrix} \epsilon_\beta & t_L \\ t_L & \epsilon_\alpha \end{pmatrix},$$

$$T_{\alpha\beta} = T_{\gamma\beta} = \begin{pmatrix} t_{LL} & t_L \\ 0 & t_{LS} \\ 0 & 0 \end{pmatrix}, \quad T_{\gamma\alpha} = \begin{pmatrix} 0 & t_{LL} & t_L \\ 0 & 0 & t_{LS} \\ 0 & 0 & 0 \end{pmatrix},$$

$$T_S = \begin{pmatrix} 0 & t_{LS} & t_S \\ 0 & 0 & t_{LS} \end{pmatrix},$$

and

$$g_0 = \begin{pmatrix} G_2 \\ G_1 \\ G_0 \end{pmatrix}, \quad g_1 = \begin{pmatrix} G_4 \\ G_3 \end{pmatrix},$$

$$g_2 = \begin{pmatrix} G_7 \\ G_6 \\ G_5 \end{pmatrix}, \quad g_3 = \begin{pmatrix} G_{10} \\ G_9 \\ G_8 \end{pmatrix}, \cdots$$

and so on. Π_2 and Π_3 respectively denote 2×2 and 3×3 identity matrices.

Now we can easily renormalize this set of equation (8) using the decimation rules $LS \to L$ and $L \to S$ [12]. We illustrate this decimation scheme in Figure 1f, and the recursion relations for this transformation are

$$\begin{aligned}
\bar{\epsilon}'_\alpha &= \bar{\epsilon}_\gamma + \tilde{T}_S P T_S + T_{\gamma\beta} P \tilde{T}_{\gamma\beta} \\
\bar{\epsilon}'_\beta &= \bar{\epsilon}_\gamma + \tilde{T}_S P T_S \\
\bar{\epsilon}'_\gamma &= \bar{\epsilon}_\alpha + T_{\alpha\beta} P \tilde{T}_{\alpha\beta} \\
T'_{\alpha\beta} &= T_{\gamma\beta} P T_S \\
T'_{\gamma\alpha} &= T_{\alpha\beta} P T_S \\
T'_{\gamma\beta} &= T_{\alpha\beta} P T_S \\
T'_S &= T_{\gamma\alpha}
\end{aligned} \tag{9}$$

where $P = (E\Pi_2 - \bar{\epsilon}_\beta)^{-1}$.

The separation between the pseudo-atoms increases with renormalization, so the matrices T's flow to null matrices, and $\bar{\epsilon}$'s attain the fixed point values $\bar{\epsilon}^*$'s as we iterate the recursion relations equation (9). If the zeroth block (which is α type block in Fig. 1e) remains undecimated even in the final stage of the renormalization corresponding to the fixed point, then we can write [11]

$$g_0 = (E\Pi_3 - \bar{\epsilon_\alpha}^*)^{-1} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} .$$

This readily gives the site-diagonal Green's function $G_{00}(E)$ and the local density of states at the zeroth site can be obtained from equation (6).

Since no two sites are locally equivalent in a quasiperiodic chain, so the local density of states is different at every site of the chain. The local density of states at an arbitrary site of the second-neighbor TB Fibonacci chain can be easily obtained using the technique of reference [11], first starting with the block or pseudo-atom to which the chosen site belongs, and then determining the renormalized local environments of this pseudo-atoms under successive application of the deflation rules $LS \to L$ and $L \to S$.

Calculation of the Lyapunov exponent:

The Lyapunov exponent $\gamma(E) = 1/\lambda(E)$ ($\lambda(E) =$ localization length) for the eigenstates of the Fibonacci chain can also be obtained from our renormalization group scheme. Apart from the inhomogeneous term on the right hand side of the equation (7), the set of equations for the amplitudes of the wave functions become identical to the set of equation (7) provided we replace G_i's by ψ_i's and take E to be real. So we can renormalize the set of equations for ψ_i's in a similar way as that for G_i's.

For finding the Lyapunov exponent [13] let us first consider a finite generation, say, nth generation Fibonacci chain, and ask the question what would be the amplitude ψ_N ($N = F_n$) at the last site for an arbitrary energy E, if we take the initial condition as $\psi_0 = 1$. Then we take the limit $N \to \infty$. ψ_N can be calculated very easily with the help of renormalization group technique. We may regard this finite generation Fibonacci chain as a segment of the infinite Fibonacci chain. Now as we renormalize the system, say, after nth iteration the two blocks containing 0th and Nth sites become neighboring blocks connected by some effective hopping matrix [14]. This actually determines ψ_N in term of ψ_0. If we take the effective hopping matrix as $T_S^{(n)}$ connecting the two blocks, then the Lyapunov exponent is given by

$$\gamma(E) = Lt_{n\to\infty} \frac{1}{\tau^n} \ln Q_{11}^{(n)} ,$$

where $Q^{(n)} = (E\Pi_3 - \bar{\epsilon_\gamma}^{(n)})^{-1}\tilde{T_S}^{(n)}$ and $\tau = (1+\sqrt{5})/2$. The value of $\gamma(E)$ is quite independent of the choice of the effective hopping matrix, since in the limit $n \to \infty$ all the hopping matrices T_S, $T_{\alpha\beta}$, $T_{\gamma\alpha}$ and $T_{\gamma\beta}$ contain the same information about the localization behavior of the eigenstates.

4 Transfer matrix formalism

The transfer matrix method is an efficient tool for finding the eigenvalues and eigenstates of one-dimensional quasiperiodic lattices within the nearest-neighbor TB framework, and in this section we formulate the transfer matrix method for the second-neighbor problem. For the nearest-neighbor case, this method gives an alternative matrix formulation for the Schrödinger equation in term of 2×2 transfer matrices. In an analogous way, we recast the Schrödinger equation (1) for the second-neighbor TB system into the following matrix form

$$\begin{pmatrix} \psi_{i+2} \\ \psi_{i+1} \\ \psi_i \\ \psi_{i-1} \end{pmatrix} = M \begin{pmatrix} \psi_{i+1} \\ \psi_i \\ \psi_{i-1} \\ \psi_{i-2} \end{pmatrix}, \tag{10}$$

where the transfer matrix M is now 4×4 matrix

$$M = \begin{pmatrix} -\frac{t_{i,i+1}}{t_{i,i+2}} & \frac{E-\epsilon_i}{t_{i,i+2}} & -\frac{t_{i,i-1}}{t_{i,i+2}} & -\frac{t_{i,i-2}}{t_{i,i+2}} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

We now proceed in the usual manner considering first the successive periodic approximant of the Fibonacci lattice, and then taking the infinite chain limit. Let M_n denotes the global transfer matrix for the nth generation Fibonacci chain. Of course, for the present problem we have to start from the generation which contains at least two atoms, otherwise second-neighbor hopping would not be possible in the system. Let us now see how these M_n's evolve with the generation index n for various models of the Fibonacci lattice.

For the on-site model, we take two types of atoms A and B arranged according to the Fibonacci sequence so that the first few global matrices are $M_2 = M_{\rm B}M_{\rm A}$, $M_3 = M_{\rm A}M_{\rm B}M_{\rm A}$, $M_4 = M_{\rm B}M_{\rm A}M_{\rm A}M_{\rm B}M_{\rm A}$, etc. The individual transfer matrices $M_{\rm A}$ and $M_{\rm B}$ correspond to A and B atoms in the lattice, and they are given by

$$M_{\rm A} = \begin{pmatrix} -\frac{t_1}{t_2} & \frac{E-\epsilon_{\rm A}}{t_2} & -\frac{t_1}{t_2} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$M_{\rm B} = \begin{pmatrix} -\frac{t_1}{t_2} & \frac{E-\epsilon_{\rm B}}{t_2} & -\frac{t_1}{t_2} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Thus the global transfer matrices M_n's for the on-site model satisfy the following simple recursion relation

$$M_{n+1} = M_{n-1}M_n, \quad \text{for} \quad n \geq 1$$

with $M_0 = M_{\rm B}$ and $M_1 = M_{\rm A}$.

The global transfer matrices for the general model of the Fibonacci chain can be expressed in term of the following five basic matrices

$$M_\alpha = \begin{pmatrix} -\frac{t_L}{t_{LS}} & \frac{E-\epsilon_\alpha}{t_{LS}} & -\frac{t_L}{t_{LS}} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$M_\beta = \begin{pmatrix} -\frac{t_S}{t_{LS}} & \frac{E-\epsilon_\beta}{t_{LS}} & -\frac{t_L}{t_{LS}} & -\frac{t_{LL}}{t_{LS}} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$M_\gamma = \begin{pmatrix} -\frac{t_L}{t_{LS}} & \frac{E-\epsilon_\gamma}{t_{LS}} & -\frac{t_S}{t_{LS}} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$M_\beta^{'} = \begin{pmatrix} -\frac{t_S}{t_{LS}} & \frac{E-\epsilon_\beta}{t_{LS}} & -\frac{t_L}{t_{LS}} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$M_\gamma^{'} = \begin{pmatrix} -\frac{t_L}{t_{LL}} & \frac{E-\epsilon_\gamma}{t_{LL}} & -\frac{t_S}{t_{LL}} & -\frac{t_{LS}}{t_{LL}} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Considering successive periodic approximants for the general model of the Fibonacci chain with periodic boundary condition, the global transfer matrices for the first few generations are given by

$$\begin{aligned} M_2 &= M_\beta^{'}M_\gamma \\ M_3 &= M_\gamma^{'}M_\beta M_\alpha \\ M_4 &= M_\beta M_\alpha M_\gamma^{'} M_\beta^{'} M_\gamma \\ M_5 &= M_\gamma^{'} M_\beta^{'} M_\gamma M_\beta M_\alpha M_\gamma^{'} M_\beta M_\alpha \\ &\vdots \end{aligned} \tag{11}$$

It seems that finding the recursion relation for M_n's becomes an intractable problem as M_n's have a very complex structure. However, we are able to find the recursion relation even in this case using the symmetry of these structures. We see that M_n's can be generated successively starting with $M_1 = M_\alpha$ applying the basic transformations $M_\alpha \to M_\beta^{'}M_\gamma$, $M_\beta \to M_\gamma^{'}$, $M_\beta^{'} \to M_\gamma^{'}$, $M_\gamma \to M_\beta M_\alpha$ and $M_\gamma^{'} \to M_\beta M_\alpha$.

Now we generate another auxiliary set of transfer matrices $\bar{M}_n$'s applying the above transformations successively starting from $\bar{M}_1 = M_\gamma^{'}$. Then for the general model

of the Fibonacci lattice, we have the following recursion relations for the global transfer matrices

$$M_{n+1} = \bar{M}_{n-1}\bar{M}_n \quad \text{and} \quad \bar{M}_{n+1} = \bar{M}_{n-1}M_n, \quad \text{for} \quad n \geq 2.$$

It should be noted that for the transfer model, we also have five basic matrices M_α, M_β, M_γ, $M_\beta^{'}$ and $M_\gamma^{'}$ which are, of course, different from the general model, but M_n's satisfy the same recursion relations as those for the general model.

Thus the global transfer matrices M_n's of the Fibonacci chain for the on-site, transfer and general model can be easily calculated simply iterating the appropriate recursion relations. Once we know the transfer matrix M_n corresponding to the nth generation chain, the eigenvalues of this finite system can be determined by the technique of reference [15]. From the Bloch condition, the allowed energy spectrum can be obtained from the relation $|y_n| \leq 1$, where

$$y_n = \frac{1}{2}\left[\mathrm{Tr}M_n \pm \sqrt{2\mathrm{Tr}({M_n}^2) - (\mathrm{Tr}M_n)^2 + 8}\right].$$

The above procedure gives the eigenvalues only for finite system size, and it becomes practically impossible to determine them with adequate accuracy when the system size becomes large. Also any dynamical map, like the well-known trace-map relation [4,9], is not known for these 4×4 transfer matrices M_n's. So the analysis similar to that of the trace-map technique is not possible in this case for finding the eigenvalues of the limiting infinite chain. On the other hand, our RSRG scheme for the Green's functions becomes exact only when the system size is infinite, and thus the energies corresponding to non-zero values of the density of states really give the eigenvalues of the infinite chain. Now corresponding to every eigenvalue of the system, the amplitudes ψ_i's of the eigenfunction can be obtained from equation (10) provided we specify the initial amplitudes ψ_0, ψ_{-1}, ψ_{-2} and ψ_{-3}. Hence, the entire spectrum of the infinite Fibonacci chain can be obtained without much effort from the density of states, and the nature of the allowed eigenstates can be determined with the help of transfer matrix method.

5 Results and discussions

With this much theoretical development, we now look into the results for some specific cases of the second-neighbor TB Fibonacci chain. In Figure 2 we have plotted the local density of states (LDOS) as a function of energy for the transfer model of the Fibonacci chain. Figure 2a is in fact a plot of LDOS for the nearest-neighbor TB system, and for numerical calculations we choose the parameters as $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$, $t_L = 1$ and $t_S = 2$. Next we add second-neighbor electronic hopping in this system, and see how it affects the LDOS. The strength of the second-neighbor hopping terms are taken as $t_{LL} = 0.1$ and $t_{LS} = 0.2$ in Figure 2b, while those in Figure 2c are $t_{LL} = 0.3$ and $t_{LS} = 1.2$. In these calculations all energies are measured in arbitrary units. Figure 2a shows that the

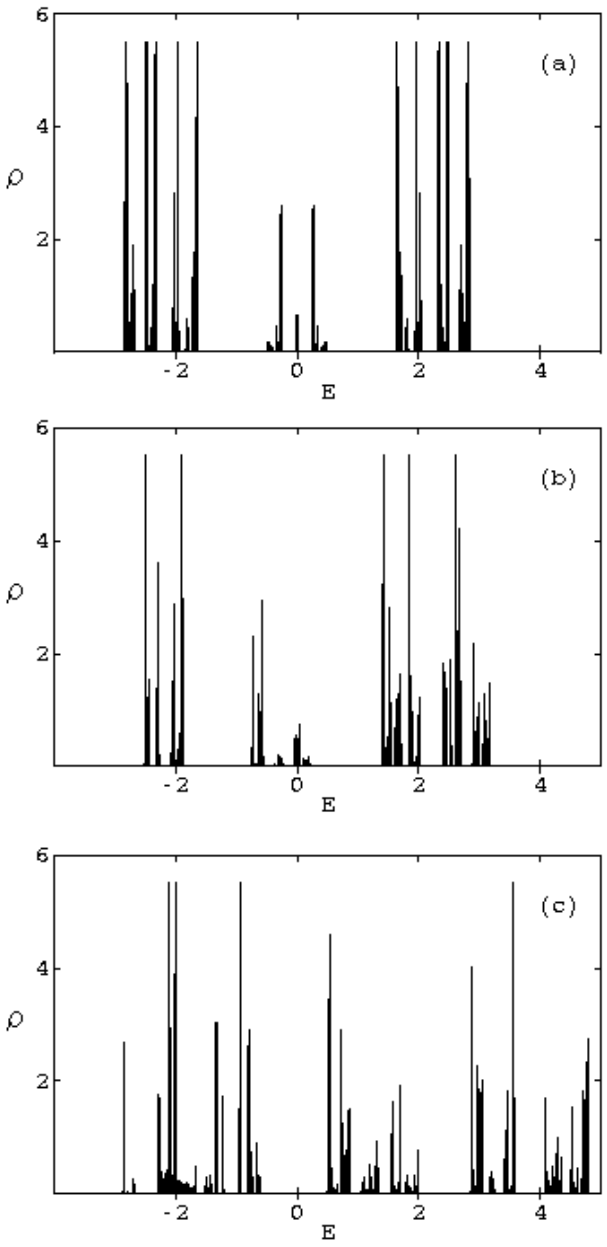

Fig. 2. Plot of LDOS *versus* E for the transfer model. TB system with only nearest-neighbor terms: (a) $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$, $t_L = 1$, $t_S = 2$. TB system with both nearest-neighbor and second-neighbor terms: (b) $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$, $t_L = 1$, $t_S = 2$, $t_{LL} = 0.1$, $t_{LS} = 0.2$, and (c) $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$, $t_L = 1$, $t_S = 2$, $t_{LL} = 0.3$, $t_{LS} = 1.2$. All energies are measured in arbitrary units.

LDOS is symmetric about the origin of energy $E = 0$, and, we see from Figures 2b and 2c that this symmetry gets destroyed by the second-neighbor electronic hopping process. However, we observe that the features characteristics of the quasiperiodic system, namely, spiky and highly fragmented density of states, are not affected by the second-neighbor electronic hopping.

We display the $\rho(E)$ *versus* E curves for the on-site model of the Fibonacci chain in Figure 3. As before, Figure 3a corresponds to the nearest-neighbor TB

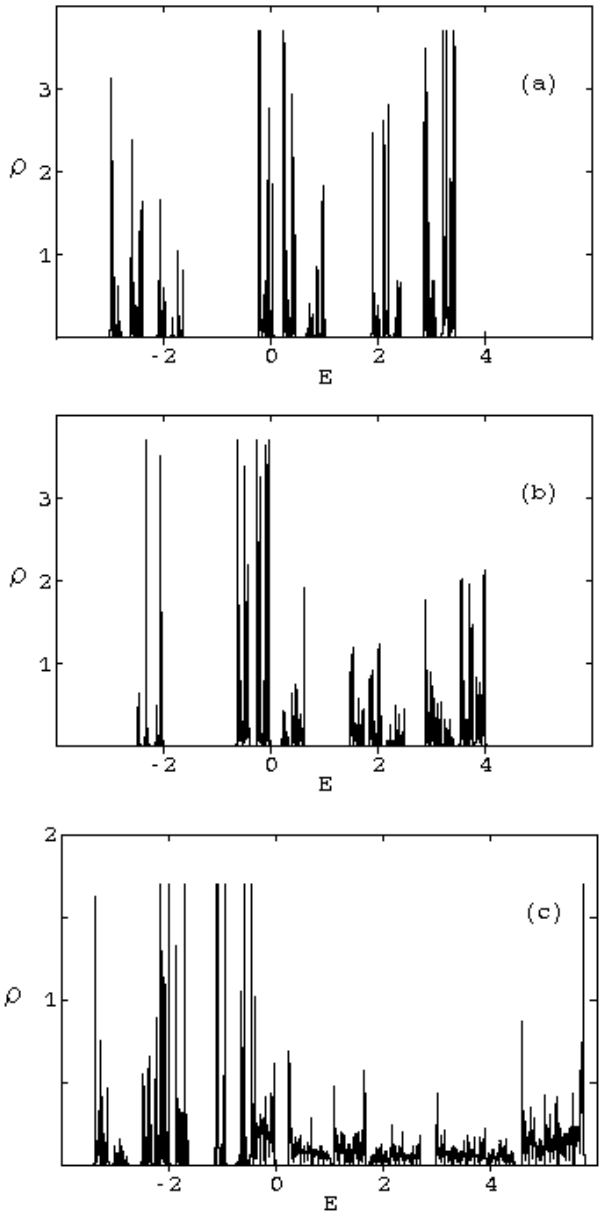

Fig. 3. Plot of LDOS *versus* E for the on-site model. TB system with only nearest-neighbor terms: (a) $\epsilon_\alpha = -\epsilon_\beta = \epsilon_\gamma = 1$, $t_L = t_S = 1.5$. TB system with both nearest-neighbor and second-neighbor terms: (b) $\epsilon_\alpha = -\epsilon_\beta = \epsilon_\gamma = 1$, $t_L = t_S = 1.5$, $t_{LL} = t_{LS} = 0.3$, and (c) $\epsilon_\alpha = -\epsilon_\beta = \epsilon_\gamma = 1$, $t_L = t_S = 1.5$, $t_{LL} = t_{LS} = 1.2$. All energies are measured in arbitrary units.

Hamiltonian, and the parameters are taken as $\epsilon_\alpha = -\epsilon_\beta = \epsilon_\gamma = 1$, $t_L = t_S = 1.5$. Figures 3b and 3c actually correspond to second-neighbor TB system, where we include second-neighbor hopping in the above nearest-neighbor system for studying the influence of this additional electronic hopping on the LDOS. We choose $t_{LL} = t_{LS} = 0.3$ in Figure 3b and $t_{LL} = t_{LS} = 1.2$ in Figure 3c. Here the energies are measured in arbitrary units. It is apparent from Figures 3a, 3b and 3c that the qualitative nature of the band structure for the on-site model remains unaltered even in the presence of second-neighbor electronic

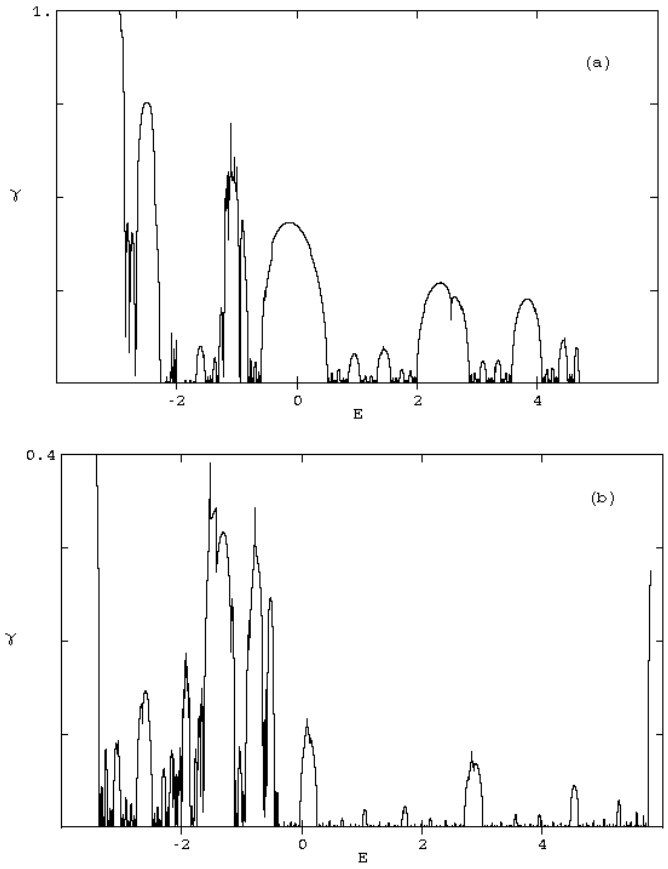

Fig. 4. Plot of γ *versus* E curves. (a) Plot for the transfer model with parameters as those in Figure 2c, and (b) plot for the on-site model with parameters as those in Figure 3c.

hopping among the atoms. Thus our study on the transfer and on-site models of the Fibonacci chain reveals that the unusual electronic properties, like the Cantor-set energy spectrum, spiky density of states, etc., are characteristics of the quasiperiodic structure, and, the generalization of the tight-binding Hamiltonian has no effect on the qualitative features of the electronic structure.

To gain further insight about the properties of the second-neighbor TB Fibonacci chain, we now study the nature of the energy eigenstates. For this purpose, in Figure 4 we have plotted the Lyapunov exponent γ as a function of energy E. Figure 4a corresponds to the transfer model with parameters as those of Figure 2c, while Figure 4b is for the on-site model described by the same parameters as those in Figure 3c. Comparing Figure 4a with Figure 2c and Figure 4b with Figure 3c, we observe that the Lyapunov exponent vanishes precisely at those energies which are the allowed eigenstates of the system. This means that the localization length becomes infinity for the allowed eigenstates of the system. It indicates that the electrons are not confined to a finite region of the lattice, and the eigenstates should have extended character. On the other hand, we see (using Eqs. (9)) that for allowed eigenvalues of the system, the effective hopping integrals flow to zero under renormalization. But we know that hopping integrals never flow to zero

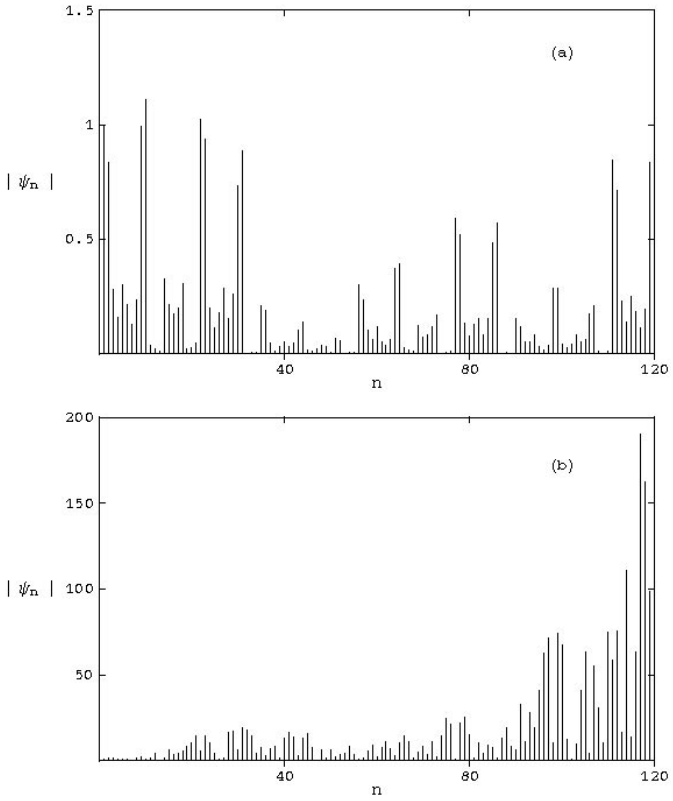

Fig. 5. Plot of ψ_n *versus* n. (a) Plot for the transfer model with parameters as those in Figure 2c corresponding to $E = -2.00440$, and (b) plot for the on-site model with parameters as those in Figure 3c corresponding to $E = -1.10328$.

on renormalization for extended eigenstates [12]. This clearly shows that the states are neither localized nor extended, and such states are termed as critical states.

The critical nature of the eigenstates can also be observed from the explicit calculation of the wave function amplitudes using the transfer matrix relation equation (10). In Figure 5a we plot $|\psi_n|$ against n for the transfer model having parameters as those of Figure 2c, while Figure 5b is the plot for the on-site model referring to the system of Figure 3c. Figures 5a and 5b respectively correspond to the energy eigenvalues $E = -2.00440$ and $E = -1.10328$, which are estimated by scanning the non-zero values for the density of states. In both these calculations the initial amplitudes are taken as $\psi_0 = 1$, $\psi_{-1} = \psi_{-2} = \psi_{-3} = 0$. The critical nature of the wave functions is quite apparent from these plots. At this point we would like to make the following comments regarding the transfer matrix method for the second-neighbor problem. The stability of the calculations in terms of 4×4 transfer matrices crucially depends on the correct estimation of the energy eigenvalues, and, also on the choice of the initial amplitudes. We have seen that even for the second-neighbor TB periodic system, the wave function diverges for every allowed eigenvalues unless we maintain the proper phase relationship among the initial amplitudes. For the quasiperiodic Fibonacci chain such phase relationship among the initial amplitudes is not known, and this introduces error in the calculation of amplitudes of the wave functions.

6 Conclusions

In this work we provide a new RSRG scheme for finding the electronic density of states of one-dimensional tight-binding systems taking both first-neighbor and second-neighbor hopping integrals in the Hamiltonian. This is an exact method and can be easily generalized to systems having higher neighbor hopping integrals. It offers a very elegant theoretical tool for computing the density of states of quasiperiodic systems, since the self-similar property of these lattices can be exploited most efficiently only by the renormalization group technique. We have studied the quasiperiodic Fibonacci chain as a prototype example for illustrating our method. The Lyapunov exponent can also be obtained from our RSRG scheme. The analysis of the renormalized hopping integrals together with the Lyapunov exponent gives information about the nature of the states. We have also developed the transfer matrix formalism for the second-neighbor tight-binding system in terms of 4×4 transfer matrices, and determined the eigenfunctions of the system. From our study we conclude that the unusual physical properties, namely, the critical eigenstates, highly fragmented density of states, Cantor-set energy spectrum etc. are the characteristic features of the quasiperiodic structure, and these features are quite independent of the details of the tight-binding model itself.

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