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The electronic properties of a Fibonacci chain

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Abstract
Using a tight-binding model and transfer-matrix technique, as well as *Lanczos* algorithm, we numerically investigate the nature of the electronic states and electron transmission in site, bond and mixing Fibonacci model chains. We rely on the *Landauer* formalism as the basis for studying the conduction properties of these systems. Calculating the *Lyapunov* exponent, we also study the localization properties of electronic eigenstates in the Fibonacci chains. The focus is on the significance of the relationship between the transmission spectra and the nature of the electronic states. Our results show that, in contrast to Anderson's localization theorem, in the Fibonacci chains the electronic states are non-localized and the transparent states occurr near the Fermi level.

Keywords: quasicrystal, Fibonacci sequence, transfer-matrix technique, *Lanczos* algorithm and *Landauer* formalism

1. Introduction

Since the discovery of the quasicrystalline phase [1], much attention has been given to the quasicrystal materials. The lack of translational symmetry in quasicrystals means the non-applicability of Bloch's theorem. Since quasicrystals exhibit an intermediate character between crystals and amorphous solids, the electronic properties of these materials are expected to display new behavior. Experimentally, quasicrystalline phases have unique electronic properties. They are characterized by a low conductivity, which increases when temperature or disorder increases. Also the building of artificial multilayer structures by molecular beam epitaxy [2], has considerably stimulated the theoretical study of the physical properties of quasiperiodic systems [3,4]. There has been in particular, detailed discussion on the nature of electronic eigenstates on quasicrystals. It is questioned whether their electronic spectra are absolutely continuous, pointlike or singular continuous, or correspondingly the electronic states are extended, localized or critical. It has been established that in these systems the three kinds of wave functions, i.e., extended, localized and critical states coexist [5-8]. Critical states are neither localized nor extended; they have self-similar wave functions in real space [9]. The effects of quasiperiodicity in the electronic spectra can be studied in the most simple quasiperiodic structure which is a Fibonacci chain (FC). The investigation of the electronic transport in FCs is an open and interesting problem. In particular, the relationship between the nature of electronic states and transport phenomena is not fully understood. The conductivity in FCs has been studied by using the Miller-Abrahams equations [10,11] and by the Kubo-Greenwood formula [12,13]. Also the existence of transparent states with the maximum value of transmission coefficient equal unity has been reported [14]. However, the question of the localization nature of the transparent states is still controversial.

In this paper we have numerically studied the electronic states belonging to various types of FCs, site, bond and mixing models. Embedding a typical Fibonacci lattice in an infinite periodic chain, we calculate the electronic transmission through these systems based on *Landauer* formalism. We find that the magnitude of the transmission, especially near Fermi level, is close to unity, i.e., close to the magnitude of transmission in a periodic system. Also the localization properties of the corresponding eigenstates in these chains is investigated. Our results show that the transparent states in these

Fibonacci model chains are close to similar states in periodic systems. The formalism we have applied in this work is based on the transfer-matrix (t-matrix) technique, where the solution of the Schrodinger equation is obtained by means of a product of 2×2 matrices.

The outline of the paper is as follows: In Sec.(2) we give a general introduction of a Fibonacci system and then describe our models for construction of several Fibonacci model chains. In Sec.(3) our methodology to calculate the t-matrices, the transmission coefficient and the *Lyapunov* exponent is described. The results and discussion are presented in Sec.(4) followed by a summary and conclusions in Sec.(5).

2. Fibonacci chain

There are several ways to generate a Fibonacci system [15-17]. In this study, to investigate the electronic properties of a FC, we have constructed; *i*) a bond Fibonacci model (BFM) in which the on-site energies are the same and the hopping integrals, t_A and t_B are organized following the Fibonacci sequence (FS). *ii*) a site Fibonacci model (SFM) containing two sort of atoms with the same hopping integrals. *iii*) a mixing Fibonacci model (MFM) in which two kinds of atoms A and B are arranged following the FS. In this model the arrangement of the hopping integrals between atoms depends on the nature of them giving rise to the two different parameters t_{AA} and $t_{AB}=t_{BA}$.

A typical FS of generation n containing $N(n)=S_n$ sites, can be built by defining the first and second generations of $S_1=A$ and $S_2=BA$. One may obtain the generation S_n from the substitution rule $S_n=S_{n-1}S_{n-2}$. For instance, the fourth generation is obtained as $S_4=BAABA$. The FCs as the simplest one-dimensional quasicrystals are the most intensively studied and new concepts on the electronic properties such as the singular continuous energy spectrum, existence of self-similarity in their transmission spectra are now well established [14,18]. The quasiperiodicity of the FCs is characterized by the golden mean $\tau_0=\frac{\sqrt{5}-1}{2}$ [19]. It is well known that the golden mean, τ_0 can be approximated by the Fibonacci numbers ($F_1=1$, $F_2=1$, $F_n=F_{n-1}+F_{n-2}$ for $n>2$), namely $\tau_0=\lim_{n\to\infty}\frac{F_n}{F_{n+1}}$. Figure 1 schematically illustrates the SFM, BFM and MFM chains, respectively where are connected to two semi-infinite periodic linear chains with null on-site energies and corresponding hopping integrals equal unity.

3. Methodology

Here we present the t-matrix formalism. We have applied this technique to investigate the electronic properties of the Fibonacci model chains. Let us start by considering a general FC in which both diagonal and off-diagonal terms are present in the Hamiltonian;

$$H=\sum_i\left[|i\rangle\varepsilon_i\langle i|+t_{i,i+1}|i\rangle\langle i+1|+t_{i,i-1}|i\rangle\langle i-1|\right], \qquad (1)$$

where ε_i is the on-site energy of the site i and $t_{i,i\pm1}$ are the nearest-neighbor hopping integrals between the sites i and $i\pm1$. In studying the electronic properties of one-dimensional quasiperiodic chains, it has been common to use the corresponding tight-binding equation Hamiltonian (1);

$$t_{i,i-1}\psi_{i-1}+(\varepsilon_i-E)\psi_i+t_{i,i+1}\psi_{i+1}=0, \qquad (2)$$

where ψ_i is the probability amplitude at site i. Solving for ψ_{i+1} we find the t-matrix formulation;

$$\begin{pmatrix}\psi_{i+1}\\ \psi_i\end{pmatrix}=\begin{pmatrix}\frac{E-\varepsilon_i}{t_{i,i+1}} & -\frac{t_{i,i-1}}{t_{i,i+1}}\\ 1 & 0\end{pmatrix}\begin{pmatrix}\psi_i\\ \psi_{i-1}\end{pmatrix}=M_i(E)\begin{pmatrix}\psi_i\\ \psi_{i-1}\end{pmatrix}, \qquad (3)$$

where $M_i(E)$ is the local t-matrix associated with site i. Defining $U_i=\begin{pmatrix}\psi_i\\ \psi_{i-1}\end{pmatrix}$ and $M(E)=\prod_{i=1}^{N}M_i(E)$ as the global t-matrix of the chain, then $U_{N+1}=M(E)U_1$ or;

$$\begin{pmatrix}\psi_{N+1}\\ \psi_N\end{pmatrix}=\begin{pmatrix}m_{11} & m_{12}\\ m_{21} & m_{22}\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_0\end{pmatrix}=\prod_{i=1}^{N}M_i(E)\begin{pmatrix}\psi_1\\ \psi_0\end{pmatrix}. \qquad (4)$$

We see that t-matrices depend on energy, E. If the eigenenergy and U_1 are known, then the whole eigenfunctions will easily be calculated from the t-matrices. Also the t-matices can give the valuable information about the nature of the wave functions. Now, we proceed to calculate of the transmission coefficient, $T(E)$, whose magnitude is directly related to the conductance through the *Landauer* formula [20];

$$G=\frac{2e^2}{h}T(E). \qquad (5)$$

Connecting the Fibonacci lattice to two semi-infinite periodic leads, then $T(E)$ is identical to the probability that an incident electron with energy E in the left-hand lead emerges in the right-hand one. Using eq.(4), the transmission coefficient (transmittance) $T(E)$ is given by [14,19,21];

$$T(q)=\frac{4(1-q^2)}{(Z+qY)^2+(1-q^2)X^2} \qquad (6)$$

where the dimensionless parameters q, X, Y and Z are given as follows;

$$q=1-\frac{E}{2t}\ ;\ X=m_{22}+m_{11}\ ;\ Y=m_{22}-m_{11}\ ;\ Z=m_{21}-m_{12}, \qquad (7)$$

where $t=1$ is the hopping integral of semi-infinite leads in the FC and $m_{ij}(i,j=1,2)$ are the matrix elements of the global t-matrix, $M(E)$, of the chain. We have calculated the energy eigenvalues spectrum, $\{E_i\}$, and the corresponding electronic eigenstates, $\{\psi_i\}$, for the FC using a direct diagonalization procedure based on the *Lanczos* algorithm [22,23]. This diagonalization method is known to be very efficient for large matrices. Considering $\{\varepsilon_i\}$ and $\{t_{i,i\pm1}\}$ according to FS, we have applied this method to the Hamiltonian (1) and the resulting energy spectrum used to calculate $M(E)$ and thereby transmittance $T(E)$ and *Lyapunov* exponent $\Gamma(E)$ via eqs.(4), (6) and (8), respectively. The localization properties of the electronic states in the Fibonacci model chains can be studied through the calculation of the *Lyapunov* exponent $\Gamma(E)=\frac{1}{N}\ln\|M(E)\|$ [19], where $\|\ \|$ denotes the modulus of the matrix $M(E)$. Using the matrix elements of $M(E)$ via eq.(4), we can easily write $\Gamma(E)$ as follows;

$$\Gamma(E)=\frac{1}{N}\ln\sqrt{m_{11}^2+m_{12}^2+m_{21}^2+m_{22}^2}\ . \qquad (8)$$

The *Lyapunov* exponent $\Gamma(E)$ characterizes the evolution of an electronic eigenstate along the chain [24]. $\Gamma(E)$ is zero for an extended or critical state, but is positive for a localized state, representing then the inverse of the localization length.

4. Results and discussion

We now apply the t-matrix formalism to calculate the transmittance $T(E)$ and *Lyapunov* exponent $\Gamma(E)$. In our models, the on-site energies $\{\varepsilon_i\}$ and the hopping integrals $\{t_{i,i\pm1}\}$ along the FC are chosen according to FS as follows;

i) bond Fibonacci model (BFM):

$$\begin{cases}\varepsilon_i=\varepsilon & for\ all\ i\\ t_{i,i\pm1}=t_A\ or\ t_B\end{cases}$$

ii) site Fibonacci model (SFM):

$$\begin{cases}\varepsilon_i=\varepsilon_A\ or\ \varepsilon_B\\ t_{i,i\pm1}=t & for\ all\ i\end{cases}$$

iii) mixing Fibonacci model (MFM):

$$\begin{cases}\varepsilon_i=\varepsilon_A\ or\ \varepsilon_B\\ t_{i,i\pm1}=t_{AA}\ or\ t_{AB}(=t_{BA})\end{cases}$$

Numerical calculations of products of t-matrices in general are unstable, and this is due to the very fast increase of the exponential part, which causes to overflow the calculations and thus the loss of all the information. Our calculations show that the double-precision numerical calculations are not sufficient to obtain the reliably accurate results. In this case, one has to apply the quadruple-precision in the numerical results. To overcome these problems and saving the CPU time, we rewrite the matrix $M(E)=M_N M_{N-1}\cdots M_2 M_1$ according to FS. In our models, there are actually four different local t-matrices $M_i(E)$, since the hopping integrals depend on three subsequent elements in the FS. Nevertheless, the t-matrix product can be rewritten in terms of two matrices as follows;

$$M_a=\begin{pmatrix}\frac{E-\varepsilon_A}{t_{AB}} & -\gamma\\ 1 & 0\end{pmatrix}\begin{pmatrix}\frac{E-\varepsilon_A}{t_{AA}} & -\gamma^{-1}\\ 1 & 0\end{pmatrix}\begin{pmatrix}\frac{E-\varepsilon_B}{t_{AB}} & -1\\ 1 & 0\end{pmatrix}$$

$$M_b=\begin{pmatrix}\frac{E-\varepsilon_A}{t_{AB}} & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\frac{E-\varepsilon_B}{t_{AB}} & -1\\ 1 & 0\end{pmatrix} \qquad (9)$$

where $\gamma=\frac{t_{AA}}{t_{AB}}$ and $t_{BA}=t_{AB}$ is set. Thus, the resulting t-matrix product is again arranged according to the FS. Therefore we only need to know the first three matrices $R_1=M_a$, $R_2=M_bM_a$ and $R_3=M_aM_bM_a$. Making use of these matrices, we can translate the atomic sequence $ABAAB\cdots$ describing the topological order of the FC to the t-matrix sequence $\cdots M_bM_aM_aM_bM_a$.

Setting $\varepsilon_A=\varepsilon_B=0$ and $t_A=-t_B=(\frac{\sqrt{5}-1}{2})t$ (golden mean τ_0), our numerical results for a BFM has been shown in figure 2. In this paper, we restrict the magnitude of the hopping integrals to the particular values of $\pm\tau_0$ in the numerical calculations, as it is the mostly used one in the literature. Figure 2(a) illustrates the density of states (DOS) of a BFM lattice of generation $n=15$ with 987 atoms that embedded in a periodic chain with 5×10^4 of identical atoms connected by hopping integrals t = 1. Considering the self-similarity in the energy spectra of Fibonacci systems and using their energy eigenvalues, one may write the following expression for the DOS of these systems [25];

$$\rho(E)=\begin{cases}\frac{1}{E_{i+1}-E_i} & if\ \ i=1\ \ and\ \ \frac{N}{2}+1\\ \frac{1}{E_i-E_{i-1}} & if\ \ i=\frac{N}{2}\ \ and\ \ N\\ \frac{2}{E_{i+1}-E_{i-1}} & otherwise\end{cases} \qquad (10)$$

Using the on-site energies $\{\varepsilon_i\}$ and the corresponding hopping integrals $\{t_{i,i\pm1}\}$ according to the FS, we have

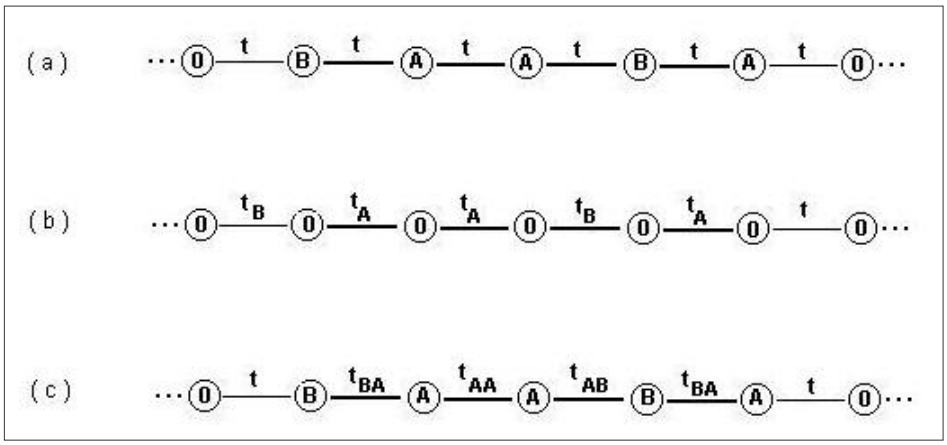

Figure 1. A schematic representation of typical Fibonacci chains. (a) the site Fibonacci, (b) the bond Fibonacci and (c) the mixing Fibonacci models of generation $n=4$ are connected to two semi-infinite periodic chains with $\varepsilon=0$ and $t=1$. The parameters $t_{i,j}$ ($i,j=A$ or B) and letters A and B have described in the text.

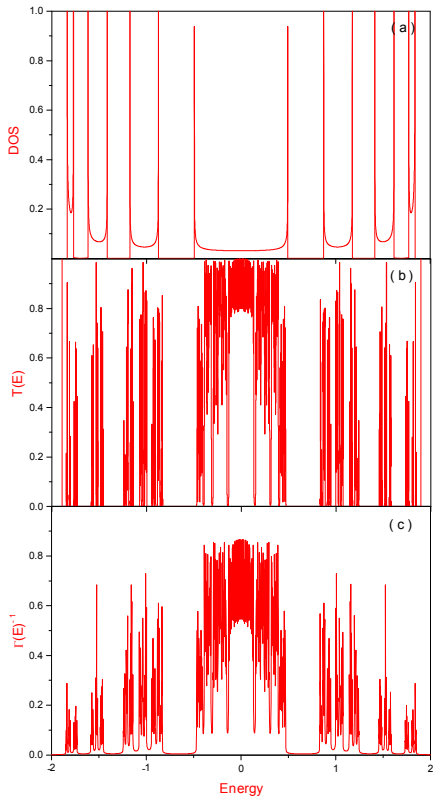

Figure 2. (a) the electronic density of states (DOS), (b) transmittance $T(E)$ and (c) the inverse of *Lyapunov* exponent $\Gamma(E)$ for a bond Fibonacci system of generation $n=15$ is connected to two semi-infinite periodic chains with 5×10^4 identical atoms. $\varepsilon_A=\varepsilon_B=0$ and $t_A=-t_B=(\frac{\sqrt{5}-1}{2})t$ have been considered.

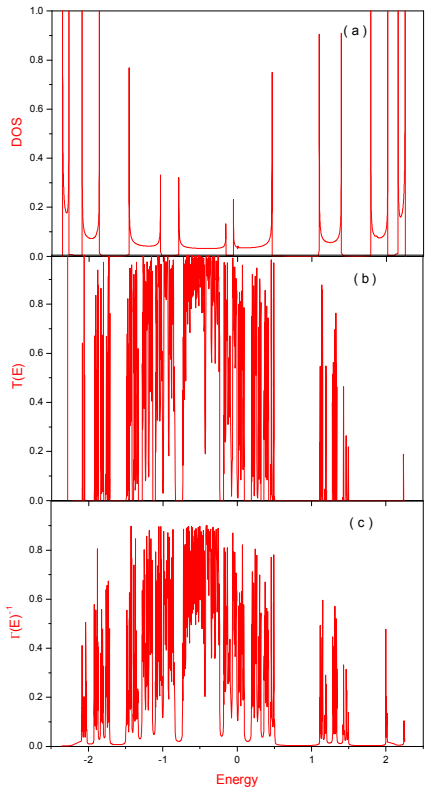

Figure 3. (a) the electronic density of states (DOS), (b) transmittance $T(E)$ and (c) the inverse of *Lyapunov* exponent $\Gamma(E)$ for a mixing Fibonacci system of generation $n=15$ is connected to two semi-infinite periodic chains with 5×10^4 identical atoms. $\varepsilon_A=-\varepsilon_B=0.25t$, $t_{AA}=-t_{AB}=(\frac{\sqrt{5}-1}{2})t$ and $t_{BA}=t_{AB}$ have been considered.

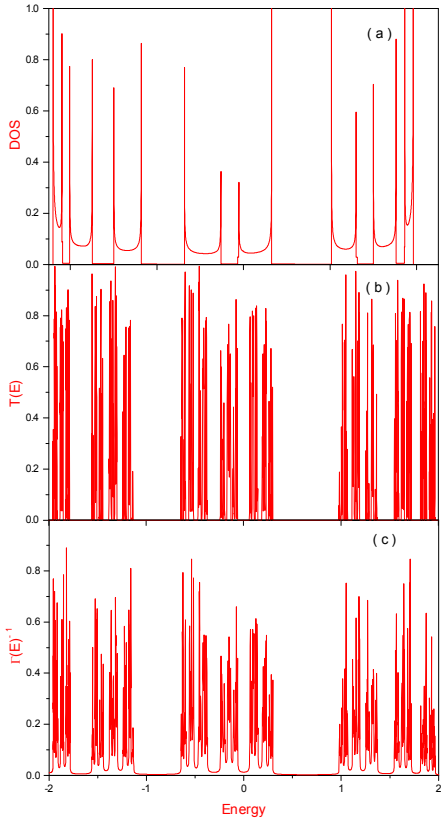

Figure 4. (a) the electronic density of states (DOS), (b) transmittance $T(E)$ and (c) the inverse of *Lyapunov* exponent $\Gamma(E)$ for a site Fibonacci system of generation $n=15$ is connected to two semi-infinite periodic chains with 5×10^4 identical atoms. $\varepsilon_A=-\varepsilon_B=0.5t$, $t_{AA}=t$ and also $t_{AB}=t_{BA}=t$ have been considered.

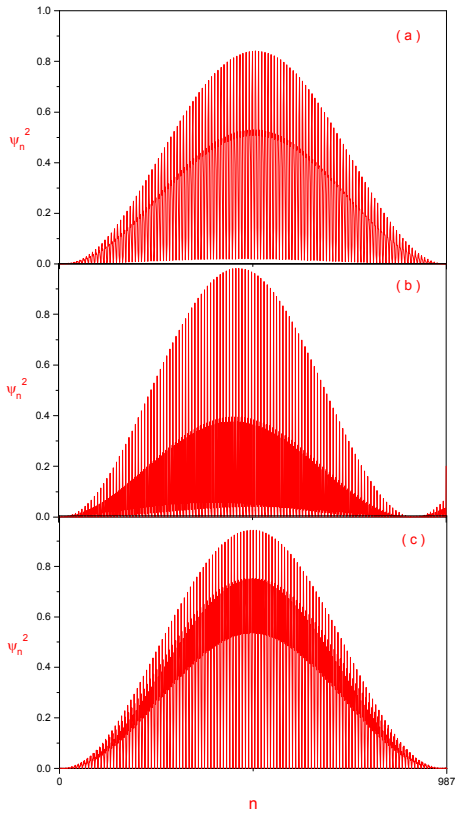

Figure 5. The magnitude of the wave functions $|\psi_n|^2$ in Fibonacci lattices with $N=F_{15}$ atoms. (a) $|\psi_{15}|^2$ for a bond Fibonacci model around the Fermi level, $E_f=0$ and at the eigenvalue number 493. (b) $|\psi_{15}|^2$ for a mixing Fibonacci model around the Fermi level, $E_f=-0.431eV$ and at the eigenvalue number 391 and (c) $|\psi_{15}|^2$ for a site Fibonacci model around the Fermi level, Eq= 0.468eV and at the eigenvalue number 370.

applied the *Lanczos* procedure to the Hamiltonian (1) with the periodic boundary conditions and the resulting energy spectrum was used to calculate the electronic DOS from eq. (10). Figures 2(b) and 2(c) show the transmittance $T(E)$ and the inverse of the *Lyapunov* exponent $\Gamma(E)$ (localization length), respectively for the BFM chain. As expected, the spectra are fully self-similar, i.e., the peak clusters and the gaps are arranged in a very similar way. In fact, the self-similarity in transmittance spectrum and thereby in the inverse of $\Gamma(E)$ is the reflection of the existence of self-similarity in the corresponding energy spectrum. Figure 2(c), with remarkable coincidence with figure 2(b), shows that the electronic eigenstates associated to the corresponding energy eigenvalues are non-localized and from point of view of electron conduction, these eigenstates are extended. However, in order to obtain a complete picture of an extended state, it is necessary to calculate the magnitude of the electronic wave functions at the position of atoms in the FC. Considering the corresponding system of figure 2, we have calculated the magnitude of wave function $|\psi_n|^2$ for energy eigenvalue E, which locates around the Fermi level. Figure. 5(a) shows $|\psi_n|^2$ at the eigenvalue number 493 (close to Fermi level, $E_f=0$) for a BFM lattice of generation $n=15$ with 987 atoms. We see from this figure that the calculated wave function is fully self-similar and

delocalized, as expected. In the literature, this delocalized state around the Fermi level is called the transparent state [14,26]. The same analysis as in figure 2 is applied to a MFM chain of generation $n=15$ with 987 atoms, in which $\varepsilon_A=-\varepsilon_B=0.25t$, $t_{AA}=-t_{AB}=(\frac{\sqrt{5}-1}{2})t$ and $t_{BA}=t_{AB}$ have been chosen. The results of this analysis are shown in figure 3. Notice that the spectra lose their symmetry around $E=0$, since the lattice is not bipartite. In this case the transparent state locates at $E_f=-0.431eV$ and the general behavior observed in figure 2 is also present here. In particular, the wave function behavior at eigenvalue number 391, as shown in figure 5(b), resembles the similar case as in figure 5(a). Finally, we have shown the similar results for a SFM chain in figures 4 and 5(c), in which $\varepsilon_A=-\varepsilon_B=0.5t$, $t_{AA}=t$ and $t_{AB}=t_{BA}=t$ have been considered.

5. Summary and conclusions

In summary, we have studied in details the electronic properties of three Fibonacci model chains. Based on t-matrix technique, *Landauer* formalism and *Lanczos* algorithm procedure, we have investigated the localization properties of eigenstates in these systems. Calculating the *Lyapunov* exponent and the magnitude of wave functions at atomic positions, we have demonstrated the existence of a transparent (extended) state with a transmission coefficient close to unity at the Fermi level, $E_f=0$ for the BFM, $E_f=-0.431eV$ for the MFM and at the $E_f=-0.468eV$ for the SFM. Our results also show the presence of fully self-similarity in the spectra of these Fibonacci chains.

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