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The nature of the phonon eigenstates in quasiperiodic chains (the role of Fibonacci lattices)

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Abstract

Using the forced oscillator method (FOM) and the transfer-matrix technique, we numerically investigate the nature of the phonon states and the wave propagation, in the presence of an external force, in the chains composed of Fibonacci lattices of type site, bond and mixing models, as the quasiperiodic systems. Calculating the *Lyapunov* exponent and the participation ratio, we also study the localization properties of phonon eigenstates in these chains. The focus is on the significant relationship between the transmission spectra and the nature of the phonon states. Our results show that in the presence of the Fibonacci lattices, at low and medium frequencies the spectra of the quasiperiodic systems are not much different from those of the periodic ones and the corresponding phonon eigenstates are extended. However, the numerical results of the calculations of the transmission coefficient $T(\omega)$, the inverse *Lyapunov* exponent $\Gamma(\omega)^{-1}$ and the participation ratio $PR(\omega)$ show that at high frequencies, in contrast with similar ones in disordered systems, the phonon eigenstates are delocalized.

Keywords: Fibonacci lattice, forced oscillator method, transfer-matrix technique, phonon density of states, wave transmission

1. Introduction

Since the discovery of the quasicrystalline phase [1], much attention has been devoted to the quasicrystal materials. The lack of translational symmetry in quasicrystals means the non-applicability of Bloch's theorem. For ordinary periodic lattice crystals, the oscillations of the atoms around their equilibrium positions can be described in terms of elementary excitations, the phonons. These are propagating waves with a well-defined frequency and wave vector. The motion of particles connected by a lattice translation and moving in one mode differs only by a phase factor in going from one unit cell to another. Therefore the vibrational modes are extended, in contrast with the localized modes that one sometimes finds in disordered systems [2]. If there is no lattice periodicity, there is no proper Brilloun zone. This leads to the question of whether in such systems there are also propagating waves, and what the difference is in the dynamics of lattice periodic and quasiperiodic systems. In particular, one may ask about the character of the vibrational spectrum and the existence of the extended and localized modes. Since quasicrystals exhibit an intermediate character between crystals and amorphous solids, the electronic and dynamical properties of these materials are expected to display new behavior. Experimentally, the building of artificial multilayers structures by molecular beam epitaxy [3], has considerably stimulated the theoretical study of the physical properties of quasiperiodic systems [4,5]. In the past years, most of the theoretical works on the quasicrystalline model systems has been focused on the study of the electronic properties [6-14]. There has also been significant progress in determining their structural and static properties [15-17], but the knowledge on their dynamical properties is still limited and little attention has been paid to the phonon modes in these systems. As is well known, the phonons determine the fundamental properties, such as the wave transmission, heat conduction and other low temperature thermodynamics properties of the underlying material. Theoretically the effects of quasiperiodicity in the vibrational spectra can be studied in the simplest quasiperiodic structure which is a Fibonacci lattice (FL).

In this paper we have numerically studied the phonon states in FLs subjected to a periodic external force. The site, bond and mixing Fibonacci model lattices are considered. Embedding the considered Fibonacci lattice in an infinite uniform harmonic chain, we calculate the phonon density of states (DOS) and the transmission coefficient, $T(\omega)$ for waves propagating through this chain. The results of DOS and $T(\omega)$ show that at low and medium frequencies, this system behaves nearly the same as the periodic one, but there are some structures at the upper edge of the spectrum. To study the nature of the phonon states in such systems we perform the calculation of the $\Gamma(\omega)$ and $PR(\omega)$ for the full range of the spectrum. The results indicate that, in contrast with the disordered systems, the phonon eigenstates at the upper edge of the spectrum are not localized. Calculating the *Lyapunov* exponent and participation ratio, we also investigate the localization properties of phonon eigenstates at the range of low and high frequencies in the Fibonacci model lattices.

The formalism we have applied in this work is based on the forced oscillator method (FOM) [18,19] and transfer-matrix (t-matrix) technique, which are powerful procedures for the study of large systems. As compared with the conventional methods, such as *Lanczos* [20,21] or *Householders* [22] method, the FOM offers a quite different scheme for computing the eigenvalues and the corresponding eigenvectors of large-scale matrices. The FOM utilizes the principle of Hamilton mechanics; a harmonic lattice dynamically driven by a periodic external force of frequency Ω will respond with large amplitudes in those eigenmodes close to this frequency [18]. In this method the eigenvalue analysis is reduced to the solution for the time development of the equations of motion. Particular advantages of the FOM lie in its simplicity, speed and memory efficiency. A complete formalism and discussion of this method may be found in Refs. [19,23]. The FOM has been applied in various fields, such as computing the linear response functions [24], phonon lacalization in disordered systems [23], to determine the band-edge structure of $\pm J$ spin glass model [25], the eigenvalues analysis and the spectral densities [19]. We have applied the FOM to study the dynamical properties of uniform harmonic chains in the presence of Fibonacci model lattices. The focus is on the nature of the phonon eigenstates in these systems.

The outline of the paper is as follows: in Sec.(2) we give a general introduction of a Fibonacci lattice and then describe our models for construction of these systems. In Sec.(3) the methodology to calculate the phonon DOS, the global t-matrix of the system, the transmission coefficient, the *Lyapunov* exponent and the participation ratio in FLs is described. The results and discussion are presented in Sec.(4) followed by a summary and conclusions in Sec.(5).

2. Fibonacci lattice

There are several ways to generate a Fibonacci system [26-28]. In this work, to investigate the dynamical properties of a FL, we have constructed; *i*) a bond Fibonacci model (BFM) in which the masses are the same and the springs, k_A and k_B are organized following the Fibonacci sequence (FS). *ii*) a site Fibonacci model (SFM) containing two different masses m_A and m_B. These masses are coupled together by the identical springs and organized following the FS along the lattice. *iii*) a mixing Fibonacci model (MFM) in which two kinds of masses m_A and m_B are arranged following the FS. In this model the arrangement of the springs between masses depends on the nature of them giving rise to the two different parameters k_{AA} and $k_{AB} = k_{BA}$.

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 then 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 FLs as the simplest one-dimensional quasicrystals are the most intensively studied and many concepts on their physical properties are now well established [6,29]. The quasiperiodicity of the FLs is characterized by the golden mean $\tau_0 = \frac{\sqrt{5}-1}{2}$ [30]. 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. These structures are connected to two semi-infinite periodic harmonic chains with identical masses m_0 and spring constants k_0.

3. Methodology

Here a short description is given of the two powerful numerical methods particularly suitable to treat physical systems with much large size, the forced oscillator method (FOM) and transfer-matrix technique.

3.1. The forced oscillator method

Consider a set of N atoms are coupled together by linear springs in the presence of a periodic external force having frequency Ω. The equations of motion of the system are given by;

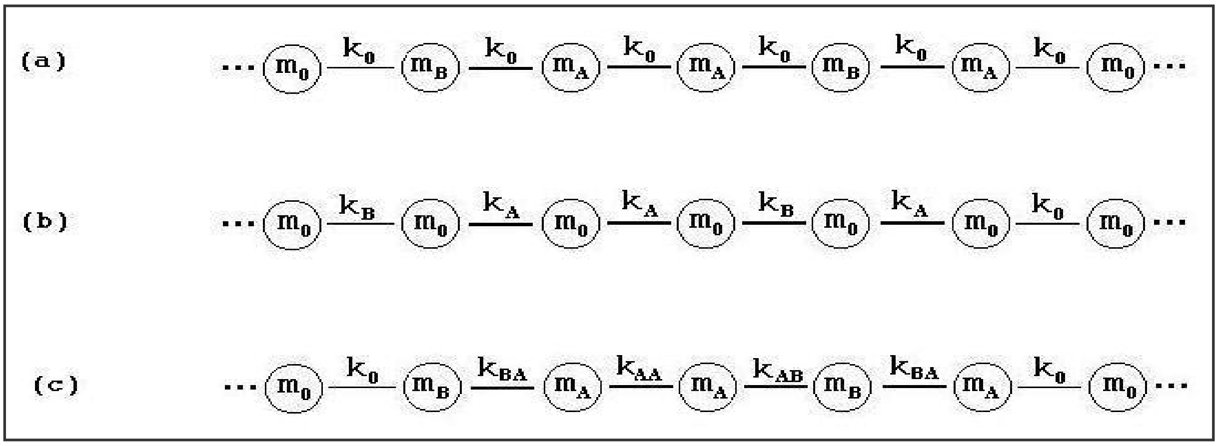

Figure 1. A schematic representation of typical Fibonacci lattices. (a) the site Fibonacci, (b) the bond Fibonacci and (c) the mixing Fibonacci models of generation $n=4$ are connected in both ends to two semi-infinite periodic chains with masses m_0 and the corresponding springs with the strength of k_0. The parameters m_{ij} and $k_{i,j}$ ($i,j=A$ or B) and letters A and B have described in the text.

$$m_i\ddot{u}_i(t)=-\sum_j k_{ij}u_j(t)+f_i\cos(\Omega t)\ , \quad (1)$$

where m_i and $u_i(t)$ are the mass and displacement of the ith atom and k_{ij} describes the strength of the spring coupling atoms i and j. The amplitude of the external force is;

$$f_i=f_0\cos(\varphi_i)\ , \quad (2)$$

where f_0 is a constant and φ_i is a random number distributed uniformly from 0 to 2π. The displacements $u_i(t)$ can be decomposed into a set of eigenmodes according to [23];

$$u_i(t)=\sum_\lambda Q_\lambda(t)\frac{e_i(\lambda)}{\sqrt{m_i}}\ , \quad (3)$$

where $Q_\lambda(t)$ and $e_i(\lambda)$ are the amplitude and the eigenvector of the mode λ, respectively. The external force excites only the eigenmodes close to its frequency Ω. After sufficient time development, the energy of the system averaged over random number φ_i is expressed as;

$$\langle E\rangle=\frac{f_0^2}{4}\sum_\lambda\frac{\sin^2[(\omega_\lambda-\Omega)/2]t}{(\omega_\lambda-\Omega)^2}=\frac{f_0^2\pi t}{8}\sum_\lambda\delta(\omega_\lambda-\Omega). \quad (4)$$

The problem thus reduces to obtain the time development of the equations of motion of the system in the presence of the external force. By discretizing time t with a step τ, the equations become;

$$v_i(n+1)=v_i(n)+\frac{\tau}{m_i}\sum_j k_{ij}u_j(n)+f_i\cos(\Omega n\tau)$$

$$u_i(n+1)=u_i(n)+v_i(n+1)\tau \quad (5)$$

where the integer n represents the number of time steps, namely, $t=n\tau$. To obtain a fine resolution the step size τ has to be sufficiently small so that for all the modes of the system the condition of $\tau\le\frac{2}{\omega_m}$ is satisfied. In fact, this condition provides a convenient method to determine ω_m, the maximum frequency of the system. Also, in the presence of the external force, it is shown that the real frequencies ω_λ of the eigenmodes are related to the frequency Ω by [23];

$$\omega_\lambda=\frac{2}{\tau}\sin(\frac{\Omega\tau}{2}). \quad (6)$$

Thus, through the following relation one can obtain the phonon DOS in terms of Ω;

$$D(\omega_\lambda)=\frac{8\langle E\rangle\cos(\Omega\tau/2)}{\pi\, n\,\tau f_0^2 N}. \quad (7)$$

3.2. The transfer-matrix technique

We have applied the t-matrix technique to investigate the properties of phonon localization in the Fibonacci model lattices. Let us start by considering a general Fibonacci lattice composed of two kinds of masses, m_A and m_B, which are arranged according to the FS, and coupled by two kinds of springs, k_{AA} and $k_{AB}=k_{BA}$. The Fibonacci lattice in both ends is connected to two semi-infinite periodic linear chains with masses m_0 and corresponding springs with constant k_0. In the absence of the periodic external force, the equations of motion read;

$$(k_{i,i-1}+k_{i,i+1}-m_i\omega^2)u_i=k_{i,i-1}u_{i-1}+k_{i,i+1}u_{i+1}\ . \quad (8)$$

Solving for u_{i+1} we find the t-matrix formulation;

$$\begin{pmatrix}u_{i+1}\\ u_i\end{pmatrix}=\begin{pmatrix}\alpha_i & -\beta_i\\ 1 & 0\end{pmatrix}\begin{pmatrix}u_i\\ u_{i-1}\end{pmatrix}=M_i(\omega)\begin{pmatrix}u_i\\ u_{i-1}\end{pmatrix} \quad (9)$$

where ω is the normal frequency of vibration,

$\beta_i = \dfrac{k_{i,i-1}}{k_{i,i+1}}$, $\alpha_i = (1 + \beta_i - \dfrac{m_i \omega^2}{k_{i,i+1}})$ and $M_i(\omega)$ is the local t-matrix associated with site i. Defining $U_i = \begin{pmatrix} u_i \\ u_{i-1} \end{pmatrix}$ and $M(\omega) = \prod_{i=1}^{N} M_i(\omega)$ as the global t-matrix of the chain, then $U_{N+1} = M(\omega) U_1$ or;

$$\begin{pmatrix} u_{N+1} \\ u_N \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_0 \end{pmatrix} = \prod_{i=1}^{N} M_i(\omega) \begin{pmatrix} u_1 \\ u_0 \end{pmatrix}. \quad (10)$$

Now, to investigate the localization properties of the phonon eigenstates, we proceed with the calculation of the transmission coefficient $T(\omega)$, the *Lyapunov* exponent $\Gamma(\omega)$ and the participation ratio $PR(\omega)$. These are very good quantities refelecting the localization properties of eigenstates in the physical systems and have been used to study the electronic eigenstates in disordered and quasiperiodic systems [8,31-33].

A. The transmission coefficient, $T(\omega)$

Let n_0 and $(n_0 + F_n)$ be the first and the last atom of the Fibonacci lattice (FL) in the infinite chain. F_n, the number of sites on the FL, is the Fibonacci number of generation n. We consider an incoming wave from the left side of the FL with frequency ω. Then in the right hand of the FL there is only outgoing wave. That is;

$$\Psi_{Left}^{(j)} = C_1 e^{i(\omega t + q r_j)} + C_2 e^{-i(\omega t + q r_j)} \qquad for \quad j \le n_0$$

$$\Psi_{Right}^{(j)} = C_3 e^{i(\omega t + q r_j)} \qquad for \quad j \ge (n_0 + F_n) \quad (11)$$

where q is a positive integer and $r_j = ja$, with $a = 2\pi\tau_0$ on the FL and is consider to 1 on the periodic sides. It is well known that $T(\omega) = \left| \dfrac{C_3}{C_1} \right|^2$ is identical to the probability that an incoming wave with frequency ω in the left-hand side emerges in the right-hand of the FL. Using Eq.(10) and follow the procedure of Ref.[30], we obtain;

$$T(\omega) = \frac{4\sin^2(\omega t + qa)}{(Z\cos(\omega t + qa) - Y)^2 + X^2 \sin^2(\omega t + qa)}, \quad (12)$$

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

$$X = m_{11} + m_{22} \quad ;$$
$$Y = m_{21} - m_{12} \quad ;$$
$$Z = m_{11} - m_{22} \quad , \quad (13)$$

where m_{ij} with $i, j = 1, 2$ are the matrix elements of the global t-matrix $M(\omega)$.

B. *The Lyapunov exponent,* $\Gamma(\omega)$

The nature of the vibrational eigenmodes can also be investigated by computing the *Lyapunov* exponent $\Gamma(\omega) = \dfrac{1}{N} \ln \| M(\omega) \|$ [30], where $\| \; \|$ denotes the modulus of the matrix $M(\omega)$. Using the matrix elements of $M(\omega)$ via Eq.(10), we can easily write $\Gamma(\omega)$ as follows;

$$\Gamma(\omega) = \frac{1}{N} \ln \sqrt{m_{11}^2 + m_{12}^2 + m_{21}^2 + m_{22}^2} \; . \quad (14)$$

The *Lyapunov* exponent $\Gamma(\omega)$ characterizes the evolution of a phonon eigenmode along the chain. $\Gamma(\omega)$ is zero for an extended or critical state, but is positive for a localized state, representing then the inverse of the localization length.

C. *The participation ratio,* $PR(\omega)$

The localization properties of eigenmodes can also be described by the participation ratio [34,35], which is defined by;

$$PR(\omega) = \frac{1}{N} \frac{(\sum_{i=1}^{N} u_i^2)^2}{\sum_{i=1}^{N} u_i^4} \quad , \quad (15)$$

$PR(\omega)$ is almost equal to 1 if the eigenmode is extended and will drop steeply to zero if the eigenmode gets localized. To calculate $T(\omega)$, $\Gamma(\omega)$ and $PR(\omega)$, we apply the time development algorithm of the FOM in the presence of the periodic external force, Eq.(2). Thus according to Ref.[23], we set $t = n\tau$ and $\omega \to \omega_\lambda$, the real vibration frequency.

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 achieve the reliably accurate results. In this case, one has to apply the quadruple-precision in the numerical results. However, 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 $M_i(\omega)$, since the spring constants depend on three subsequent elements in the FS. Thus, the t-matrix product can be rewritten in terms of two matrices as follows;

$$M_a = \begin{pmatrix} \gamma + 1 - \frac{m_A \omega^2}{k_{AB}} & -\gamma \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \gamma^{-1} + 1 - \frac{m_A \omega^2}{k_{AA}} & -\gamma^{-1} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2 - \frac{m_B \omega^2}{k_{AB}} & -1 \\ 1 & 0 \end{pmatrix}$$

$$M_b = \begin{pmatrix} 2 - \frac{m_A \omega^2}{k_{AB}} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2 - \frac{m_B \omega^2}{k_{AB}} & -1 \\ 1 & 0 \end{pmatrix}, \qquad (16)$$

where $\gamma = \frac{k_{AA}}{k_{AB}}$ and $k_{BA} = k_{AB}$ 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 $R_1 = M_a$, $R_2 = M_b M_a$ and $R_3 = M_a M_b M_a$. 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 $\cdots M_b M_a M_a M_b M_a$.

4. Results and discussion

In our models, the masses $\{m_i\}$ and the hopping integrals $\{k_{i,i\pm1}\}$ along the FL are chosen according to FS as follows;

i) site Fibonacci model (SFM):

$$\begin{cases} m_i = m_A \text{ or } m_B \\ k_{i,i\pm1} = k_0 \quad \text{for all } i \end{cases}$$

ii) bond Fibonacci model (BFM)

$$\begin{cases} m_i = m_0 \quad \text{for all } i \\ k_{i,i\pm1} = k_A \text{ or } k_B \end{cases}$$

iii) mixing Fibonacci model (MFM):

$$\begin{cases} m_i = m_A \text{ or } m_B \\ k_{i,i\pm1} = k_{AA} \text{ or } k_{AB} (= k_{BA}) \end{cases}$$

In this work we describe our numerical results about the SFM and MFM lattices. We find the similar results for the BFM lattices. However, in order to shorten the discussions, these results are not mentioned here. Using eqs.(6) and (7), we have calculated the phonon DOS for the harmonic chains composed of type SFM and MFM lattices. Figure 2(a) illustrates the DOS for a periodic chain with the identical masses m_0 which are connected to the linear springs k_0 . Setting $m_A = \tau_0$ (golden mean value), $m_B = 1$ and $k_{AA} = k_{AB} = k_0$, figure 2(b) shows the DOS in the presence of a SFM lattice of generation $n = 16$ with 1597 atoms that embedded in the periodic chain with 5×10^4 of identical masses $m_0 = 3$ connected by the springs $k_0 = 1$. Also figure 2(c) shows the numerical results of the DOS for a chain composed

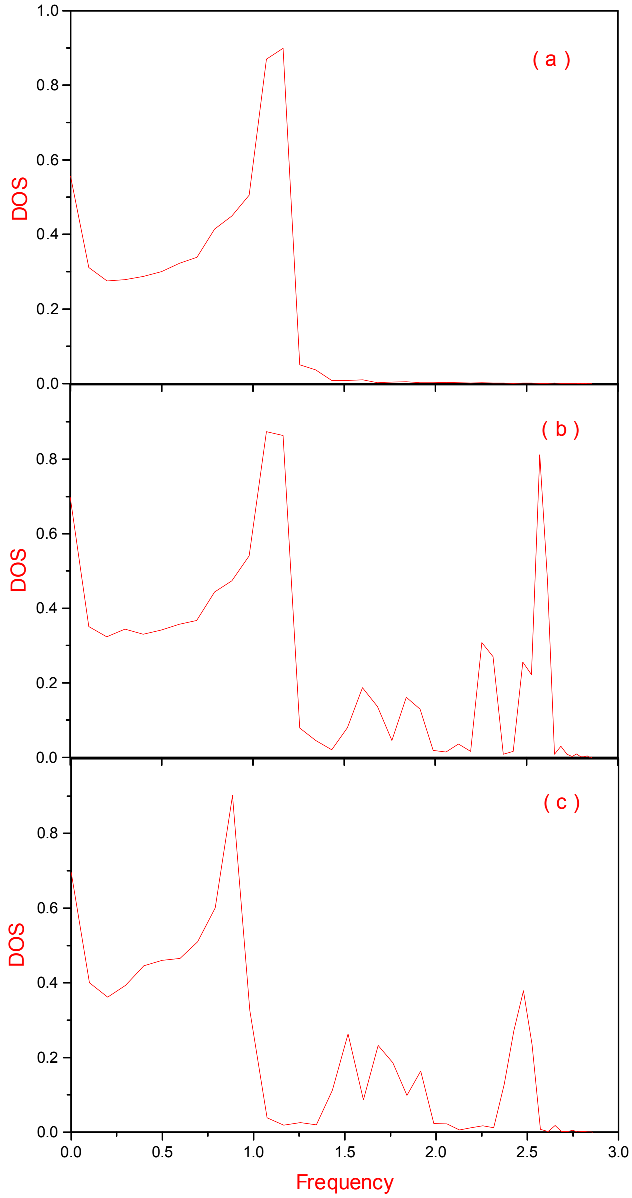

Figure 2. The phonon density of states (DOS) for (a) a linear periodic harmonic chain with masses $m_0 = 3$ and the corresponding springs with the strength of, $k_0 = 1$ (b) a SFM lattice of generation $n = 16$ is connected in both ends to two semi-infinite periodic chains with 5×10^4 identical atoms. Values of $m_A = \tau_0$, $m_B = 1$ and $k_{AA} = k_{AB} = k_0$ have been considered. Panel (c) shows the DOS for a MFM lattice of generation $n = 16$ with parameters $m_A = \tau_0$, $m_B = 1$, $k_{AA} = 1 + \tau_0$ and, $k_{AB} = k_{BA} = \tau_0$ as described in the text.

of a MFM lattice of generation $n = 16$. In this figure $m_A = \tau_0$, $m_B = 1$, $k_{AA} = 1 + \tau_0$ and $k_{AB} = k_{BA} = \tau_0$ have been considered. Following Sec.(2), we restrict the ratio of m_A / m_B and the magnitudes of the spring constants to the particular values τ_0 and $1 + \tau_0$ in the numerical calculations.

As we can see from the figure 2, at low and medium frequencies the spectra are not much different from those

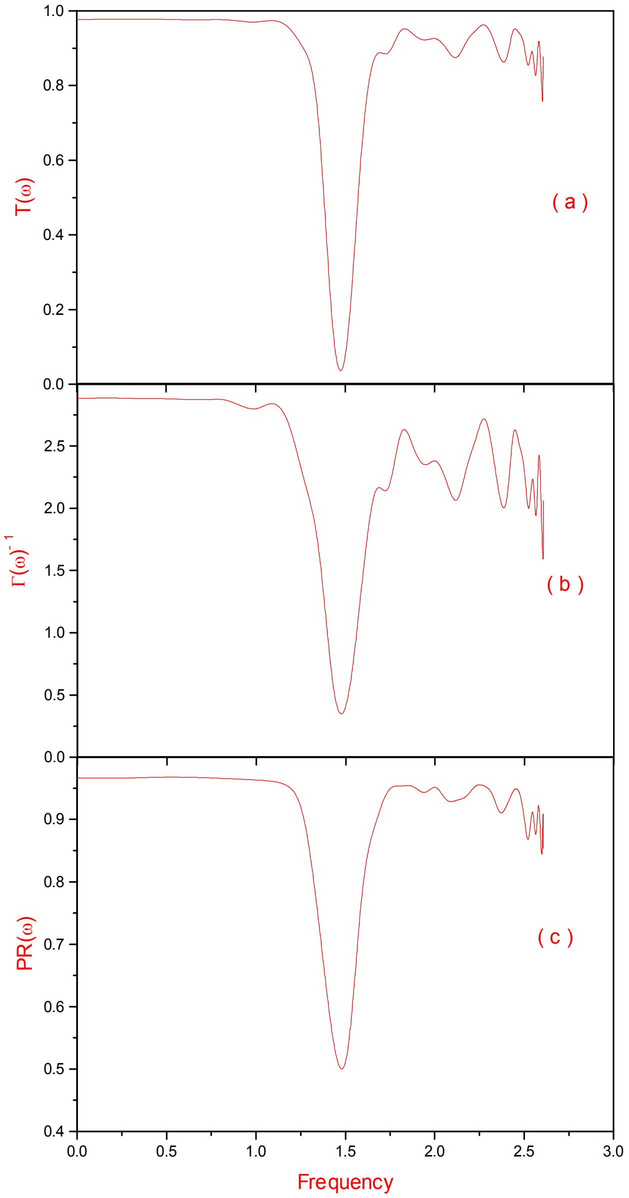

Figure 3. Plots (a)-(c) show the transmission coefficient, $T(\omega)$ the inverse of the *Lyapunov* exponent $\Gamma(\omega)^{-1}$ (the localization length) and the participation ratio $PR(\omega)$ for a SFM lattice with the same parameters as the figure 2(b), respectively.

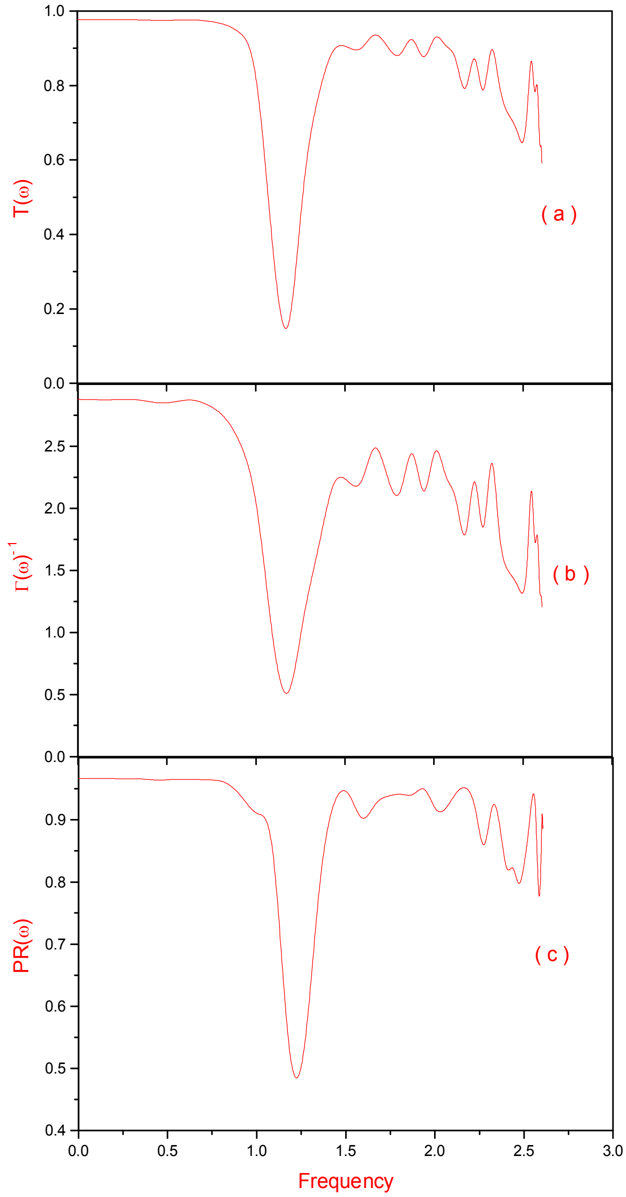

Figure 4. Plots (a)-(c) show the transmission coefficient, $T(\omega)$ the inverse of the *Lyapunov* exponent. $\Gamma(\omega)^{-1}$ (the localization length) and the participation ratio $PR(\omega)$ for a MFM lattice with the same parameters as the figure 2(c), respectively.

of the uniform periodic systems. The occurrence of some structures at the upper edge of the spectrum reflects the effects of the presence of the embedded Fibonacci lattice on the phonon eigenstates of the large periodic chain. Thus, at low and medium frequencies, i.e., in the frequency range of $\omega < 1.5$ in figure 2(b) and $\omega < 1.25$ in figure 2(c), the phonon eigenstates are extended. Our further investigations of the numerical results of the calculations of the transmission coefficient $T(\omega)$, the inverse *Lyapunov* exponent $\Gamma(\omega)^{-1}$ and the participation ratio $PR(\omega)$ show that at the upper edges of the spectrum, the phonon eigenstates in these chains are delocalized.

Figure 3 shows the numerical results of the $T(\omega)$, $\Gamma(\omega)^{-1}$ and the $PR(\omega)$ corresponding to figgure.2(b) for the SFM lattice with the same parameters. It is well known that these quantities correctly describe the localization properties of the energy and frequency spectra. Our results of calculations of $T(\omega)$, $\Gamma(\omega)^{-1}$ and the $PR(\omega)$ suggest that the phonon eigenstates of the harmonic chain in presence of a SFM lattice, especially at high frequencies are not localized and comparatively have the features of the extended states. At low and medium frequencies these quantities reflect the characterizations of the extended eigenstates in the periodic chain, as at the low and medium frequencies in figure 2. In figure 4 we have also shown the similar results of calculation of $T(\omega)$, $\Gamma(\omega)^{-1}$ and the $PR(\omega)$ due to a MFM lattice corresponding to figure 2(c) with the same parameters. As we can see $T(\omega)$, $\Gamma(\omega)^{-1}$ and the $PR(\omega)$ show similar characterizations, in particular at high frequencies. This figure also suggests that the phonon eigenstates in the chains composed of MFM lattices, at high frequencies are delocalized.

5. Summary and conclusions

In summary, we have studied in details the phonon properties of the harmonic chains composed of Fibonacci lattices. Based on the forced oscillator method (FOM) and transfer-matrix technique, we have investigated the localization properties of phonon eigenstates for harmonic periodic chains in the presence of Fibonacci lattices of types site, bond and mixing models. Calculating the transmission coefficient $T(\omega)$, the inverse *Lyapunov* exponent $\Gamma(\omega)^{-1}$ and the participation ratio $PR(\omega)$, we have demonstrated, in contrast with similar ones in disordered systems, the existence of the delocalized phonon eigenstates at high frequencies range in the spectra of these systems.

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