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Dynamical properties of three component Fibonacci quasicrystal

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Abstract. We present a real space renormalization group (RSRG) method to study the lattice dynamics of a three component Fibonacci (3CF) quasicrystal. Phonon dispersion relations corresponding to different models of this lattice are obtained. Some features of the phonon dispersion curves are compared with experiments on real quasicrystal. It is observed that the positions of the strongest Bragg peaks calculated analytically are in perfect agreement with our RSRG calculations.

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

1 Introduction

The discovery of quasicrystal by Shechtman *et al.* [1] triggered the extensive theoretical [2–17] as well as experimental [18–20] researches on various physical properties of semi-periodic [21] systems. Particularly, one-dimensional quasiperiodic or aperiodic lattices have attracted most of the attention. The interest in 1D systems really shot up after the success of Merlin *et al.* [18] in growing model systems, where quasiperiodicity or aperiodicity is built up. Most of these studies are concerned with the electronic, optical and phonon properties of the substitutional quasiperiodic or aperiodic structures. The studies of such self-similar systems are also meaningful from both theoretical and experimental point of views. From experimental side, it has been possible to construct Fibonacci [18] and Thue-Morse [19], etc., superlattices by epitaxial growth method. These artificial superlattices are a new kind of solids usually grown by depositing very thin (10 nm) layers of two or more constituent materials (say GaAs-AlAs). Thus an aperiodicity is introduced by arranging two layers of materials according to some substitutional sequences (for example, Fibonacci, Thue-Morse, etc., sequences) in the z-direction. A lot of various kinds of experiments have been performed on these superlattices. The varieties of all these theoretical and experimental studies give some exotic physical properties [2] like Cantor-set energy spectrum, critical wavefunction and scaling behavior of the integrated density of states, etc., which are completely different from crystalline or amorphous solids.

Besides the studies of the electronic and phonon properties of these materials, comparatively less works have been done to study the dynamical response function of the quasiperiodic or aperiodic lattices. The main difficulty to tackle these types of problems, is understandably the absence of translational invariance. Because of the lack of translational symmetry, we can not use Bloch theorem here. Therefore, we are to take help of the other procedures like trace map [2] technique and real space renormalization group (RSRG) method. A large number of theoretical works have used the trace map technique. Another powerful tool is the RSRG method. RSRG technique can be successfully used exploiting the self-similar properties of the quasicrystals to calculate the electronic density of states, the dynamic response function and the localization length, etc., of these lattices. We know that the dynamic structure factor $S(q,\omega)$ is a very important physical quantity because it is directly related to the inelastic neutron scattering cross-section and it also gives the excitation modes of the system [22,23]. Patel and Sherrington [24] worked out $S(q,\omega)$ for a ferromagnetically coupled spins on a finite 2D Penrose lattice. Ashraff and Stinchcombe [25] and Ashraff *et al.* [26] derived an analytical expression for $S(q,\omega)$ for a 1D Fibonacci chain using generating function approach. The main results of their derivation are that the magnon dispersion consists of a main branch along with many satellite branches of much weaker intensity. There are well defined propagating modes for small wavevector separated by a set of gaps from the stripes of the dispersion less modes at higher frequencies. Using spectral moment method Benoit *et al.* [27] rediscovered similar characteristics in a Fibonacci quasilattice. Karmakar *et al.* [28] developed a real space renormalization group (RSRG) method to calculate $S(q,\omega)$ for phonon on a Fibonacci chain. Consequently, Ghosh and Karmakar [29] calculated $S(q,\omega)$ for a period doubling lattice.

Most of the theoretical models use the tight-binding Hamiltonians to calculate the electronic properties of the

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two component quasiperiodic [2,30–33] or aperiodic [34] lattices. In the literature, there are a few works which have considered the three component quasilattices [35,36] as typical examples to investigate their electronic properties and there are some theoretical as well as experimental works on the study of the static structure factor of the three component quasiperiodic Fibonacci [20] lattice. But the investigation of the dynamic structure factor of the three component quasiperiodic lattices, to the best of our knowledge, has not been attempted so far. Therefore, the theoretical model for studying the three component quasiperiodic systems is worthwhile as we know that all the thermodynamically stable real quasicrystals are ternary alloys (AlMnPd, etc.). The experimental X-ray spectra of the quasicrystal are found to give the bright Bragg diffraction peaks at the theoretically predicted values of q_{mn}, where m and n are integers. For example, in case of the two component Fibonacci lattice the brightest Bragg peaks are situated at $q_{mn} = \frac{2\pi}{D}(m + n\tau)$. D is the average lattice spacing $= (\tau d_A + d_B)/\tau^2$, where d_A and d_B are respectively the thicknesses of A and B layers arranged according to a Fibonacci lattice. τ is golden mean ratio $= (1+\sqrt{5})/2$. Apart from the static structure factor, another important physical quantity, which gives the dynamical properties of a crystal or quasicrystal is $S(q,\omega)$ because it is directly related to the inelastic differential scattering cross section. And so the results of our theoretical calculation of the dynamic structure factor can be compared with the experimental findings. Moreover, it is easy to find the phonon spectrum from the study of the dynamic structure factor $S(q,\omega)$.

In this paper, we have exploited the self-similar property of the three component Fibonacci (3CF) quasicrystal to calculate the static and the dynamic structure factor by applying the real space renormalization group (RSRG) method. This method also helps us to find the phonon dispersion relation and the allowed eigenmodes for this 3CF lattice. The allowed phonon modes can also be found by solving the trace map equation, first developed by Kohmoto *et al.* [2]. The trace map is a polynomial of eigen modes and in the periodic approximants method [2], the degree of the polynomial increases as the number of size of the approximant increases. Therefore, it is difficult to solve the trace map equation for large system size. And in the infinite limit, it is practically impossible to solve the trace map equation. But from the calculation of the dynamic structure factor, we can easily find the phonon spectrum. The most important results of this work are that the phonon spectrum consists of an infinite number of densely populated gaps and pseudo Brillouin zone boundaries observed by experiments on real quasicrystals. The dispersion less modes in the optical branch of the phonon spectrum are another interesting observations found experimentally by Goldman *et al.* [37] and Boudard *et al.* [38].

The paper has been organized as follows. In Section 2 we describe the lattice and the model. Section 3 briefly discusses the major point of the real space renormalization group (RSRG) technique to calculate the dynamic response function. The results and the discussions are presented in Section 4. Finally we conclude in Section 5.

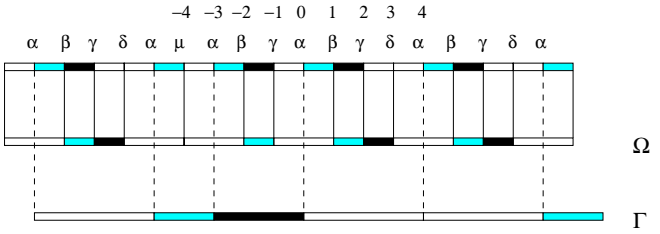

Fig. 1. Portion of an infinite three component Fibonacci (3CF) chain illustrating the decimation scheme. The original lattice is split into two equivalent self-similar Ω and Γ sublattices. The white, dotted and black bars represent A, B and C bonds respectively.

2 The lattice and the model

Three component Fibonacci (3CF) lattice [35] can be obtained by the inflation rules $B \to C$, $C \to A$ and $A \to AB$. It can also be constructed using the stacking rule $S_{l+1} = S_l S_{l-2}$ with $S_{-1} = B$, $S_0 = C$ and $S_1 = A$. The total number of elements in any sequence S_{l+1} is $F_{l+1} = F_l + F_{l-2}$ with $F_{-1} = F_0 = F_1 = 1$. The number of A in any sequence S_l is F_{l-1}, that of B is F_{l-2} and the number of C is F_{l-3}. If N_l^A and N_l^B be the number of A and B respectively in any sequence S_l then the ratio N_l^B/N_l^A is $F_{l-2}/F_{l-1} = \sigma$ (say) in the infinite limit of l (*i.e.*, $l \to \infty$). Similarly $N_l^C/N_l^A = \sigma^2 = F_{l-3}/F_{l-1}$. Here σ is the only real root of the algebraic equation $\sigma^3+\sigma-1 = 0$. Now according to the inflation rules $B \to C$, $C \to A$ and $A \to AB$, the first few generations of the three component Fibonacci sequences are B, C, A, AB, ABC, $ABCA$ and so on. If we arrange three kinds of atoms according to a three component Fibonacci sequence, then the lattice is known as the three component Fibonacci lattice. Substitutional matrix corresponding to the transformations $A \to AB$, $B \to C$ and $C \to A$ can be written as a 3×3 matrix with detM$= -1$ as follows

$$\begin{pmatrix} A' \\ B' \\ C' \end{pmatrix} = \begin{pmatrix} 1\ 1\ 0 \\ 0\ 0\ 1 \\ 1\ 0\ 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix}.$$

The characteristic roots of the above transformation matrix satisfy the equation $y^3 - y^2 - 1 = 0$. The only real root y is equal to 1.46557 and the other two imaginary roots are $y_\pm = -0.232786 \pm 0.792552\, I$. To implement the real space renormalization group (RSRG) scheme, we start from a more general model. We take three types of bonds with bond lengths d_A, d_B and d_C arranged according to the three component Fibonacci lattice. Five kinds of masses m_α, m_β, m_γ, m_δ and m_μ are put between the bonds AB, BC, CA, AA and BA respectively (see Fig. 1) and three kinds of spring constants k_A, k_B and k_C corresponding to the A, B and C bonds are taken in our general model of the three component Fibonacci model. The so-called

on-site model can be obtained from our general consideration by putting $m_\alpha = m_\delta = m_A$, $m_\beta = m_\mu = m_B$, $m_\gamma = m_C$ and $k_A = k_B = k_C = k$. The transfer model is obtained by taking $m_\alpha = m_\beta = m_\gamma = m_\delta = m_\mu = m$ and $k_A \neq k_B \neq k_C$. The mixed model is the combination of the transfer and on-site models, *i.e.*, $m_\alpha = m_\delta = m_A$, $m_\beta = m_\mu = m_B$, $m_\gamma = m_C$ and $k_A \neq k_B \neq k_C$.

If we take the spring mass model in the harmonic approximation with nearest neighbor interaction then the equations of motion look like

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

where u_i is the amplitude of eigen modes at the ith lattice site, ω is the phonon angular frequency, $k_{i,i\pm1}$ are the spring constants and m_i is the mass of the ith atom in the lattice. And the single particle Green's functions $G_{ij}(\omega)$ can be written as

$$\epsilon_i G_{ij} = -\delta_{ij} + k_{i,i+1}G_{i+1j} + k_{i,i-1}G_{i-1j}, \tag{2}$$

where $\epsilon_i = k_{i,i+1} + k_{i,i-1} - m_i\omega^2$.

Now the dynamic structure factor $S(q,\omega)$ is defined as

$$S(q,\omega) = \lim_{N\to\infty}\lim_{\delta\to 0} G_N(q,\omega - \mathrm{i}\delta) \tag{3}$$

where

$$G_N(q,\omega) = 1/N\sum_{ij} G_{ij}(\omega)\mathrm{e}^{\mathrm{i}q(r_i - r_j)}. \tag{4}$$

N is the system size and r_i is the distance of ith atom from the origin. It is obvious from equation (4) that for a periodic lattice with lattice parameter b the expression for the dynamic structure factor $S(q,\omega)$ is

$$S(q,\omega) = \mathrm{Im}\left[1/[m(\omega - \mathrm{i}\delta)^2 - 2k + 2k\cos qb]\right]. \tag{5}$$

But for a quasiperiodic system there is no translational symmetry. Therefore, we can not write the expression for the dynamic structure factor $S(q,\omega)$ in a compact form. But we can exploit the self-similar property of the quasiperiodic three component Fibonacci lattice and calculate the dynamic structure factor of the lattice. It will be shown that the calculation of the $S(q,\omega)$ essentially boils down to the iteration of certain recursion relations and the dynamic structure factor can be calculated with arbitrary accuracy.

3 RSRG scheme for the determination of S(q, ω)

Let us now consider the sum $G^i(q,\omega) = \sum_j \mathrm{e}^{\mathrm{i}q(r_i - r_j)}G_{ij}(\omega)$ [29]. This sum is independent of the index i in a periodic system due to translational invariance. However, in case of a quasiperiodic system, it depends on the index i, as no two sites are equivalent in the quasiperiodic lattice and from equation (2) we obtain,

$$\epsilon_i G^i(q,\omega) = -F_i + k_{i,i+1}\mathrm{e}^{-\mathrm{i}q(r_{i+1} - r_i)}G^{i+1}(q,\omega) + k_{i,i-1}\mathrm{e}^{\mathrm{i}q(r_i - r_{i-1})}G^{i-1}(q,\omega) \tag{6}$$

where all F_i's are initially equal to unity. The use of new notations F_i's for representing unity does not directly follow from equation (2). We have introduced these notations by hand and we will see how it facilitates the determination of $S(q,\omega)$ in quasiperiodic lattices. Even though all F_i's are initially same, they will become different upon renormalization. However, from the symmetry of the lattice we observe that there will be only five distinct types of F_i's, and we can identify them as F_α, F_β, F_γ, F_δ and F_μ corresponding to the α, β, γ, δ and μ sites of the lattice.

It is now necessary to determine all $G^i(q,\omega)$'s from equation (6) for finding $G_N(q,\omega)$ and we can write

$$G_N(q,\omega) = (1/N)\sum_i G^i(q,\omega). \tag{7}$$

In the quasiperiodic 3CF chain $G^i(q,\omega)$'s are all distinct and instead of determining them directly from equation (6), we use RSRG technique for evaluating $G^i(q,\omega)$. We split the original chain into two self-similar sublattices Ω and Γ as shown in Figure 1. The Ω-sublattice is obtained by eliminating the sites using the decimation rules $AB \to A$, $C \to B$ and $A \to C$, while the corresponding rules for the Γ-sublattice are $BCA \to A$, $BA \to B$ and $BCA \to C$. Both Γ and Ω sublattices again form two new 3CF chains at some inflated length scale. All the sites of the original three component Fibonacci lattice are distributed among these two sublattices, and thus they are complementary to each other (see Fig. 1). This complementary nature of Ω and Γ sublattices also ensures that no information is lost by introducing this splitting procedure. Now it is possible to generate two sets of renormalized equations for $G^i(q,\omega)$'s, one corresponding to Ω-sublattice while the other for the Γ-sublattice. The equations for Ω-sublattice can be obtained from equation (6) by eliminating all $G^i(q,\omega)$'s belonging to Γ-sublattice and the resulting equations can be cast in the same form as that of the original set of equations (2), provided we rename the sites appropriately and renormalize the parameters as follows,

$$\begin{aligned}
&\epsilon_\alpha^{'} = \epsilon_\beta - k_B^2/\epsilon_\alpha; \quad \epsilon_\beta^{'} = \epsilon_\gamma; \quad \epsilon_\gamma^{'} = \epsilon_\delta - k_A^2/\epsilon_\alpha\\
&\epsilon_\delta^{'} = \epsilon_\mu - k_A^2/\epsilon_\alpha - k_B^2/\epsilon_\alpha; \quad \epsilon_\mu^{'} = \epsilon_\gamma - k_A^2/\epsilon_\alpha\\
&F_\alpha^{'} = F_\beta - F_\alpha k_B\mathrm{e}^{\mathrm{i}qa_B}/\epsilon_\alpha; \quad F_\beta^{'} = F_\gamma\\
&F_\gamma^{'} = F_\delta - F_\alpha k_A\mathrm{e}^{\mathrm{i}qa_A}/\epsilon_\alpha\\
&F_\delta^{'} = F_\mu - F_\alpha(k_A\mathrm{e}^{-\mathrm{i}qa_A} + k_B\mathrm{e}^{\mathrm{i}qa_B})/\epsilon_\alpha\\
&F_\mu^{'} = F_\gamma - F_\alpha k_A\mathrm{e}^{-\mathrm{i}qa_A}/\epsilon_\alpha\\
&k_A^{'} = -k_Ak_B/\epsilon_\alpha; \quad k_B^{'} = k_C; \quad k_C^{'} = k_A\\
&a_A^{'} = a_A + a_B; \quad a_B^{'} = a_C; \quad a_C^{'} = a_A
\end{aligned} \tag{8}$$

Similarly for the Γ-sublattice the recursion relations can be written as,

$$\begin{aligned}
\epsilon_\alpha^{'} &= M - k_A^4/(\epsilon_\alpha^2 X); \quad \epsilon_\beta^{'} = \epsilon_\alpha - k_B^2/M^{'} - k_A^2/\epsilon_\mu \\
\epsilon_\gamma^{'} &= \epsilon_\alpha - k_B^2\epsilon_\beta - k_A^2\epsilon_\gamma - k_B^2k_C^2/(\epsilon_\beta^2 X) - k_A^2k_C^2/(\epsilon_\gamma^2 M^{'}) \\
\epsilon_\delta^{'} &= WA - k_B^2k_C^2/(\epsilon_\beta^2 X) - k_A^4/(\epsilon_\delta X) \\
\epsilon_\mu^{'} &= W^{'} - k_B^2k_C^2/(\epsilon_\beta^2 X) \\
F_\alpha^{'} &= N + k_A^2 Y \mathrm{e}^{2\mathrm{i}qa_A}/(\epsilon_\delta X) \\
F_\beta^{'} &= F_\alpha - k_B N^{'}\mathrm{e}^{-\mathrm{i}qa_B}/M^{'} - F_\mu k_A \mathrm{e}^{\mathrm{i}qa_A}/\epsilon_\mu \\
F_\gamma^{'} &= F_\alpha - F_\beta k_B \mathrm{e}^{-\mathrm{i}qa_B}/\epsilon_\beta - F_\gamma k_A \mathrm{e}^{\mathrm{i}qa_A}/\epsilon_\gamma \\
&\quad + Y k_B k_C \mathrm{e}^{-\mathrm{i}q(a_B+a_C)}/(\epsilon_\beta X) \\
&\quad + k_A k_C N^{'}\mathrm{e}^{\mathrm{i}q(a_A+a_C)}/(\epsilon_\gamma M^{'}) \\
F_\delta^{'} &= ZA + k_B k_C \mathrm{e}^{-\mathrm{i}q(a_B+a_C)}/(\epsilon_\beta X) + k_A^2 Y \mathrm{e}^{2\mathrm{i}qa_A}/(\epsilon_\delta X) \\
F_\mu^{'} &= Z^{'} + Y k_B k_C \mathrm{e}^{-\mathrm{i}q(a_B+a_C)}/(\epsilon_\beta X) \\
k_A^{'} &= -k_A^2 k_B k_C/(\epsilon_\beta\epsilon_\delta X); \quad k_B^{'} = -k_A k_B/\epsilon_\mu \\
k_C^{'} &= k_A k_B k_C/(\epsilon_\gamma M^{'}) \\
a_A^{'} &= 2a_A + a_B + a_C; \quad a_B^{'} = a_A + a_B \\
a_C^{'} &= a_A + a_B + a_C,
\end{aligned} \tag{9}$$

where

$$\begin{aligned}
X &= \epsilon_\gamma - k_A^2/\epsilon_\delta - k_C^2/\epsilon_\beta \\
Y &= F_\gamma - k_A F_\delta \mathrm{e}^{-\mathrm{i}qa_A}/\epsilon_\delta - k_C F_\beta \mathrm{e}^{\mathrm{i}qa_C}/\epsilon_\beta \\
M &= \epsilon_\alpha - k_B^2/\epsilon_\mu - k_A^2/\epsilon_\delta \\
N &= F_\alpha - k_B F_\mu \mathrm{e}^{-\mathrm{i}qa_B}/\epsilon_\mu - k_A F_\delta \mathrm{e}^{\mathrm{i}qa_A}/\epsilon_\delta \\
M^{'} &= \epsilon_\beta - k_C^2/\epsilon_\gamma; \quad N^{'} = F_\beta - F_\gamma k_C \mathrm{e}^{-\mathrm{i}qa_C}/\epsilon_\gamma \\
WA &= \epsilon_\alpha - k_B^2/\epsilon_\beta - k_A^2/\epsilon_\delta \\
ZA &= F_\alpha - k_B F_\beta \mathrm{e}^{-\mathrm{i}qa_B}/\epsilon_\beta - k_A F_\delta \mathrm{e}^{\mathrm{i}qa_A}/\epsilon_\delta \\
W^{'} &= \epsilon_\alpha - k_B^2/\epsilon_\beta - k_A^2/\epsilon_\mu \\
Z^{'} &= F_\alpha - k_B F_\beta \mathrm{e}^{-\mathrm{i}qa_B}/\epsilon_\beta - k_A F_\mu \mathrm{e}^{\mathrm{i}qa_A}/\epsilon_\mu.
\end{aligned} \tag{10}$$

Here $\epsilon_i = k_{i,i+1} + k_{i,i-1} - m_i\omega^2$, where i refers to α, β, γ, δ and μ .

Let us represent the above two transformations by $T_{\Omega(\Gamma)}$ and denote the renormalized Green's functions as $G^i_{\Omega(\Gamma)}$. Now we can recast $G_N(q,\omega)$ as,

$$G_N(q,\omega) = p_{(\Omega)} G_N^{(\Omega)}(q,\omega) + p_{(\Gamma)} G_N^{(\Gamma)}(q,\omega) \tag{11}$$

where $G_N^{(\lambda)}(q,\omega) = (1/N_\lambda)\sum_{i\in(\lambda)} G^i_{(\lambda)}(q,\omega)$. Here λ can be either Ω or Γ, and $N_{\Omega(\Gamma)}$ is the number of sites in the Γ (Ω)-sublattice. The coefficient $p_{(\Omega)}$ and $p_{(\Gamma)}$ denote the fraction of total sites which belong to Ω and Γ sublattices respectively, *i.e.*, $p_{(\Omega)} = N_\Omega/N$ and $p_{(\Gamma)} = N_\Gamma/N$. The expressions for $G_N(q,\omega)$ and $G_N^{(\lambda)}(q,\omega)$ are structurally same, the former being defined in terms of the parameters of the original 3CF lattice, while the latter refers to those of the renormalized $\Gamma(\Omega)$-sublattice. Equation (11) shows that $G_N(q,\omega)$ becomes equal to a linear combination of $G_N^{(\Omega)}(q,\omega)$ and $G_N^{(\Gamma)}(q,\omega)$, with coefficients $p_{(\Omega)}$ and $p_{(\Gamma)}$, where $p_{(\Omega)} = \sigma$ and $p_{(\Gamma)} = \sigma^3$. Since each of these sublattices again forms a new 3CF chain, we can treat them at the same footing as the original chain. Thus for the renormalized $\Omega(\Gamma)$ sublattice, $G_N^{\Omega(\Gamma)}$ takes the same role as that of $G_N(q,\omega)$ in the original lattice. As we can split further each of these new chains into Γ and Ω sub-sublattices, it is again possible to express both $G_N^{(\Omega)}(q,\omega)$ and $G_N^{(\Gamma)}(q,\omega)$ in the form of equation (11). Thus we have,

$$\begin{aligned}
G_N(q,\omega) &= p_{(\Omega\Omega)} G_N^{(\Omega\Omega)}(q,\omega) + p_{(\Omega\Gamma)} G_N^{(\Omega\Gamma)}(q,\omega) \\
&\quad + p_{(\Gamma\Omega)} G_N^{(\Gamma\Omega)}(q,\omega) + p_{(\Gamma\Gamma)} G_N^{(\Gamma\Gamma)}(q,\omega).
\end{aligned} \tag{12}$$

Here we denote the two branches resulting from Ω-sublattice as $(\Omega\Omega, \Omega\Gamma)$, while those from Γ-sublattice as $(\Gamma\Omega, \Gamma\Gamma)$. The coefficients can be written as $p_{(\mu\nu)} = p_{(\mu)}p_{(\nu)}$, with $\mu, \nu = \Omega$ or Γ.

If we continue the splitting procedure, it will give rise to a tree like structure and it is possible to label each sublattice by its path in this tree. In other words, we label a sublattice by specifying the sequence of Ω and Γ branches that constitute the path leading to the sublattice. The idea of above labeling comes from the fact that this branching process actually gives a family classification for the sites of the 3CF chain, and we can consider this tree as the genealogical tree for this lattice. So finally we can write $G_N(q,\omega)$ as,

$$G_N(q,\omega) = \sum_{\text{all paths}} p_{(\text{path})} G_N^{(\text{path})}(q,\omega) \tag{13}$$

where the sum is over all possible paths in the genealogical tree for a given number of branching. We terminate each path in the genealogical tree using the criteria that the corresponding renormalize coupling constants k_A, k_B and k_C becomes zero at this stage of iteration. In this limit, the computation of each term in the equation (13) becomes trivial (see Eq. (6)) and one can express every $G_N^{(\text{path})}$ into the following general form,

$$\begin{aligned}
G_N^{(\text{path})} &= -\big(x_\alpha F_\alpha^*/\epsilon_\alpha^* \\
&\quad + x_\beta F_\beta^*/\epsilon_\beta^* + x_\gamma F_\gamma^*/\epsilon_\gamma^* + x_\delta F_\delta^*/\epsilon_\delta^* + x_\mu F_\mu^*/\epsilon_\mu^*\big)
\end{aligned} \tag{14}$$

where ϵ_i^*'s and F_i^*'s represent the appropriate renormalized parameters and x_α, x_β, x_γ, x_δ and x_μ are the concentrations of α, β, γ, δ and μ sites in the 3CF chain. Then $G_N(q,\omega)$ can be easily evaluated using the above RSRG scheme and the dynamic structure factor for the quasiperiodic 3CF chain can be obtained from equation (3).

The merit of this scheme is that one has to generate all possible paths in the genealogical tree using a simple algorithm, then iterate the recursion relations (8) and (9) sequentially along these paths, and finally determine $G_N(q,\omega)$ using equation (13). There is no approximation involved in this method and the dynamic structure factor for quasiperiodic lattices can be obtained with arbitrary accuracy, the accuracy level being set by the smallness of the renormalized values of k_A, k_B and k_C.

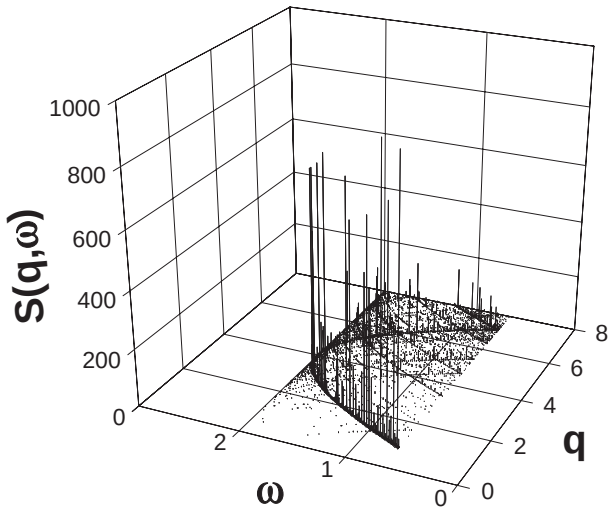

Fig. 2. The dynamic structure factor $S(q,\omega)$ for a bond model. The parameters are same as in Figure 4a.

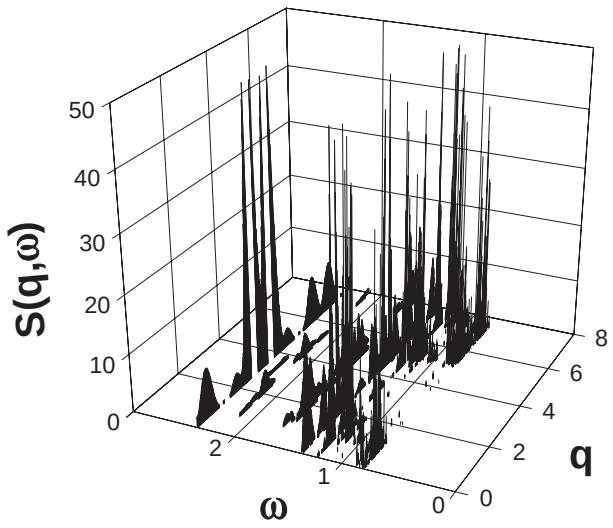

Fig. 3. The dynamic structure factor for on-site model. The parameters are same as in Figure 4e.

The dispersion relations for the system can be easily obtained from $S(q,\omega)$ using the fact that the ω and q values corresponding to every non-zero values of $S(q,\omega)$ constitute a point in the dispersion curve. Thus scanning the entire $\omega - q$ plane for non-zero $S(q,\omega)$ one can get the dispersion curve for the 3CF chain, and the whole spectrum of normal mode frequencies becomes available.

4 Results and discussions

The 3D plot for the dynamic structure factor $S(q,\omega)$ of 3CF lattice as a function of ω and q has been given for the bond and the on-site models respectively in Figures 2 and 3. The calculation of the dynamic response function facilitates an easy determination of the phonon dispersion (ω *vs.* q) curves. As for examples, we have shown in Figures 4a–e the phonon dispersion curves for different models of the three component Fibonacci chain. In Figure 4a we have plotted ω *vs.* q by scanning the function $S(q,\omega)$ for non-zero values corresponding to the models characterized by the parameters $m_\alpha = m_\beta = m_\gamma = m_\delta = m_\mu = 1$, $k_A = k_B = k_C = 1$, $d_A = 1$, $d_B = \sigma$ and $d_C = \sigma^2$, where σ is the only real root of the algebraic equation $\sigma^3+\sigma-1 = 0$. In Figure 4b the phonon dispersion relation for the transfer model with the parameters $m_A = m_B = m_C = 1$, $k_A = 1$, $k_B = 2$, $k_C = 2.5$ and $d_A = d_B = d_C = 1$ is shown. The dispersion curve for the mixed model defined by the parameters $m_A = 1$, $m_B = 0.5$, $m_C = 2$, $k_A = 1$, $k_B = 2$, $k_C = 2.5$ and $d_A = d_B = d_C = 1$ is plotted in Figure 4c. The parameters $m_A = m_B = m_C = 1$, $k_A = 1$, $k_B = 2$, $k_C = 2.5$, $d_A = 1$, $d_B = \sigma$ and $d_C = \sigma^2$ are taken for plotting the phonon dispersion relation in Figure 4d. Figure 4e shows the phonon dispersion curve for the on-site model with the parameters $m_\alpha = m_\delta = m_A = 1$, $m_\beta = m_\mu = m_B = 0.5$, $m_\gamma = m_C = 2$, $k_A = k_B = k_C = 1$ and $d_A = d_B = d_C = 1$. Figure 5 is a plot of the static structure factor $S(q)$ *vs.* q for the three component Fibonacci lattice. Actually the peaks of the static structure factor are delta peaks for quasiperiodic lattices. But we see that there are widths in the static structure factor in Figure 5. The widths of the static structure factor come due to the finite value of the imaginary part (δ in Eq. (3)) included in the calculation. If one decreases the value of the imaginary part (δ) the peaks become sharp and in the limit $\delta \to 0$, it becomes delta peak. We have checked numerically that the theoretically predicted values of wavevector $q_{n_1,n_2,n_3}(= 2\pi D^{-1}(n_1 d_A + n_2 d_B + n_3 d_C))$ for the maximum intensity in the static structure factor are in excellent agreement with our RSRG calculations.

The common features to all these dispersion curves are that they consist of infinite number of gaps. In each case the phonon dispersion relation reveals that at very low and very high q values, *i.e.*, when the wavelength of the incident radiation is too big or too small compared to the lattice parameters, the scattering is insensitive to the quasiperiodic ordering and features similar to a periodic one are reproduced. For intermediate values of q the quasiperiodicity comes into play. This is reflected by the existence of numerous gaps in the phonon spectrum. We also observe optical modes in the phonon dispersion curves. The optical modes in the spectrum is the superposition of an infinite number of curves corresponding to the very large system size and hence it is very much complicated. Except for the curve of Figure 4a, there are also the dispersion less optical modes clearly visible in the dispersion relations of Figures 4b–e. The origin of the dispersion less modes can be explained as follows. In case of transfer, on-site or mixed models, the spring constants k_A, k_B and k_C become unequal under renormalization procedure. We have checked numerically that under renormalization, the spring constant k_A becomes very large (*i.e.*, $k_B/k_A \ll 1$) compared to the other spring constants k_B or k_C at some stage of iteration of equations (8) or (9). Therefore, at this length scale, the whole chain can be thought to be consisting of diatomic molecules with strong coupling k_A and those molecules are connected with very weak coupling

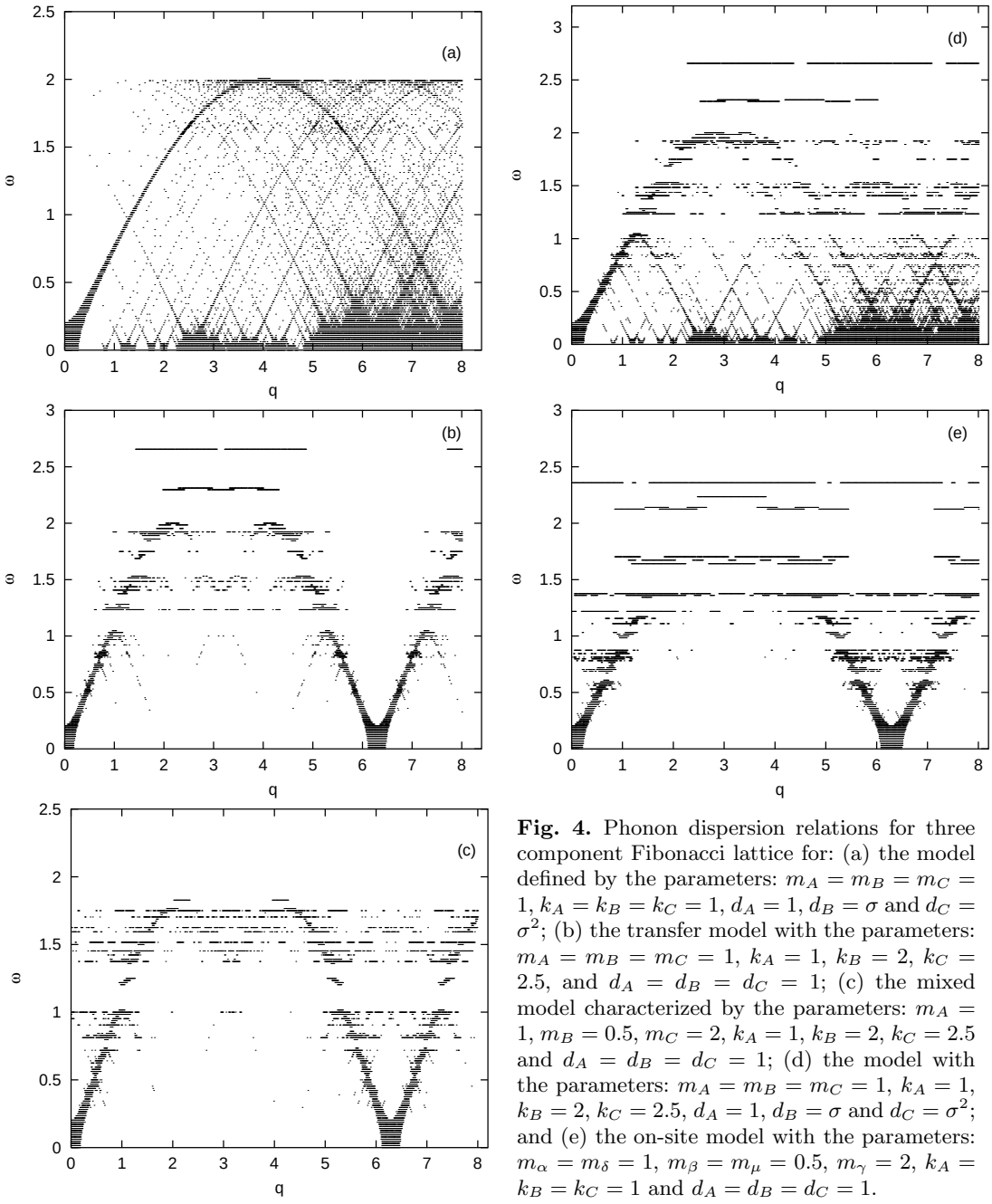

Fig. 4. Phonon dispersion relations for three component Fibonacci lattice for: (a) the model defined by the parameters: $m_A = m_B = m_C = 1$, $k_A = k_B = k_C = 1$, $d_A = 1$, $d_B = \sigma$ and $d_C = \sigma^2$; (b) the transfer model with the parameters: $m_A = m_B = m_C = 1$, $k_A = 1$, $k_B = 2$, $k_C = 2.5$, and $d_A = d_B = d_C = 1$; (c) the mixed model characterized by the parameters: $m_A = 1$, $m_B = 0.5$, $m_C = 2$, $k_A = 1$, $k_B = 2$, $k_C = 2.5$ and $d_A = d_B = d_C = 1$; (d) the model with the parameters: $m_A = m_B = m_C = 1$, $k_A = 1$, $k_B = 2$, $k_C = 2.5$, $d_A = 1$, $d_B = \sigma$ and $d_C = \sigma^2$; and (e) the on-site model with the parameters: $m_\alpha = m_\delta = 1$, $m_\beta = m_\mu = 0.5$, $m_\gamma = 2$, $k_A = k_B = k_C = 1$ and $d_A = d_B = d_C = 1$.

k_B or k_C. So the vibrations are essentially composed of diatomic molecules. In such case, it has been shown in reference [39] that there will be dispersion less modes in the optical branches, *i.e.*, the optical modes will be flat with very small spread. This spread is because of the fact that the ratio k_B/k_A is not zero and so these molecules are very weakly coupled, the result is a small spread of the order of k_B/k_A in the optical band frequencies as q varies. In Figure 4a, we have taken equal mass and equal spring constant (*i.e.*, $m_i = m$ for all i and $k_A = k_B = k_C = k$) with the different bond lengths d_A, d_B and d_C. In this case under the iterations of the recursion relations (please see recursion relations for the spring constants from Eqs. (8) and (9)) the numerical values of the spring constants will not differ from one another. Therefore, as the conditions of either $k_B/k_A \ll 1$ or $k_C/k_A \ll 1$ are not satisfied in this case, the dispersion less modes are not observed in Figure 4a.

5 Conclusions

In conclusion, we have presented the results of the dynamical properties of a three component Fibonacci lattice. The phonon dispersion curves corresponding to different models of the three component Fibonacci (3CF) chain, give an

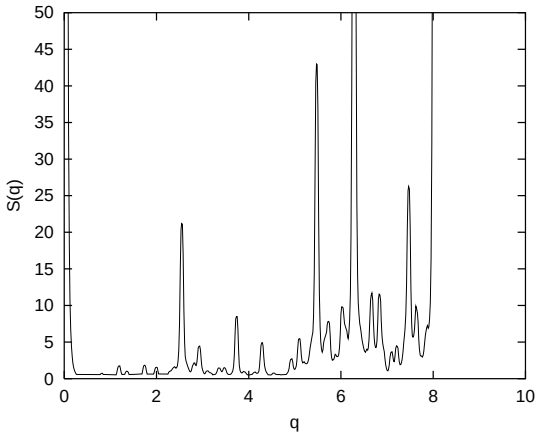

Fig. 5. Static structure factor for the bond lengths $d_A = 1$, $d_B = \sigma$ and $d_C = \sigma^2$. The maximum of the peaks occur at $q_{n_1,n_2,n_3} = 2\pi D^{-1}(n_1 d_A + n_2 d_B + n_3 d_C)$, where $D = d_A + \sigma d_B + \sigma^2 d_C$ and n_1, n_2 and n_3 are integers.

infinity of gaps. The pseudo-Brillouin zone boundaries are clearly visible in the phonon spectrum. The dispersion less modes are observed in case of transfer, on-site and mixed models because of the fact that one of the spring constants k_A, k_B and k_C becomes very large compared to the others and the optical branch [39] becomes flat with very small spread in band frequencies. Under this condition the whole lattice can be thought as consisting of molecules with strong coupling among the constituent atoms, whereas the molecules among themselves are weakly coupled. Actually in this length scale, the eigen modes are standing waves spreading all over the lattice and the theory of propagating waves are not applicable here. We have also presented the static structure factor using same formalism. The peaks of the static structure are found to occur in the theoretically observed values of the wavevector q. All these gross features are found to be compatible with the experimental results on real quasicrystal [37,38].

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