Dynamic structure factor of a Fibonacci lattice: A renormalization-group approach

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We present a real-space renormalization-group method for evaluating the exact dynamic structure factor $S(q,\omega)$ of a quasiperiodic Fibonacci chain. Contrary to earlier work that takes account only of the global aspects of the symmetry of the chain, our method additionally takes care of the local environmental aspects of the symmetry by separating the original lattice into a finite number of self-similar interpenetrating sublattices, followed by elimination of the coupling between them. Our method also yields correctly the positions of the Bragg peaks of the Fibonacci chain. Moreover, the present method allows the sites of the chain to be grouped into classes following a "genealogical" classification, the members of a given class being equivalent up to a certain length scale. Based on this classification, the proof of the existence of a *key site,* which has only been conjectured in our earlier work using numerical search, has been given.

I. INTRODUCTION

Quasiperiodic crystals have become a well-known subject of interest during the past few years after the discovery of the icosahedral symmetry in a rapidly quenched alloy of Al and Mn by Schechtman *et al.*[1] Quasiperiodic systems in one dimension are currently being investigated quite exhaustively.[2–12] Growth of quasiperiodic superlattices[4] has presented an experimental realization of quasicrystalline lattices even in one dimension and the interest in one-dimensional quasilattices has increased after this success.

In this communication we present an idea relying solely on the real-space renormalization-group (RSRG) method[13,14] to evaluate the exact dynamic structure factor $S(q,\omega)$ of an infinite Fibonacci chain in which both the global and local symmetry aspects of a Fibonacci chain are taken into account correctly. Ashraff and Stinchcombe (AS) have adopted a generating-function approach[11] together with real-space decimation to calculate the dynamic response $S(q,\omega)$ of a Fibonacci quasicrystal. However, the fact that in a quasiperiodic chain every site sits in a different environment has been considered only in an averaged sense, as in their previous work on density of states.[6] In our formalism, apart from being able to calculate $S(q,\omega)$, one can also compute the local and average densities of states (LDOS and ADOS). However, another aspect of the present method is that it provides a way of classifying the different sites of a quasiperiodic chain, which we call the "genealogical" classification, for reasons to be explained later. This classification enables us to group the sites of a chain into "families," the size of the families depending on the length scale chosen. It follows that, in the limit of infinite length scale, each site constitutes its own family, which is clearly in accord with the quasiperiodic nature of the chain. A similar classification in the context of energy spectrum of hierarchical lattices has recently been given by Niu and Nori.[9]

The method can be easily applied to periodic and other non-Fibonaccian lattices[10] that have self-similar structures. However, in this work we shall confine ourselves to the Fibonacci lattice. We develop our scheme by computing the dynamic structure factor and later explain how the LDOS and ADOS result from the same scheme.

II. RSRG SCHEME TO CALCULATE $S(q,\omega)$

A. The Fibonacci chain

The lattice under consideration consists of two types of bonds, long (L) and short (S), arranged according to a Fibonacci sequence and three types of atoms of masses m_α, m_β, and m_γ situated at the L-L, L-S, and S-L vertices, respectively. The spring constant takes two different values, k_L and k_S, depending on the nature of the bonds. The dynamic structure factor is defined by[11]

$$S(q,\omega)=\lim_{\delta\to 0}\lim_{N\to\infty}\mathrm{Im}G_N(q,\omega-i\delta)\ , \tag{1}$$

where

$$G_N(q,\omega)=(1/N)\sum_{l,l'}[\exp iq(r_l-r_{l'})]G_{ll'}(\omega) \tag{2}$$

r_l being the position of the lth site and N the number of sites. Here $G_{ll'}(\omega)$ are the single-site Green's functions which satisfy the equations of motion

$$\left[\sum_{\substack{l\neq i\\ \langle il\rangle}}k_{il}-m_i\omega^2\right]G_{ij}(\omega)=-\delta_{ij}+\sum_{\substack{k\neq i\\ \langle ki\rangle}}k_{ik}G_{kj}(\omega) \tag{3}$$

in the harmonic approximation. In this method we split the original lattice into two sublattices, each of which is a scaled version of the original Fibonacci lattice. The sum in Eq. (2) over the original lattice points is then expressed as a combination of two independent sums over these two sublattices. The terms connecting the two sublattices in the original sum of Eq. (2) are eliminated using Eq. (3). Each sum now runs solely over the lattice points of one sublattice and is similar to the original sum corresponding to a renormalized lattice. For convenience in implementing the RSRG scheme, we rewrite Eq. (2) as

$$G_N(q,\omega)=(1/N)\sum_{l,l'} F_l \mathcal{G}_{ll'}(q,\omega) , \tag{4}$$

where

$$\mathcal{G}_{ll'}(q,\omega)=[\exp iq(r_l-r_{l'})]G_{ll'}(\omega) .$$

It should be mentioned at this stage that, as the process of decoupling of the sublattices is carried out by eliminating appropriate Green's functions using Eq. (3), an additional factor F_l is generated in front of each term in the summation at every stage of renormalization. In order to take care of the situation, we introduce beforehand a factor F_l as a coefficient to every $\mathcal{G}_{ll'}(q,\omega)$ inside the summation. All F_l's are equal to unity at the beginning and grow during the process of renormalization. We have been able to derive recursion relations for these F_l's which play the key role in the present RSRG scheme. The dependence of F_l on the index l only follows from Eq. (3). At any length scale, F_l's are not all distinct but can have three values only, viz., F_α, F_β, and F_γ, depending on the local symmetry of the sites in the renormalized lattice.

To implement the scheme, we split the original Fibonacci lattice into two sublattices, which we call Ω and Γ, using the transformation $LS\rightarrow L$ and $L\rightarrow S$ as shown in Fig. 1. The Γ sublattice is formed by the β-type sites, whereas, α and γ sites form the vertices of the Ω sublattice. The scale factors for the Ω and Γ sublattices are τ and τ^2, respectively, where, $\tau=(\sqrt{5}+1)/2$ is the golden ratio. The self-similar structure of the Fibonacci lattice and the fact that it can be split into a finite number of similar sublattices is crucial in implementing the RSRG scheme. We now partition the sum in Eq. (4) as

$$G_N(q,\omega)=(1/N)\left[\sum_{l,l'\in\Omega} F_l\mathcal{G}_{ll'}+\sum_{l,l'\in\Gamma} F_l\mathcal{G}_{ll'} + \sum_{\substack{l\in\Omega\\ l'\in\Gamma}} F_l\mathcal{G}_{ll'}+\sum_{\substack{l\in\Gamma\\ l'\in\Omega}} F_l\mathcal{G}_{ll'}\right] . \tag{5}$$

Equation (5) shows that the last two sums involve intersublattice connections which are finally eliminated and can be expressed as

$$G_N(q,\omega)=p_\Omega\left[(1/N_\Omega)\sum_{l,l'\in\Omega}(F_l)_\Omega\mathcal{G}_{ll'}\right] + p_\Gamma\left[(1/N_\Gamma)\sum_{l,l'\in\Gamma}(F_l)_\Gamma\mathcal{G}_{ll'}\right] , \tag{6}$$

where $(F_l)_\Omega$ and $(F_l)_\Gamma$ denote the "new" coefficients in the decoupled sums for Ω and Γ sublattices, respectively. In Eq. (6), $N_{\Omega(\Gamma)}$ is the number of atoms in the $\Omega(\Gamma)$ sublattice and $p_\Omega=\tau-1$ and $p_\Gamma=2-\tau$. Now, the sum within each parenthesis is similar to the original sum if we use appropriate renormalized parameters. Since both Ω and Γ maintain the Fibonacci character, we can again split each of the sums into two parts using the above idea and this process can be continued. We evaluate each sum in the limit when both k_L and k_S flow to zero under renormalization. The recursion relations for the Ω sublattice are given by

$$\begin{aligned}
&\varepsilon'_\alpha=\varepsilon_\gamma+w_\beta(k_L^2+k_S^2) , \quad \varepsilon'_\beta=\varepsilon_\gamma+w_\beta k_S^2 , \quad \varepsilon'_\gamma=\varepsilon_\alpha+w_\beta k_L^2 ,\\
&k'_L=w_\beta k_L k_S , \quad k'_S=k_L ,\\
&F'_\alpha=F_\gamma+F_\beta w_\beta[k_L\exp(iqa_L)+k_S\exp(-iqa_S)] ,\\
&F'_\beta=F_\gamma+F_\beta w_\beta k_S\exp(-iqa_S) ,\\
&F'_\gamma=F_\alpha+F_\beta w_\beta k_L\exp(iqa_L) ,\\
&a'_L=\tau a_L , \quad a'_S=\tau a_S .
\end{aligned} \tag{7}$$

Here,

$$\begin{aligned}
&\varepsilon_\alpha=m_\alpha\omega^2-2k_L ,\\
&\varepsilon_\beta=m_\beta\omega^2-(k_L+k_S) ,\\
&\varepsilon_\gamma=m_\gamma\omega^2-(k_L+k_S) ,\\
&w_i=-1/\varepsilon_i ,
\end{aligned}$$

where $i=\alpha$, β, or γ. a_L and a_S are the long and short bond lengths, respectively. A similar set of recursion relations has also been obtained for the Γ sublattice.

In the limit k_L and $k_S\rightarrow 0$, the sum typically looks like

$$[x_\alpha(\omega-\varepsilon^*_\alpha)^{-1}+x_\beta(\omega-\varepsilon^*_\beta)^{-1}+x_\gamma(\omega-\varepsilon^*_\gamma)^{-1}] , \tag{8}$$

where x_α, x_β, and x_γ are the concentrations of the α, β, and γ sites and ε_i^* is the corresponding renormalized on-site term in that limit. We would like to emphasize that the bond lengths a_L and a_S have to bear the ratio τ for a uniform scaling of the entire Fibonacci chain. This implies that the structure factor of an ordered chain cannot be obtained from the recursion relations listed above by merely taking the periodic limit. However, the above relations yield results for an ordered lattice only in the limit $q\rightarrow 0$ because, in this long-wavelength limit, the response becomes insensitive to the lattice structure. In this limit, as expected, one finds that the structure factor agrees well with the analytical result for an ordered chain.

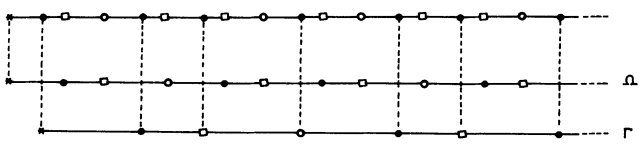

FIG. 1. Section of an infinite Fibonacci chain illustrating the sublattice splitting.

B. The case of an ordered chain

As an elementary illustration of the present approach, we have looked at the expression for $S(q,\omega)$ in the case of an equispaced linear chain of atoms of mass m and coupling constant k_0. In this case, the chain trivially decomposes into two identical linear chains under a scale factor equal to 2, leading to the following analytical form of $S(q,\omega)$:

$$S(q,\omega)=\mathrm{Im}\lim_{N\rightarrow\infty}\lim_{\delta\rightarrow 0}(1/\varepsilon^*)\prod_{n=0}^{\infty}[1-2k_n\cos(qa_n)/\varepsilon_n] , \tag{9}$$

where $\varepsilon_0 = m\omega^2 - 2k_0$, and the recursion relations are given by

$$\varepsilon_{n+1} = \varepsilon_n - 2k_n^2/\varepsilon_n ,$$

$$k_{n+1} = -k_n^2/\varepsilon_n ,$$

and

$$a_{n+1} = 2a_n ,$$

and ε^* is the fixed point for ε. This expression may be compared with the well-known formula

$$S(q,\omega) = \mathrm{Im}[m\omega^2 - 2k(1-\cos qa)]^{-1} . \quad (10)$$

The numerical performance of the RSRG expression (9) has been compared with that of Eq. (10) and the results are in excellent agreement.

III. RESULTS FOR THE FIBONACCI CHAIN

Our RSRG method can be easily employed to obtain the ADOS given by the equation

$$\mathcal{D}(\omega) = (-1/\pi)\mathrm{Im}\left[(1/N)\sum_l G_{ll}(\omega)\right]$$

of a Fibonacci chain. Since this sum does not involve any off-diagonal matrix element of the Green's function, the splitting procedure is simpler here. All the F_l's are equal to unity at all stages of the RSRG transformation and only the recursions of the ε's and k's are relevant for both the sublattices.

In order to calculate the LDOS at an arbitrary site of the Fibonacci chain, we follow the sequence of sublattices Ω, Γ, etc., to which the site successively belongs during the process of renormalization. At every intermediate step we use the appropriate set of recursion relations depending on whether the chosen site happens to belong to an Ω or Γ sublattice at that stage. The local Green's functions are obtained in the limit k_L and $k_S \to 0$, and are given by $G_{00} = 1/\varepsilon^*$, where ε^* is the renormalized on-site term in that limit.

We have computed the LDOS at an arbitrary site and also the ADOS of a 30th-generation Fibonacci chain. The LDOS and ADOS reflect the familiar three subband splitting corresponding to the transfer model which is now quite well understood.[5-7]

The surface plot of $S(q,\omega)$ has been presented in Fig. 2. It exhibits a highly complex structure in which the zero response corresponds to the gaps in the density of states. The dispersion relation for the Fibonacci chain can also be obtained from the nonzero values of $S(q,\omega)$. In Fig. 3, we have plotted energy (ω) against the wave vector (q) for $S(q,\omega) > 0.5$. For elastic scattering, the Bragg peaks occur at[15]

$$q_{nm} = [2\pi/(1+\tau^{-2})](n + m/\tau) ,$$

where n and m are integers and the q values corresponding to $\omega \to 0$ as obtained from Fig. 3 are in complete agreement with the above expression. If we look at the location of the Bragg peaks using the results of Ashraff and Stinchcombe,[11] we do not find agreement with q_{nm} mentioned above. The reason for this, as we mentioned in the Introduction, lies in the fact that the local environment effects have been included in an averaged manner in the AS theory. These effects turn out to be of crucial importance in fixing the values of q_{nm} as we find from the present calculation.

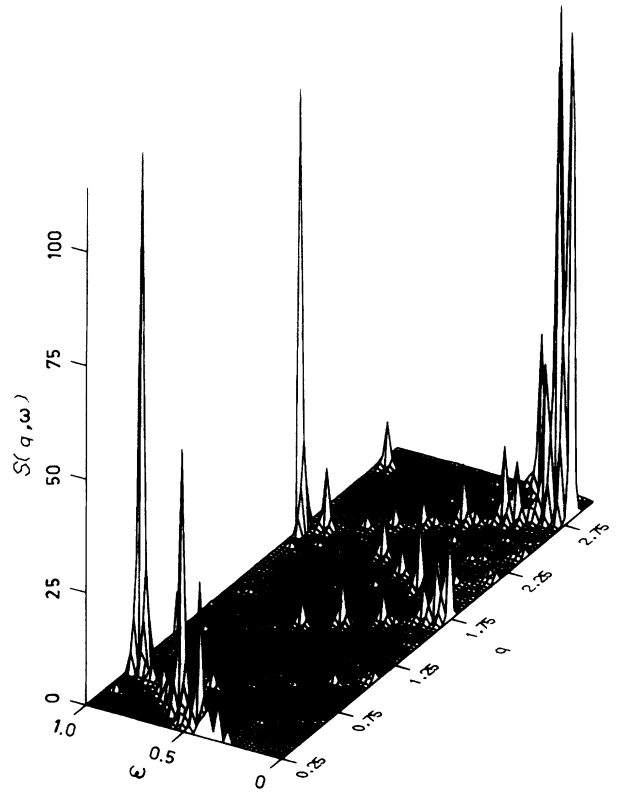

FIG. 2. Surface plot of $S(q,\omega)$ in arbitrary units for an infinite Fibonacci chain with $m_\alpha = m_\beta = m_\gamma = 1$, $k_S/k_L = 2$, and $a_L/a_S = \tau$. ω and q are measured in units of $\sqrt{k_L}$ and a_S^{-1}, respectively.

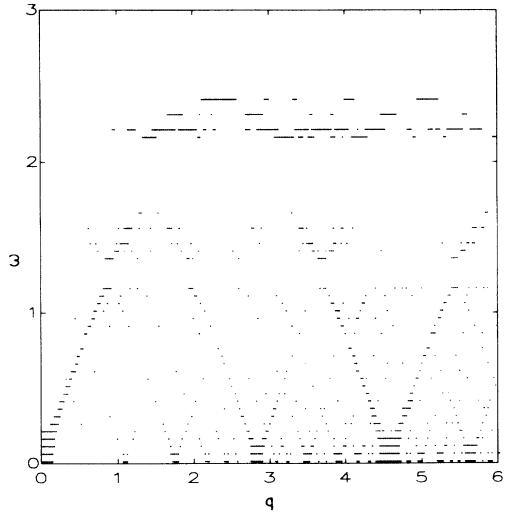

FIG. 3. Dispersion relation for the Fibonacci chain. Here the parameters of the system are the same as in Fig. 2.

IV. THE GENEALOGY OF A FIBONACCI LATTICE

In our approach, the sites in the original Fibonacci chain get grouped into Ω and Γ branches after the first step of renormalization. In the second step we have four branches, one Ω-Γ pair originating from the Ω branch and the other from the Γ branch. The continuation of this process gives rise to a treelike structure which may be called the genealogical tree for the Fibonacci lattice. If we continue the branching procedure for an infinite number of steps, we find that every site percolates down *one particular branch,* uniquely specified by the infinite sequence $(a,a',a'',\ldots)$, where, a, a', a'', etc., can be Ω or Γ. Interpreted in terms of the original Fibonacci chain, this result implies that every site is unlike every other site, a feature characteristic of quasiperiodic lattices. On the other hand, if the iteration is carried out a finite number of times, say n, then the sites are found to be divided into groups, each group now being labeled by a finite sequence of indices $(a,a',a'',\ldots,a^n)$, where each a, a', etc., can again be either Ω or Γ. All sites that are characterized by the same set of indices follow the same path down the genealogical tree during the process of renormalization. They may be considered as being members of the same "family" up to a length scale τ^{l+2m}, where l is the number of times the index Ω appears in the sequence and $m=n-l$. Again interpreting in terms of the original Fibonacci lattice, this means that all sites that are members of the same family may be considered as "equivalent" as far as the environment is considered up to this length scale.

We now make an important observation. Among all sites there will be one which throughout follows an infinite periodic sequence of Ω and Γ branching under successive renormalization. The existence of a periodic sequence ($\Omega\Gamma\Omega\Gamma\ldots$ to ∞) indicates that the local environment around that particular site is exactly restored (up to infinite distance) to the starting environment after every alternate branch. Now, one can easily identify that the transformation $\Omega\Gamma$ corresponds the composite transformation I-II-I in the language of Ref. 7 (where I is $LS\rightarrow L'$ and $L\rightarrow S'$, and is II is $SL\rightarrow L'$ and $L\rightarrow S'$). Thus, the site following the infinite periodic sequence of branching ($\Omega\Gamma\Omega\Gamma\ldots$) is actually the key site discussed in Ref. 7. This method thus provides proof of the existence of a site of special symmetry in an infinite Fibonacci chain which had been only conjectured earlier, based on numerical search.

V. SUMMARY

We have developed a renormalization-group method to evaluate the frequency-dependent response of the quasiperiodic Fibonacci chain. The method brings out the required features of $S(q,\omega)$ and the correct location of the Bragg peaks corresponding to the case of elastic scattering. The present method also provides a way of classifying all the sites of an infinite quasiperiodic chain into distinct families depending on the length scale of observation and gives proof of existence of a site of special symmetry conjectured elsewhere.[7]

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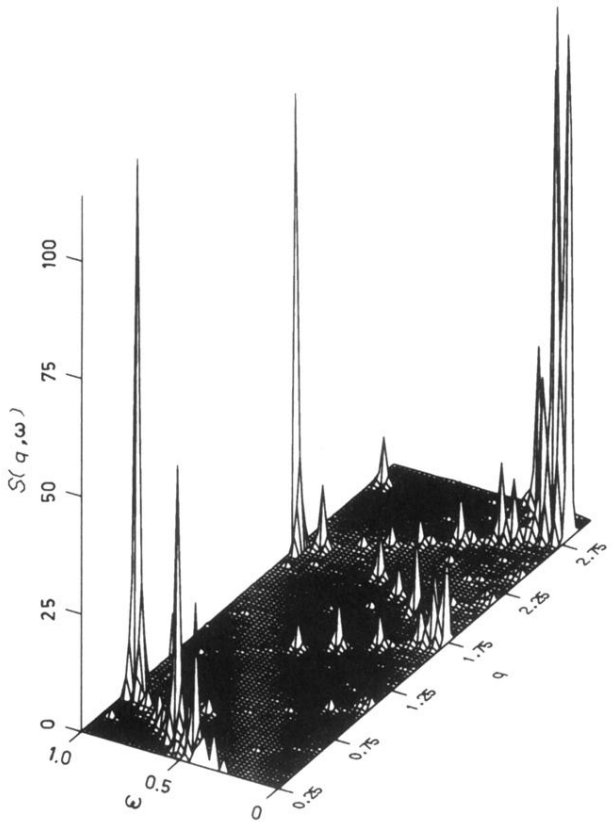

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