Frequency dependent response of a Thue-Morse aperiodic lattice

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We present an exact calculation for the dynamic structure factor of a Thue-Morse aperiodic lattice using a real space renormalization-group (RSRG) method proposed by S. N. Karmakar, A. Chakrabarti, and R. K. Moitra [Phys. Rev. B **46**, 3660 (1992)]. However, the ordering inherent in a Thue-Morse sequence prohibits a direct application of the RSRG method. We overcome this difficulty by observing that the Thue-Morse lattice can be obtained from a more general deterministic structure that is constructed using a four-letter substitution rule. This general deterministic sequence has the advantage that, first, both the aperiodic Thue-Morse sequence as well as the quasiperiodic period-doubling sequence can be extracted from it at two different limits, and second, within a decimation renormalization technique, it can be split into two equivalent self-similar sublattices. This facilitates the application of the renormalization method. Exact recursion relations for the Hamiltonian parameters for these sublattices are provided. Results are given both for this general nonperiodic structure and the Thue-Morse lattice as its special case. In addition, within the same framework we calculate the average density of states of the Thue-Morse lattice. Some features in the response of the aperiodic chains are found to be compatible with experiments on real quasicrystals.

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I. INTRODUCTION

After the discovery of icosahedral symmetry in melt-spun alloys of aluminum and manganese by Shectman *et al.*,[1] extensive research on various properties of qusicrystals have enriched the literature. In particular, one-dimensional quasiperiodic lattices have attracted most of the attention.[2–15] The interest in one-dimensional problems really shot up after the success of Merlin *et al.*[16] in growing model systems where quasiperiodic order is built by depositing GaAs and AlAs layers in a Fibonacci sequence using the molecular beam epitaxy technique. X-ray and neutron scattering experiments were performed and the positions of the Bragg peaks were identified. The recent nanostructure technology has really been successful in providing ''testing ground'' for the theories. A calculation even in one dimension has thus become meaningful from the standpoint of an experimentalist. The pioneering work of Kohmoto *et al.*[2] has triggered vigorous research activity in the field of electron and phonon spectra of one dimensional quasiperiodic and other aperiodic lattices, though some other aspects of these systems have also been investigated.[17,18] Studies of electron states and the phonon spectrum in these systems are mostly concerned with the calculation of the respective densities of states and the characterization of the wave functions. Unlike a randomly disordered system, the wave functions in a quasicrystal in one dimension is, in general, power-law localized.[2–4] The energy spectrum is a cantor set with zero Lebesgue measure and exhibits a multifractal character in most of the cases.[2–15] However, the presence of positional correlation between the constituents in certain class of one-dimensional quasiperiodic lattices is shown to be responsible for the existence of extended ''Blochlike'' eigenstates.[19–21]

Apart from the electronic and other properties mentioned above, comparatively less effort has been given to study the dynamic response of these sytems. The main obstacle is, understandably, the absence of periodicity. An important quantity is the dynamic structure factor $S(q,\omega)$, which can be directly related to the inelastic neutron scattering cross section and also gives information about the excitation modes of the system.[22,23] Experiments on quasicrystals have provided important information in this regard.[23] Over the past years there have been a few theoretical studies on $S(q,\omega)$ for disordered and quasiperiodic lattices.[24–27] Although most of the work concerns the calculation of spin dynamics on a quasiperiodic lattice, the extension to the phonon problem is quite straightforward. The behavior of the phonon modes, as obtained from such calculations, may be tested by inelastic neutron scattering experiments.

Patel and Sherrington[24] worked out $S(q,\omega)$ for a system of ferromagnetically coupled spins on a finite (2D) Penrose lattice. Well-defined propagating spin waves with isotropic dispersion close to the zone centers were found. For the 1D Fibonacci sequence Ashraff and Stinchcombe[25] and Ashraff, Luck, and Stinchcombe[26] derived an analytical expression for $S(q,\omega)$ using a generating function approach. They showed that the magnon dispersion consists of a main branch along with many satellite branches of much weaker intensity. One finds[26] propagating modes at small wave vector, separated by a set of gaps from stripes of dispersionless modes at higher frequencies. Benoit, Poussigue, and Azougarh[27] used the spectral moments method[28] to rediscover similar features in a Fibonacci quasilattice. Karmakar, Chakrabarti, and Moitra[29] developed a real space renormalization-group (RSRG) method for calculating the dynamic structure factor $S(q,\omega)$ for phonons on a Fibonacci chain. Subsequently, Ghosh and Karmakar[30] calculated $S(q,\omega)$ for a period-doubling lattice.[31] Compared to the 1D quasiperiodic Fibonacci chain, no attempt has been made so far to calculate the dynamic response of the 1D aperiodic lattices.[6] A typical

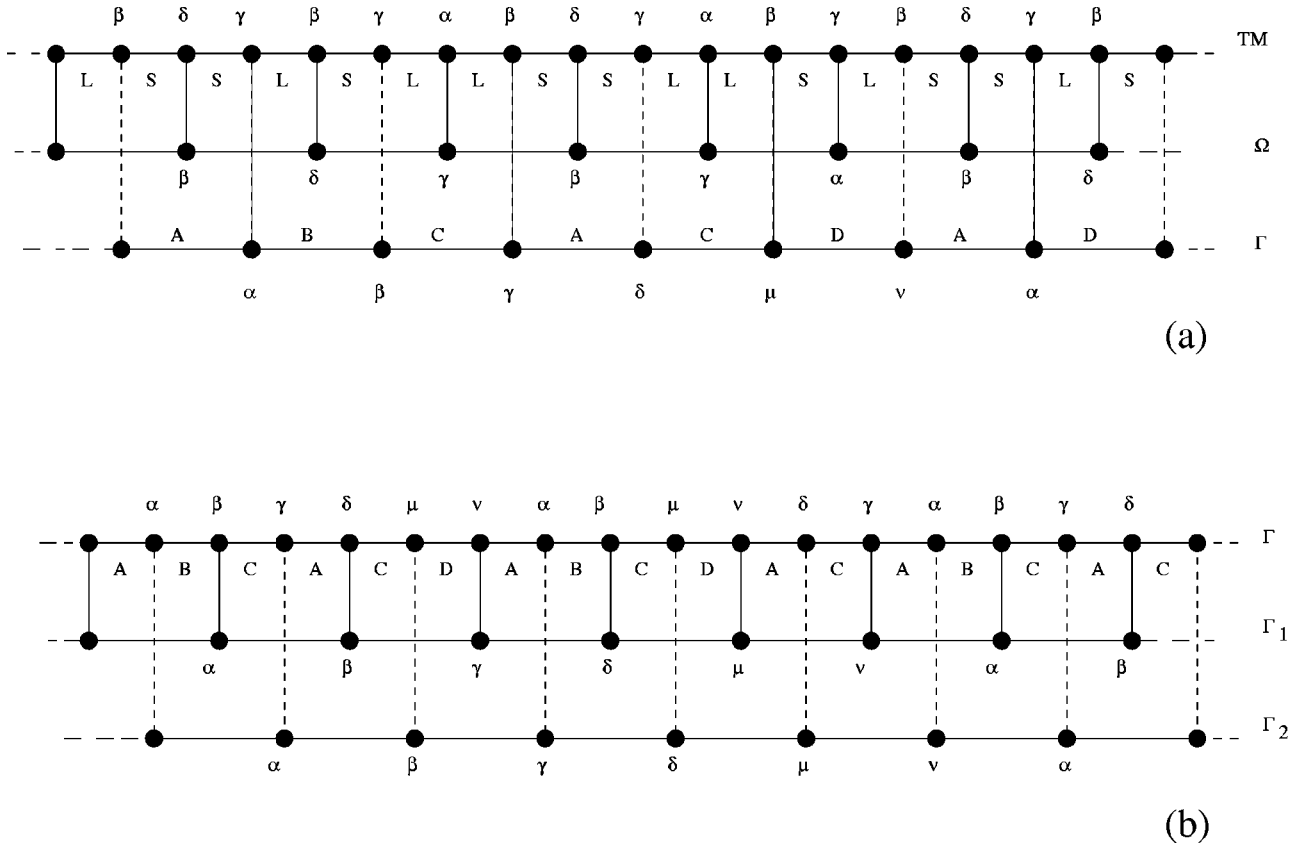

FIG. 1. (a) Portion of an infinite Thue-Morse chain illustrating the decimation scheme. (b) Splitting of a Γ lattice into two equivalent sublattices Γ_1 and Γ_2.

example of an aperiodic chain is the Thue-Morse (TM) lattice,[31] which is generated using a two-letter substitution rule, viz. $L \rightarrow LS$ and $S \rightarrow SL$, L being the seed. Hence the first few generations look like $G_0 = L$, $G_1 = LS$, $G_2 = LSSL$, $G_3 = LSSLSLLS$ and so on. The essential difference between a TM sequence and the classical Fibonacci sequence is the existence of positional correlations between the constituents in the former that enables an infinite TM sequence to sustain a countable infinity of extended eigenmodes[32] though there is no translational periodicity. These eigenstates have profound influence on the transport properties of such lattices.

In this paper, we calculate the dynamic structure factor of an infinite TM lattice, since such calculations in the case of aperiodic lattices, to the best of our knowledge and belief, is really lacking. Our motivation behind this work is twofold. First, we think it would be rather interesting to see the effect of the positional correlation in a TM lattice that makes the energy spectrum of such structures radically different from the canonical case of a Fibonacci quasicrystal, on the response characteristics. Second, recent experiments on actual quasicrystals reveal several interesting characteristics and one might ask, to what extent such features represent in a 1D structure. We will follow essentially the method developed in Ref. 29. However, it is important to note that a straightforward application of the RSRG decimation scheme[29,30] is not possible in a TM lattice. This is because the scheme relies heavily on the splitting of the original lattice into two equivalent self-similar lattices, each of which is an exact replica of the parent lattice. This is true for a Fibonacci lattice as well as a quasiperiodic period-doubling[30] (PD) lattice but cannot be achieved for a TM lattice [see Fig. 1(a)]. We give a prescription for making the scheme work for a TM lattice as well. It is shown that both the TM and the PD sequence can be obtained as special cases of a more general four-letter substitutional sequence. The growth rule for this latter sequence is proposed by us. This four-letter sequence can be shown to split under renormalization into two self-similar sublattices, each of which now becomes an exact replica of the parent lattice. The application of the RSRG scheme now becomes possible. Then $S(q,\omega)$ both for the TM and the PD lattices (as well as the nonperiodic lattice proposed by us) can be obtained within the same formalism just by tuning the initial conditions suitably. However, in what follows, we explicitly discuss $S(q,\omega)$ for a TM lattice, and in some cases present the results for its parent lattice.

In Sec. II we describe the models. In Sec. III the method of calculation is described and the results are given in Sec. IV. We conclude in Sec. V.

II. THE MODEL

We consider a spring-mass model system in one dimension, where two types of springs ''L'' and ''S'' and having spring constants k_L and k_S, respectively, are arranged following a TM sequence described earlier. Point masses m_α,

m_β, m_γ, and m_δ are attached to the vertices flanked by springs of type *L-L*, *L-S*, *S-L*, and *S-S*, respectively. The lattice is shown in Fig. 1(a). When $k_L=k_S$, $m_\alpha=m_\gamma=m_A$, and $m_\beta=m_\delta=m_B$ we get back the standard onsite model, whereas, for $m_\alpha=m_\beta=m_\gamma=m_\delta$ and $k_L\neq k_S$ the bond or the transfer model results.

In Fig. 1(a) we also show a decimation renormalization on such a TM structure resulting in a scaled version of the original lattice (Ω). The lattice Ω is obtained by using the TM growth rule in the opposite sense, i.e., by folding an *LS* pair into a new *L* and an *SL* pair into a new *S*. In this process, a set of sites is eliminated. The decimated sites themselves form an aperiodic structure (Γ), which clearly does not resemble a TM sequence. In terms of the original TM chain the Γ lattice is found to be composed of the pairs of springs *SS*, *LS*, *LL*, and *SL*. We rename these as *A*, *B*, *C*, and *D*, respectively. The Γ lattice then represents a deterministic sequence of ''bonds,'' which is completely different from a TM sequence, having four letters as its constituents. We have worked out a rule that generates the Γ sequence. The rule is $A\rightarrow AB$, $B\rightarrow CA$, $C\rightarrow CD$, and $D\rightarrow AC$. The seed is *A*. Naturally, using this set of rules backward one can renormalize a Γ lattice as well. In Fig. 1(b) we show the renormalization formalism. Most interestingly we find that both the sublattices Γ_1 and Γ_2 exactly resemble the Γ lattice. Not only that, as special cases, if we choose $A=D$ and $B=C$, we get back the TM sequence, whereas a choice $A=C$ and $B=D$ generates the quasiperiodic period-doubling lattice. Thus we have been able to generate a nonperiodic deterministic sequence that gives rise to a quasiperiodic and an aperiodic sequence at suitable limits. The property of the Γ lattice as discussed above enables us to calculate the $S(q,\omega)$ for this lattice in a straightforward manner using our earlier RSRG method.[29] We present the calculation for the TM lattice. The results presented for the TM lattice have been obtained by using the RSRG recursion relations for the Γ lattice with suitable initial values of the parameters. Some of the results for the Γ lattice itself have been presented for a comparative study.

III. CALCULATION OF $S(q,\omega)$ FOR Γ AND THUE-MORSE LATTICES

The dynamic structure factor that we are going to calculate is defined by

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

where

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

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 that satisfy the equations of motions,

$$-\epsilon_i G_{ij}=-\delta_{ij}+k_{i,i+1}G_{i+1,j}+k_{i,i-1}G_{i-1,j} \tag{3}$$

in the harmonic approximation, where $\epsilon_i=m_i\omega^2-k_{i,i+1}-k_{i,i-1}$, m_i being the mass of the ith mass point, and k_{ij} is the spring constant between the ith and jth atom. The basic spirit of the RSRG calculation lies in splitting the sum involved in Eq. (2) into a sum over two self-similar sublattices. These sublattices are obtained from the original lattice by decimating a chosen subset of sites. Once these sublattices are formed we can express the summmation in Eq. (2) as a combination of two independent sums over these two sublattices. The terms connecting these two sublattices can be eliminated by the use of the Green's function equations of motion written above. The method works in a straightforward manner for Fibonacci and the period-doubling lattices, as has already been shown in the literature.[29,30]

In order to calculate the dynamic structure factor of the Γ lattice, we need to define six values of ϵ_i corresponding to the six varieties of sites in a Γ lattice, depending on the nearest-neighbor environment. These are [Fig. 1(b)] ϵ_α, ϵ_β, ϵ_γ, ϵ_δ, ϵ_μ, and ϵ_ν located between the pairs of ''bonds'' *A-B*, *B-C*, *C-A*, *A-C*, *C-D*, and *D-A*, respectively. The spring constants for the bonds *A*, *B*, *C*, and *D* are denoted by k_A, k_B, k_C, and k_D. Now as one implements the RSRG decimation technique on the Γ lattice using the Green's-function equations of motion, an additional factor f_l appears in front of each term in the summation. To handle these factors we rewrite Eq. (2) as

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

where

$$\mathcal{G}_{ll'}=e^{iq(r_l-r_{l'})}G_{ll'}. \tag{5}$$

All the f_l's are equal to one at the beginning, and grow as the renormalization progresses. To facilitate the RSRG process we need to specify six values for the factors f_l corresponding to the six sites we have already defined. The f_l's are designated as f_α, f_β, f_γ, f_δ, f_μ, and f_ν, respectively. We have been able to derive recursion relations for each of these factors, as will be presented shortly. The sum in Eq. (2) is now partitioned as

$$G_N(q,\omega)=(1/N)\Bigg[\sum_{l\in\Gamma_1,l'\in\Gamma_1} f_l\mathcal{G}_{ll'}+\sum_{l\in\Gamma_2,l'\in\Gamma_2} f_l\mathcal{G}_{ll'}+\sum_{l\in\Gamma_1,l'\in\Gamma_2} f_l\mathcal{G}_{ll'}+\sum_{l\in\Gamma_2,l'\in\Gamma_1} f_l\mathcal{G}_{ll'}\Bigg]. \tag{6}$$

The last two terms in the above equation can be expressed completely in terms of the first two terms by using the set of Eq. (3). Now we are left with two sums, for one of which the indices run over the Γ_1 sublattice only, while for the other sum the indices belong entirely to the Γ_2 sublattice. The sum looks like

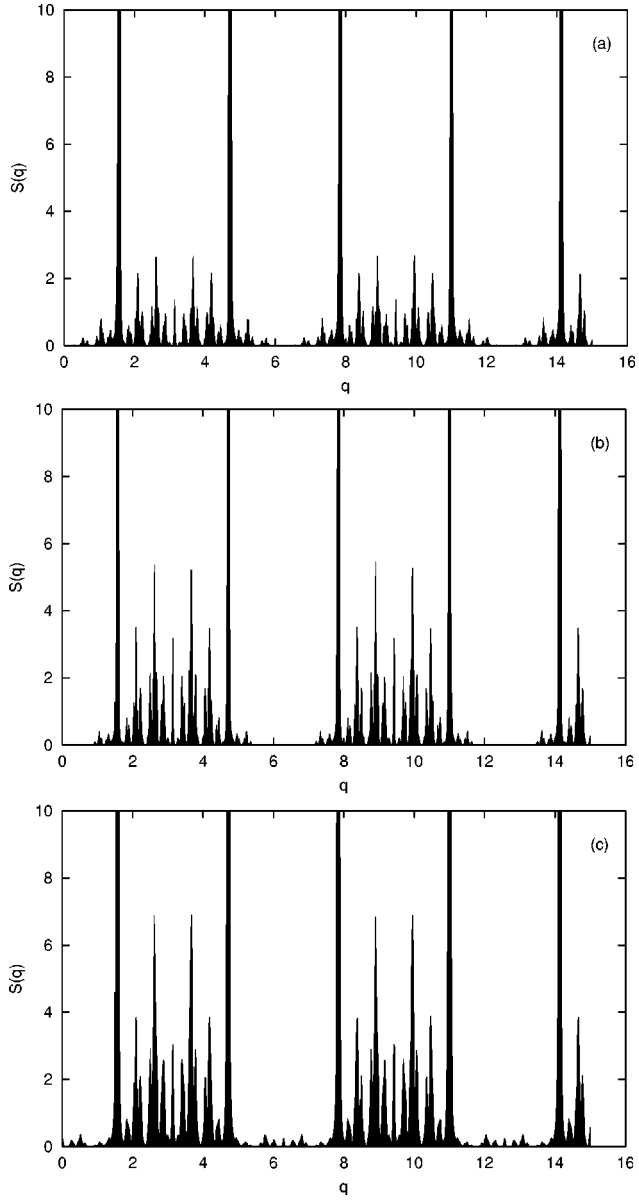

FIG. 2. $S(q,\omega)$ vs q for a Thue-Morse lattice for different fixed values of ω (a) On-site model: $m_\alpha=m_\beta=m_\delta=1$, $m_\gamma=m_\mu=m_\nu=2$, $k_A=k_B=k_C=k_D=1$, and $\omega=1.104\,18$. (b) Transfer model: $m_i=1$ for $i=\alpha$, β, γ, δ, μ, and ν, $k_A=k_D=1$, $k_B=k_C=2$. (c) Mixed model: $m_\alpha=m_\beta=m_\delta=1$, $m_\gamma=m_\mu=m_\nu$, $k_A=k_D=1$, $k_B=k_C=2$, and $\omega=1.174\,59$. In each case the respective values of ω correspond to delocalized modes in infinite chain.

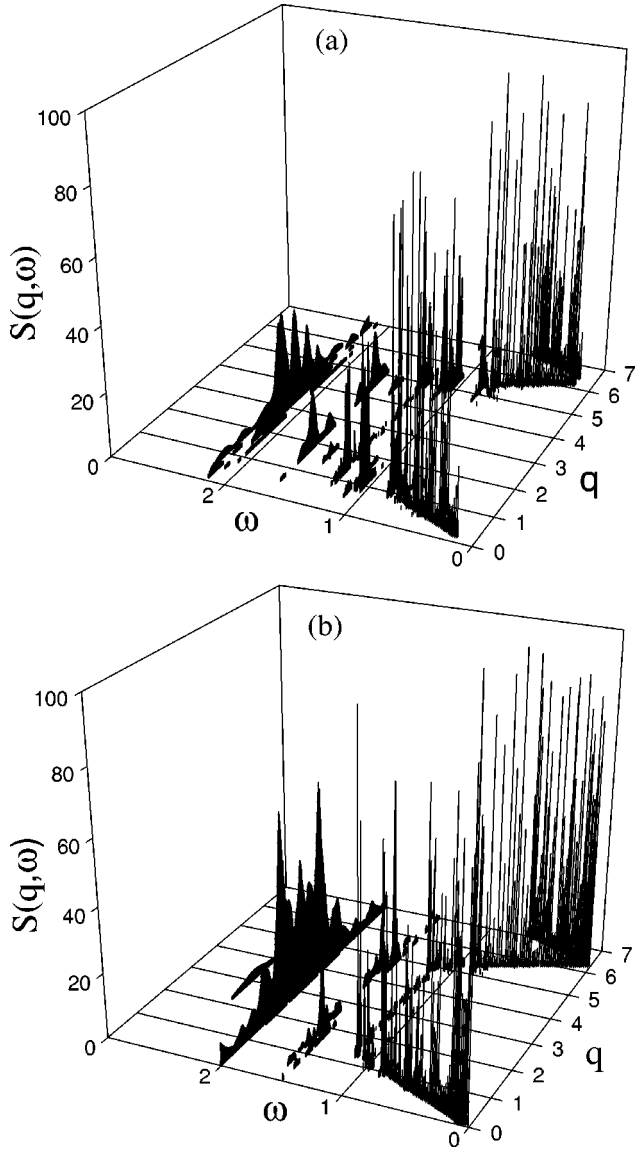

FIG. 3. $S(q,\omega)$ for (a) the Γ lattice with $m_\alpha=1$, $m_\beta=2$, $m_\gamma=2.5$, $m_\delta=1$, $m_\mu=m_\nu=2$, $k_A=1$, $k_B=2$, $k_C=2.5$, and $k_D=1.5$ and (b) the on-site model of the Thue-Morse lattice. The parameters are the same as in Fig. 2(a).

$$G_N(q,\omega)=p_1\left[1/(N_{\Gamma_1})\sum_{ll'}(f_l)_{\Gamma_1}\mathcal{G}_{ll'}\right]+p_2\left[1/(N_{\Gamma_2})\sum_{ll'}(f_l)_{\Gamma_2}\mathcal{G}_{ll'}\right], \tag{7}$$

where $(f_l)_{\Gamma_1}$ and $(f_l)_{\Gamma_2}$ are the new coefficients for the sublattices Γ_1 and Γ_2, respectively. Here, both the factors p_1 and p_2 are equal to 1/2. Since each of the resulting sublattices is a replica of the original Γ lattice, we can carry on the same splitting procedure for each of them. The RSRG process can be viewed as a branching ''genealogical tree'' with each branch splitting up into a Γ_1-Γ_2 pair with the progress of renormalization. The sum is then evaluated in the limit when the spring constants k_i flow to zero under iteration. The recursion relations for the Γ_1 sublattice are given by:

$$\epsilon'_\alpha=\epsilon_\beta+k_C^2/(-\epsilon_\gamma)+k_B^2/(-\epsilon_\alpha),$$

$$\epsilon'_\beta=\epsilon_\delta+k_C^2/(-\epsilon_\mu)+k_A^2/(-\epsilon_\gamma),$$

$$\epsilon'_\gamma=\epsilon_\nu+k_A^2/(-\epsilon_\alpha)+k_D^2/(-\epsilon_\mu),$$

$$\epsilon'_\delta=\epsilon_\beta+k_C^2/(-\epsilon_\mu)+k_B^2/(-\epsilon_\alpha),$$

$$\epsilon'_\mu=\epsilon_\nu+k_A^2/(-\epsilon_\delta)+k_D^2/(-\epsilon_\mu),$$

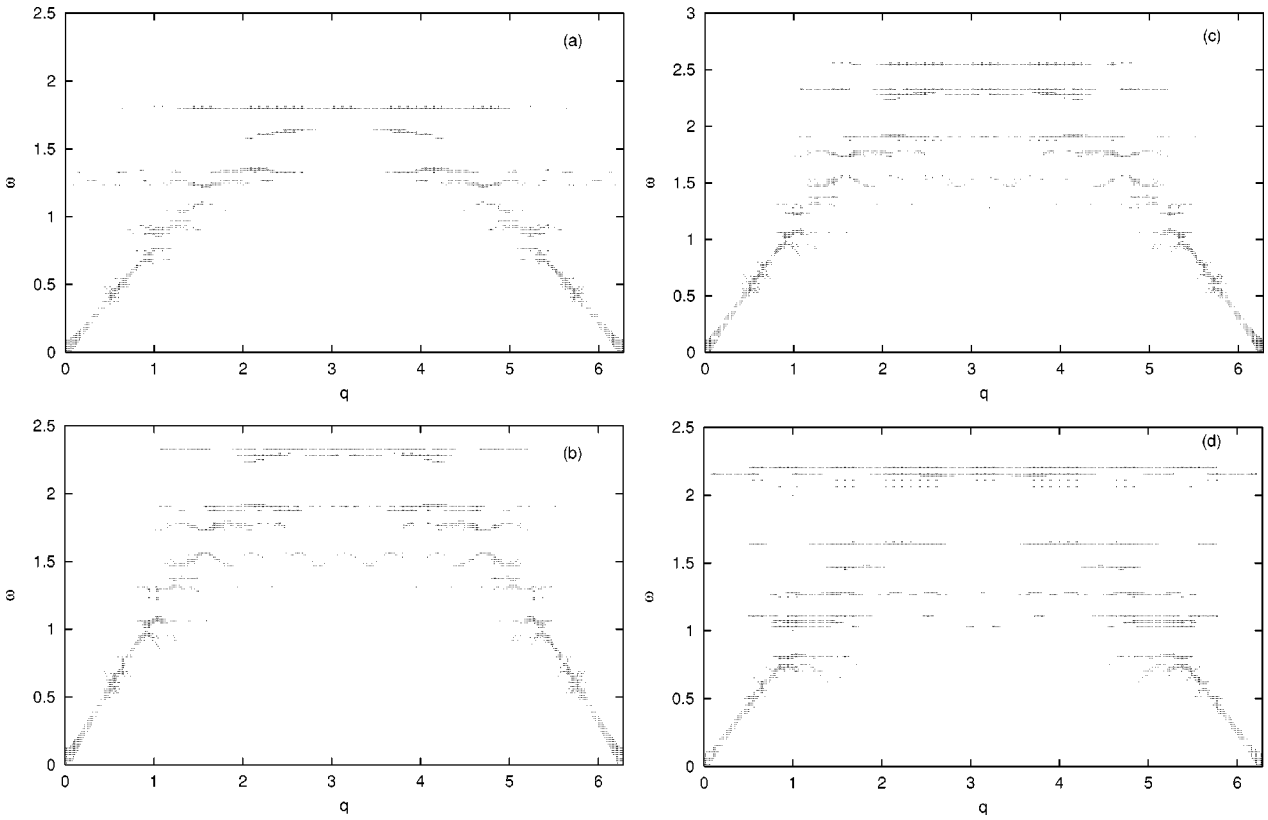

FIG. 4. Dispersion relation for (a) Thue-Morse lattice: on-site model, (b) TM transfer model, and (c) mixed model. In each case the parameters are the same as in Figs. 2(a)–(c). (d) Γ lattice with the parameters same as in Fig. 3(a).

$$\epsilon'_\nu=\epsilon_\gamma+k_A^2/(-\epsilon_\alpha)+k_C^2/(-\epsilon_\delta),$$

$$f'_\alpha=f_\beta+f_\gamma k_C e^{-iqa_C}/(-\epsilon_\gamma)+f_\alpha k_B e^{iqa_B}/(-\epsilon_\alpha),$$

$$f'_\beta=f_\delta+f_\mu k_C e^{-iqa_C}/(-\epsilon_\mu)+f_\gamma k_A e^{iqa_A}/(-\epsilon_\gamma),$$

$$f'_\gamma=f_\nu+f_\alpha k_A e^{-iqa_A}/(-\epsilon_\alpha)+f_\mu k_D e^{iqa_D}/(-\epsilon_\mu),$$

$$f'_\delta=f_\beta+f_\mu k_C e^{-iqa_C}/(-\epsilon_\mu)+f_\alpha k_B e^{iqa_B}/(-\epsilon_\alpha),$$

$$f'_\mu=f_\nu+f_\delta k_A e^{-iqa_A}/(-\epsilon_\delta)+f_\mu k_D e^{iqa_D}/(-\epsilon_\mu),$$

$$f'_\nu=f_\gamma+f_\alpha k_A e^{-iqa_A}/(-\epsilon_\alpha)+f_\delta k_C e^{iqa_C}/(-\epsilon_\delta),$$

$$k'_A=k_B k_A/(-\epsilon_\alpha),$$

$$k'_B=k_C k_A/(-\epsilon_\gamma),$$

$$k'_C=k_C k_D/(-\epsilon_\mu),$$

$$k'_D=k_A k_C/(-\epsilon_\delta),$$

$$a'_A=a_A+a_B,$$

$$a'_B=a_A+a_C,$$

$$a'_C=a_C+a_D,$$

$$a'_D=a_C+a_A. \tag{8}$$

Similarly, for the Γ_2 sublattice the recursion relations are

$$\epsilon'_\alpha=\epsilon_\gamma+k_A^2/(-\epsilon_\delta)+k_C^2/(-\epsilon_\beta),$$

$$\epsilon'_\beta=\epsilon_\mu+k_D^2/(-\epsilon_\nu)+k_C^2/(-\epsilon_\delta),$$

$$\epsilon'_\gamma=\epsilon_\alpha+k_B^2/(-\epsilon_\beta)+k_A^2/(-\epsilon_\nu),$$

$$\epsilon'_\delta=\epsilon_\mu+k_D^2/(-\epsilon_\nu)+k_C^2/(-\epsilon_\beta),$$

$$\epsilon'_\mu=\epsilon_\delta+k_C^2/(-\epsilon_\gamma)+k_A^2/(-\epsilon_\nu),$$

$$\epsilon'_\nu=\epsilon_\alpha+k_B^2/(-\epsilon_\beta)+k_A^2/(-\epsilon_\gamma),$$

$$f'_\alpha=f_\gamma+f_\delta k_A e^{-iqa_A}/(-\epsilon_\delta)+f_\beta k_C e^{iqa_C}/(-\epsilon_\beta),$$

$$f'_\beta=f_\mu+f_\nu k_D e^{-iqa_D}/(-\epsilon_\nu)+f_\delta k_C e^{iqa_C}/(-\epsilon_\delta),$$

$$f'_\gamma=f_\alpha+f_\beta k_B e^{-iqa_B}/(-\epsilon_\beta)+f_\nu k_A e^{iqa_A}/(-\epsilon_\nu),$$

$$f'_\delta=f_\mu+f_\nu k_D e^{-iqa_D}/(-\epsilon_\nu)+f_\beta k_C e^{iqa_C}/(-\epsilon_\beta),$$

$$f'_\mu=f_\delta+f_\gamma k_C e^{-iqa_C}/(-\epsilon_\gamma)+f_\nu k_A e^{iqa_A}/(-\epsilon_\nu),$$

$$f'_\nu=f_\alpha+f_\beta k_B e^{-iqa_B}/(-\epsilon_\beta)+f_\gamma k_A e^{iqa_A}/(-\epsilon_\gamma),$$

$$k'_A=k_C k_B/(-\epsilon_\beta),$$

$$k'_B = k_A k_C/(-\epsilon_\delta),$$

$$k'_C = k_D k_A/(-\epsilon_\nu),$$

$$k'_D = k_C k_A/(-\epsilon_\gamma),$$

$$a'_A = a_B + a_C,$$

$$a'_B = a_A + a_C,$$

$$a'_C = a_D + a_A,$$

$$a'_D = a_C + a_A. \tag{9}$$

In the above set of equations $\epsilon_i = m_i\omega^2 - k_{i,i+1} - k_{i,i-1}$, and i stands for α, β, γ, δ, μ, and ν. The symbols a_j refer to the bond lengths with $j = A$, B, C, and D, respectively. It is to be noted that once we set the parameters in the original Γ chain to represent a TM lattice, the renormalized version Γ_1 preserves the TM ordering. We continue with the splitting process and in the limit $k_i \to 0$, the sum in Eq. (7) typically looks like

$$G_N(q,\omega) = -\sum_{\text{all paths}} p_{(\text{path})} \sum_{i=\alpha,\beta,\gamma,\delta,\mu,\nu} \frac{x_i F_i^*}{\epsilon_i^*}. \tag{10}$$

The ''*'' refers to the fixed point values of the respective quantities and x_i is the concentration of the ith type of site, where i stands for α, β, γ, δ, μ, and ν. The summation above is over all possible paths in the genealogical tree for a given number of branching. Thus, with the help of Eqs. (1) and (10), we finally determine the dynamic structure factor $S(q,\omega)$ for the Γ as well as the TM chain. It is equally straightforward to calculate $S(q,\omega)$ for a PD chain. However, the detailed results for the latter are presented elsewhere,[30] and we skip that discussuion here. The dispersion relation is almost trivially obtained from $S(q,\omega)$ by noting that, for every nonzero value of $S(q,\omega)$ one comes across a set of ω and q values. This set constitutes the dispersion curves when scanned over the entire regime in the ω-q plane.

IV. RESULTS AND DISCUSSION

In Figs. 2(a)–2(c), we plot $S(q)$ against q for three different models of the TM chain for three different frequencies. In each case we start with the Γ lattice with proper initial conditions so as to reproduce three different models of the TM lattice. The on-site model correspods to the case where $m_\alpha = m_\beta = m_\delta$, $m_\gamma = m_\mu = m_\nu$, and $k_A = k_B = k_C = k_D$; for the transfer model $m_\alpha = m_\beta = m_\gamma = m_\delta = m_\mu = m_\nu$ and $k_A = k_D$ and $k_B = k_C$ and the mixed model has the combination $m_\alpha = m_\beta = m_\delta$, $m_\gamma = m_\mu = m_\nu$, $k_A = k_D$, and $k_B = k_C$. It is now well known that an infinite TM lattice supports a countable infinity of extended eigenstates. Results for both the electronic as well as the phonon cases are available. We pick up three eigenfrequencies corresponding to three different extended modes from the available results.[32,33] These eigenfrequencies can be evaluated exactly. In each case the periodic behavior of $S(q)$ against q is clearly seen. The fractal character of $S(q)$ can be revealed on scanning the values of q between any two intervals in finer details. In Fig. 3 we show the three-dimensional plots for $S(q,\omega)$ for Γ and TM lattices. In Figs. 4(a)–4(c), we show the dispersion curves of the TM on-site, transfer, and the mixed models, respectively, while, Fig. 4(d) shows the dispersion relation for the general model of a Γ lattice for comparision. For this case we choose m_α, m_β, etc. as well as k_A, k_B, k_C, and k_D in a completely arbitrary fashion. In each case the 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 aperiodic ordering, and features similar to a periodic case are reproduced. For intermediate values

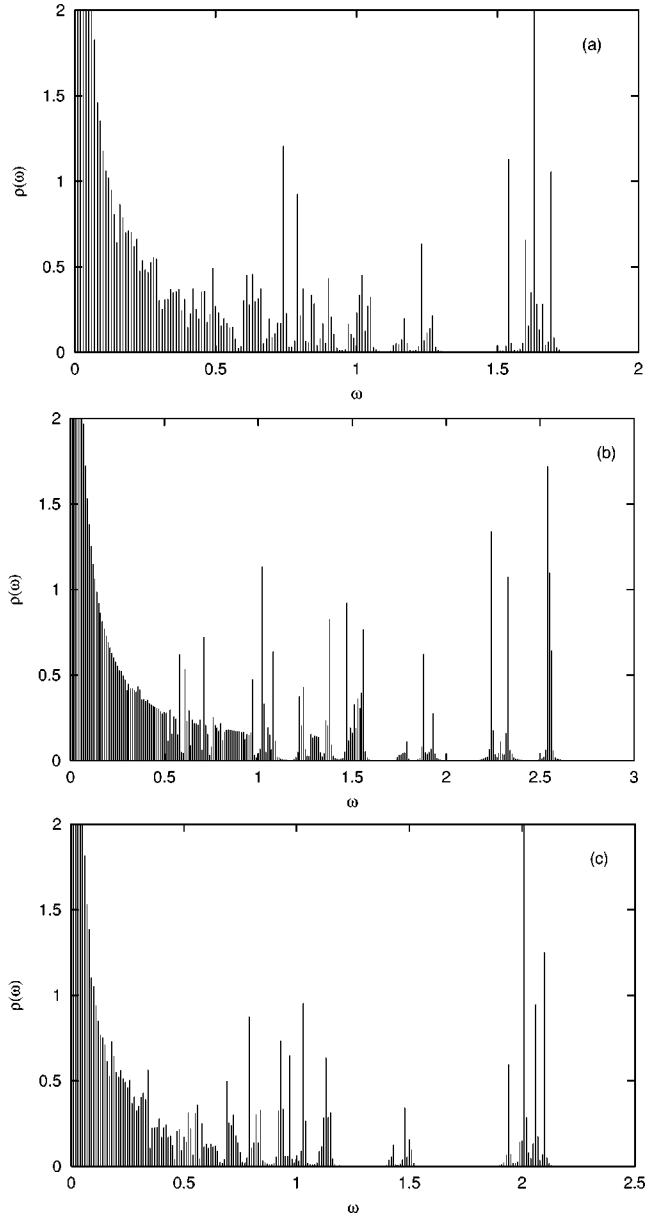

FIG. 5. Average density of states for the TM lattice: (a) on-site model, (b) transfer model, and (c) bond model. The parameters in each case are the same as those used in Fig. 2.

of q the aperiodicity comes into play. This is reflected by the occurence of numerous pseudogaps. In each case the dispersion curves consist of a main branch on which infinite number of satellite branches are superimposed. For the on-site model [Fig. 4(a)], the acoustic branch peaks near what one may call a ''pseudo'' Brillouin-zone boundary,[34] which resembles that of an ordered chain. For the transfer and the mixed models, such boundaries are hard to locate. The optical branch in each case exhibits a fragmented but practically dispersionless character. It is interesting to note that such dispersionless features are also present in case of real quasicrystal.[34,35]

It is well known[36] that flat (dispersionless) optical modes may occur in the vibrational spectrum of a periodic linear chain of atoms, or even in a 3D model. This happens if the intracellular interactions are much stronger than those between the cells. In such cases, independent ''molecular'' vibration takes place in each primitive cell, independent of wavelength of the normal mode.

An infinite TM lattice can be built up by higher and higher order periodic approximants. By renormalizing an nth order periodic approximant $n-1$ times we can map the lattice onto a binary ''ordered'' sequence of bonds $LSLS\cdots$ and so on. One can now calculate the effective coupling constants k_L and k_S by using the recursion relations (8) and (9). This helps in offering a possible explanation to the existence of flat optical branches, viz., those values of Ω for which the intramolecular coupling k_S becomes much greater than the intermolecular coupling k_L are likely to constitute the dispersionless modes. For all these frequencies, the entire lattice vibrates in segments (which form the ''molecules'') and there is a very weak coupling between any two consecutive segments. If we deal with an infinite lattice, then the entire lattice is likely to execute a collective ''molecular'' vibration.

As the band structure of such lattices is highly fragmented, cantorlike, it is really difficult to predict a sharp separation between the acoustic and the optical branches. However, we have checked our prediction for a few values of the frequency, and it seems that our explanation works well. For example, in the on-site model, the frequency 1.78 falls in the dispersionless optical mode. The ratio of the renormalized coupling constants k_S/k_L is of the order of 100 from the third stage of renormalization onwards, which supports our conjecture.

The density of states

The RSRG method used in the calculation of $S(q,\omega)$ can be used straightaway to find out the local density of states (LDOS) and the average density of states (ADOS) of such an aperiodic lattice. The ADOS is given by

$$\rho(\omega) = -\frac{1}{\pi}\lim_{\delta\to 0}\ \mathrm{Im}\left[\frac{1}{N}\sum_i\ G_{ii}(\omega - i\delta)\right]. \qquad (11)$$

This sum does not include any off-diagonal matrix elements. We therefore set all F_i equal to unity at each stage of the renormalization. To calculate the LDOS at any specific site of the TM chain (or even the Γ lattice), one must take into account the successive sequence of branching, i.e., of the sequence of Ω, Γ_1, and Γ_2 through which the chosen site evolves under renormalization. At every stage the appropriate set of recursion relations Eq. (8), or Eq. (9) has to be used. The LDOS is obtained from the local Green's function $G_{00}=1/\epsilon_i^*$ in the limit when k_i's flow to zero under iteration. However, we show in Fig. 5 the ADOS for the TM sequence for the on-site, the transfer, and the mixed models, respectively.

V. CONCLUSIONS

In conclusion, we have presented the computation of the dynamic structure factor of a general substitutional sequence that reproduces the Thue-Morse ordering at special limit. The difficulty involved in dealing directly with the TM structure is thus bypassed. The dispersion curves for both the TM lattice as well as its parent (Γ) lattice are presented. The dispersion curves reveal the presence of infinite number of gaps in both the acoustic and the optical branches. The optical branches exhibit a dispersionless feature which is common even to the real quasicrystals. As a by-product of our scheme we calculate the average density of states for various models of a Thue-Morse lattice.

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