Vibrational properties of a general aperiodic Thue-Morse lattice: Role of the pseudoinvariant of the trace map

Anathnath Ghosh* and S. N. Karmakar†
Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Calcutta 700064, India
(Received 11 May 1999)

Using the real-space renormalization group (RSRG) scheme of Ghosh and Karmakar [Phys. Rev. B **58**, 2586 (1998)], we analytically determine the trace-map relation for a general spring-mass model of the aperiodic Thue-Morse (TM) lattice, and, interestingly observe that this map has a pseudoinvariant. This pseudoinvariant has a crucial role on the nature of the eigenmodes of this lattice. When the pseudoinvariant vanishes identically, as in the case of the on-site, transfer, or mixed model of the TM lattice, all normal modes are found to be delocalized, whereas the eigenmodes are critical for more general models with nonzero pseudoinvariant. Our RSRG scheme also gives the average phonon density of states $\rho(\omega)$ and Lyapunov exponent $\gamma(\omega)$ (= inverse localization length) of the eigenmodes.

I. INTRODUCTION

The discovery of quasicrystalline order in rapidly quenched AlMn alloy[1] stimulated a lot of theoretical interest in the properties of quasiperiodic systems, specially, in one dimension. Studies of such simple model one-dimensional systems become really meaningful after the recent advancements in the fabrication techniques, and it is now possible to synthesize high-quality superlattices[2] arranging different kind of films in a one-dimensional quasiperiodic order. These materials form an intriguing new class of solids in that their macroscopic properties have unusual features characteristic of the quasiperiodic structure, which may be of great technological importance. In fact, theoretical works reveal that quasiperiodic systems have many unique properties, like the critical wave functions, Cantor-set energy spectrum, etc., and the common wisdom is that these are the signature of the underlying quasiperiodic structure.

The well-studied one-dimensional quasiperiodic systems are the Fibonacci,[3–6] period-doubling,[7] and Thue-Morse,[8–10] etc. lattices obtained from the so-called substitutional sequences. The electronic,[11] phonon,[12] optical,[13] etc. properties of these lattices are very conveniently studied with the help of the transfer matrix technique or real-space renormalization group method. Within the transfer matrix formalism, the dynamical trace-map technique introduced by Kohmoto *et al.*[3] turns out to be a very efficient mathematical tool for investigating the physical properties of this class of systems. For the on-site model,[11] the transfer matrices form a set of real 2×2 unimodular matrices, and the nonlinear dynamical trace-map relation, corresponding to the quasiperiodic inflation transformations, can be easily obtained from the unimodular property of the transfer matrices. The major simplification in the trace-map technique results from the fact that it provides a reduced dynamical system, which contains all information of the original physical system.

In some cases, the dimensionality of the dynamical system is further reduced due to the existence of invariant or pseudoinvariant[11,14] (constant of motion) for the dynamical map. But such trace-map relations are usually not known for the transfer or other general models, and the determination of the trace-maps become extremely difficult since the transfer matrices in general do not have the unimodular property. Recently we[10] have introduced a real-space renormalization group (RSRG) technique for finding the trace-map relation corresponding to a very general model of any quasiperiodic system, and explicitly obtained the trace-map relation for a general Thue-Morse (TM) chain. Using this trace-map relation, we have also calculated the electronic energy spectrum for the TM lattice under periodic boundary conditions.

In this present paper, we study in details the vibrational properties of a general spring-mass model[12,15] for the TM lattice using the RSRG method. We analytically observe that the trace map for this general aperiodic TM chain has a pseudoinvariant, and it has an important role on the nature of the eigenmodes of this system. We see that the models for which the pseudoinvariant vanishes support only delocalized eigenmodes, whereas for other cases the states are critical. As an example, all the eigenmodes are delocalized for the on-site, transfer, and mixed models (see text below) of the TM lattice. Axel *et al.*[16] studied the phonon properties of the TM lattice only for the on-site model. However, for understanding the physical properties of real systems, it is necessary to consider much more general models for the system, and it is then possible to verify theoretical predictions about the phonon properties of the lattice (see Ref. 17) by measuring the x-ray or neutron diffraction patterns from the TM superlattices. In this work we investigate the nature of the eigenmodes, phonon spectrum, density of states, and localization behavior of the modes for various models of the TM lattice.

This paper has been organized as follows. In the next section we describe the general model of the TM lattice, and also outline the standard transfer matrix formalism for determining the trace-map relation. In Sec. III, we briefly introduce the RSRG decimation procedure for finding the trace-map relation for the general model of this system, and show that the dynamical map has a pseudoinvariant. In the following section we study the phonon spectrum by trace-map

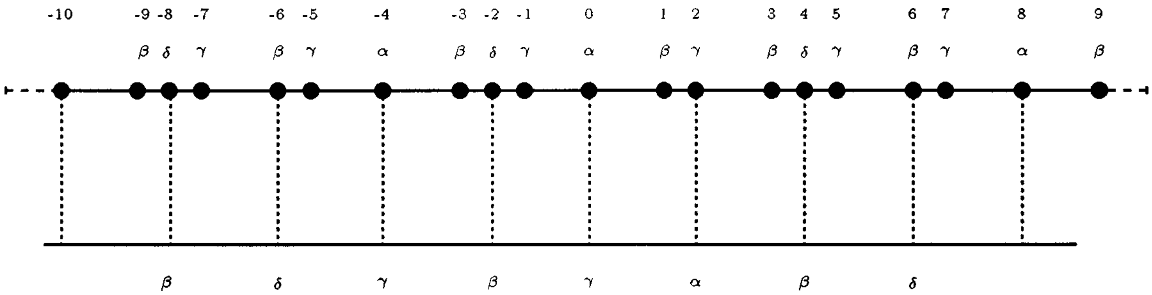

FIG. 1. Section of a Thue-Morse chain illustrating decimation technique.

technique, and also determine the phonon density of states using the RSRG method. In Sec. V, we analyze the nature of the eigenmodes and then calculate the localization length $\xi(\omega)$ of the eigenmodes. Finally we conclude in Sec. VI.

II. THE MODEL AND TRACE MAP BY TRANSFER MATRIX FORMALISM

We describe the classical vibrations of the TM lattice by the usual spring-mass model[15] with nearest-neighbor coupling, and the equations of motion are given by

$$\epsilon_i u_i = K_{i,i+1} u_{i+1} + K_{i,i-1} u_{i-1}, \tag{1}$$

where $\epsilon_i = K_{i,i+1} + K_{i,i-1} - m_i\omega^2$, $K_{i,i\pm1}$'s are spring constants, m_i's are the atomic masses, and u_i's denote amplitudes of vibrations, i being the site index. The transfer model is obtained when all m_i's are equal and K_i's are either K_L or K_S arranged in TM sequence. For the well-known on-site model, $K_{i,i\pm1}$'s are all equal, and m_i's take two values M_A or M_B such that TM aperiodicity is preserved among them. Mixed model is a combination of the above two models, in which both the spring constants and atomic masses are simultaneously arranged according to the TM sequence.

Now we introduce the general model for the TM lattice as follows. The TM sequence can be constructed from two symbols A and B by the inflation rules $A \rightarrow AB$ and $B \rightarrow BA$ starting with the symbol $A(B)$. Also we can generate it by the stacking rules $S_{n+1} = S_n \overline{S_n}$ and $\overline{S_{n+1}} = \overline{S_n} S_n$ with $S_0 = A$ and $\overline{S_0} = B$. The sequence $\overline{S_n}$ is the complement of S_n obtained by interchanging A and B in S_n. So according to these rules, the first few generations of the TM sequence are $S_0 = A$, $S_1 = AB$, $S_2 = ABBA$, $S_3 = ABBABAAB$, etc. Similarly, $\overline{S_0} = B$, $\overline{S_1} = BA$, $\overline{S_2} = BAAB$, $\overline{S_3} = BAABABBA$, etc. are the complementary sequences. Clearly the nth generation sequence $S_n(\overline{S_n})$ contains total 2^n number of symbols. We can represent the symbols A and B as long (L) and short (S) bonds in a lattice, and build the TM chain by arranging these two types of bonds L and S in TM order. A portion of the TM chain is displayed in Fig. 1. In the Thue-Morse chain we can identify four types of sites α, β, γ, and δ corresponding to the lattice points flanked by LL, LS, SL, and SS bonds, respectively (see Fig. 1). Now we define the general spring-mass model for the TM lattice by four types of masses m_α, m_β, m_γ, and m_δ corresponding to α, β, γ, and δ sites of the lattice, respectively, and by two spring constants K_L and K_S for the long and short bonds, respectively. The on-site, transfer, and mixed models are the special cases of this general models, and can be obtained by setting (i) $m_\alpha = m_\beta = m_\gamma = m_\delta = m$ and $K_L \neq K_S$ for transfer model, (ii) $m_\alpha = m_\gamma = m_A$, $m_\beta = m_\delta = m_B$ and $K_L = K_S = K$ for on-site model, and (iii) $m_\alpha = m_\gamma = m_A$, $m_\beta = m_\delta = m_B$, and $K_L \neq K_S$ for mixed model.

Now first we briefly describe how the trace-map relation for the on-site model can be obtained by transfer matrix method, and then indicate what are the difficulties for finding the trace-map relation of the general model by this method. If $M_n(\overline{M_n})$ denotes the global transfer matrix for the nth generation TM sequence $S_n(\overline{S_n})$, then for on-site model M_n's can be expressed in terms of two basic transfer matrices M_A and M_B corresponding to A and B atoms in the lattice. The matrices M_A and M_B are unimodular, and we have

$$M_A = \begin{pmatrix} \epsilon_A & -1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad M_B = \begin{pmatrix} \epsilon_B & -1 \\ 1 & 0 \end{pmatrix},$$

where $\epsilon_{A(B)} = 2K - m_{A(B)}\omega^2$ and $K_L = K_S = K$. So for on-site model, the global transfer matrices $M_0 = M_A$, $M_1 = M_B M_A$, $M_2 = M_A M_B M_B M_A$, etc. are also unimodular, and they satisfy the following recursion relations:

$$M_{n+1} = \overline{M}_n M_n \quad \text{and} \quad \overline{M}_{n+1} = M_n \overline{M}_n \quad \text{for} \quad n \geqslant 0. \tag{2}$$

The trace-map relation for on-site model can be easily found from the above recursion relations using the unimodular property of M_n's, and it is given by[18]

$$a_{n+3} = 4a_{n+1}^2 (a_{n+2} - 1) + 1 \quad \text{for} \quad n \geqslant 0, \tag{3}$$

where $a_n = \frac{1}{2}\mathrm{Tr}\, M_n = \frac{1}{2}\mathrm{Tr}\, \overline{M}_n$.

As in the electronic case, the global transfer matrices M_n's for the general spring-mass model of the TM lattice can be expressed in terms of the following four basic transfer matrices,[10]

$$ll = \begin{pmatrix} \dfrac{\epsilon_\alpha}{K_L} & -1 \\ 1 & 0 \end{pmatrix}, \quad ls = \begin{pmatrix} \dfrac{\epsilon_\beta}{K_S} & -\dfrac{K_L}{K_S} \\ 1 & 0 \end{pmatrix},$$

$$sl = \begin{pmatrix} \dfrac{\epsilon_\gamma}{K_L} & -\dfrac{K_S}{K_L} \\ 1 & 0 \end{pmatrix}, \quad ss = \begin{pmatrix} \dfrac{\epsilon_\delta}{K_S} & -1 \\ 1 & 0 \end{pmatrix}, \tag{4}$$

where $\epsilon_\alpha = 2K_L - m_\alpha\omega^2$, $\epsilon_\beta = K_L + K_S - m_\beta\omega^2$, $\epsilon_\gamma = K_L + K_S - m_\gamma\omega^2$, and $\epsilon_\delta = 2K_S - m_\delta\omega^2$. Under Born–von Karman boundary conditions, the first few global transfer matrices for the general model are

$$\begin{aligned} M_0 &= ll, \\ M_1 &= sl.ls, \\ M_2 &= ll.sl.ss.ls, \\ M_3 &= sl.ls.ll.sl.ls.sl.ss.ls, \\ &\vdots, \end{aligned} \tag{5}$$

while $\overline{M}_n$ can be obtained from M_n by interchanging s and l. In Ref. 10 we have shown that for general model of the TM lattice, the global transfer matrices satisfy the following complex recursion relations:

$$\begin{aligned} M_{n+1} &= \overline{N}_n N_n, \quad N_{n+1} = \overline{M}_n N_n, \\ \overline{M}_{n+1} &= N_n \overline{N}_n, \quad \overline{N}_{n+1} = M_n \overline{N}_n, \end{aligned} \tag{6}$$

for $n \geqslant 0$. The auxiliary transfer matrices N_n and $\overline{N}_n$ can be generated successively starting from $N_0 = ls$ and $\overline{N}_0 = sl$ applying the matrix transformations

$$\begin{aligned} ll &\rightarrow sl.ls, \quad ls \rightarrow ss.ls, \\ sl &\rightarrow ll.sl, \quad ss \rightarrow ls.sl. \end{aligned} \tag{7}$$

The matrices M_n and $\overline{M}_n$ are unimodular, but N_n and $\overline{N}_n$ are not unimodular. Now it is not known how one should proceed from the recursion relations (6) in order to find the trace-map relation for the general model of the TM lattice. One faces the same difficulty also for the transfer and mixed models as the global transfer matrices for these systems again satisfy recursion relations of the form (6).

III. TRACE MAP BY RSRG METHOD: PRESENCE OF PSEUDOINVARIANT

In this section we calculate the trace-map relation for the general spring-mass model of the TM lattice using RSRG technique already developed in Ref. 10. Our RSRG decimation scheme corresponds to the deflation transformations $LS \rightarrow L$, $SL \rightarrow S$, and it ensures that the renormalized lattice also has the TM symmetry. We illustrate this decimation scheme in Fig. 1. Under decimation Eqs. (1) get renormalized and the parameters of the general model satisfy the following recursion relations:

$$\begin{aligned} \epsilon'_\alpha &= \epsilon_\gamma - \omega_\beta(K_L^2 + K_S^2), \\ \epsilon'_\beta &= \epsilon_\delta - K_S^2(\omega_\beta + \omega_\gamma), \\ \epsilon'_\gamma &= \epsilon_\alpha - K_L^2(\omega_\gamma + \omega_\beta), \\ \epsilon'_\delta &= \epsilon_\beta - \omega_\gamma(K_L^2 + K_S^2), \\ K'_L &= K_L K_S \omega_\beta, \quad K'_S = K_L K_S \omega_\gamma, \end{aligned} \tag{8}$$

where $\epsilon_\alpha = 2K_L - m_\alpha\omega^2$, $\epsilon_\beta = K_L + K_S - m_\beta\omega^2$, $\epsilon_\gamma = K_L + K_S - m_\gamma\omega^2$, $\epsilon_\delta = 2K_S - m_\delta\omega^2$, and $\omega_i = 1/\epsilon_i$ with $i = \alpha$, β, γ or δ.

Now we introduce five quantities $W_n = \epsilon_\alpha^{(n)}/K_L^{(n)}$, $X_n = \epsilon_\beta^{(n)}/K_L^{(n)}$, $Y_n = \epsilon_\gamma^{(n)}/K_L^{(n)}$, $Z_n = \epsilon_\delta^{(n)}/K_L^{(n)}$, and $R_n = K_S^{(n)}/K_L^{(n)}$, where the superscript n denotes the stage of renormalization with $n=0$ as the initial system. Then we can recast the above recursion relations into the following form:

$$\begin{aligned} W_{n+1} &= (X_n Y_n - 1 - R_n^2)/R_n, \\ X_{n+1} &= (X_n Y_n Z_n - X_n R_n^2 - Y_n R_n^2)/(Y_n R_n), \\ Y_{n+1} &= (W_n X_n Y_n - Y_n - X_n)/(R_n Y_n), \\ Z_{n+1} &= R_{n+1} W_{n+1}, \\ R_{n+1} &= X_n / Y_n. \end{aligned} \tag{9}$$

In Ref. 10 we have shown that $W_n = \mathrm{Tr} M_n$, and using Eqs. (9) the trace-map relation for the general model of the TM lattice can be written as

$$W_{n+3} = W_{n+1}^2 (W_{n+2} - 2) + 2 + I_{n+1}, \tag{10}$$

where

$$I_{n+1} = \frac{(1+R_{n+1}) W_{n+1} [W_{n+1}(1+R_{n+1}) - X_{n+1} - Y_{n+1}]}{R_{n+1}}, \tag{11}$$

for $n \geqslant 0$. The trace-map relation Eq. (10) is equivalent to the original relation (8) or (9), and it contains all the information about the dynamics of the general TM lattice. Interestingly, we see that this map has a pseudoinvariant[14] given by

$$J_{n+1} = \frac{W_{n+1}(1+R_{n+1}) - X_{n+1} - Y_{n+1}}{R_{n+1}}, \tag{12}$$

as it transforms like $J_{n+1} = -Y_n J_n$ under renormalization. Thus if J_n vanishes at some stage of iteration, it will remain zero in all subsequent higher generations. This tells us that if $I_n = 0$ for some value of n, then it will remain zero for all higher values of n. As an example, the pseudoinvariant J_{n+1} vanishes for $n \geqslant 0$ in the case of transfer, on-site, and mixed models. So we have $I_{n+1} = 0$ $(n \geqslant 0)$ for these three models of the TM lattice, and putting $a_n = W_n/2$ in Eq. (10) we get Eq. (3) as the trace-map relation for them, the initial conditions being different in each case.

Let us now study the behavior of the pseudoinvariant Eq. (12). The notion of the pseudoinvariant used here is not similar to that of Kolar and Ali.[14] They introduced the notion of pseudoinvariant as a recurrent expression that transforms as $J_{n+1} = 4Y_n^2 J_n$, so that non-negative J_n remains non-negative and nonpositive J_n remains nonpositive, while its magnitude may vary with n. On the other hand, we have taken the transformation relation $I_{n+1} = I_n$ corresponding to an invariant quantity I $(\equiv I_n)$ of a map as our starting point (see Refs. 3 and 11) and termed it as pseudoinvariant when the right-hand side of this equation is multiplied by some n-dependent quantity. In this sense Eq. (12) defines a pseudoinvariant for the map Eq. (9). Thus unlike the invariant I, the pseudoinvariant J_n is not a constant of motion for the map. It implies that $J_n=$ const defines a manifold, which evolves with iteration, excepting the case $J_n=0$. The trace-map relation Eq. (9) of TM lattice is a four-dimensional map, and from the recursion relation for J_n, it follows that $J_n=0$ determines a three-dimensional invariant manifold in this space. The orbits of the map remain on this manifold and nonescaping orbits determine the eigenvalues of the system. Now we examine what are the situations for which J_n vanishes. We see that

$$J_0=\begin{cases} \omega^2(m_B-m_A)/K & \text{for on-site model} \\ m\omega^2(1/K_S-1/K_L) & \text{for transfer model} \\ \omega^2(m_B/K_S-m_A/K_L) & \text{for mixed model,} \end{cases}$$

and the above expressions for the pseudoinvariant are very similar to those for the invariant I of the quasiperiodic Fibonacci lattice.[11] Like the invariant I for the Fibonacci lattice, the pseudoinvariant J_0 also vanishes for the simple periodic model, and solutions are extended states which can be obtained rather trivially. There are some studies[19] that show that if the invariant vanishes for any quasiperiodic model, then the system may support delocalized states. For on-site, transfer, and mixed models of the TM lattice, we observe that though the pseudoinvariant $J_0\neq 0$, all other J_n's ($n=1, 2, 3, \ldots$, etc.) are identically zero. So we expect that these systems may support delocalized modes, and in Sec. V we actually prove that all eigenmodes are delocalized for transfer, on-site, and mixed models of the TM lattice.

From an extensive search, it is evident that most of the choices of the parameters m_α, m_β, m_γ, m_δ, K_L, and K_S give $J_0\neq 0$, $J_1=J_2=\cdots=0$, and these models of the TM lattice also support delocalized modes. However, there are some models for which the pseudoinvariants do not vanish and we numerically observe that the eigenmodes are critical in these cases. For these cases, the trace dynamics are quite complex, and we found that the use of the original RSRG Eqs. (8) is much more convenient for characterizing the nature of the states, which we shall discuss in Sec. V.

IV. PHONON SPECTRUM AND DENSITY OF STATES

A. Phonon spectrum

Let us now describe how the allowed frequencies[10,16] of the TM lattice can be determined from the trace-map relation. For Born–von Karman boundary condition, the allowed eigenfrequencies for the nth generation TM lattice can be obtained from the equation $a_n=1$. This relation determines all the 2^n eigenfrequencies of the nth generation chain consisting of 2^n atoms, and in general this equation has to be solved numerically. However, for transfer, on-site, or mixed model, the trace-map relation has a simple form Eq. (3), and it gives a lot of information about the phonon spectrum. It can be shown that the eigenvalue condition $a_n=1$ is equivalent to the set of equations,[10]

$$a_1^2=a_2^2=\cdots=0 \quad \text{and} \quad a_2-1=0. \tag{13}$$

We have to set the initial values a_1 and a_2 appropriately corresponding to transfer, on-site, and mixed models of the system, and these values are (i) for transfer model: $a_1=(\epsilon_{\beta(\gamma)}^2-K_L^2-K_S^2)/(2K_LK_S)$ and $a_2=[\epsilon_\alpha\epsilon_\beta^2\epsilon_\delta-2\epsilon_\beta\epsilon_\delta K_L^2-2\epsilon_\alpha\epsilon_\beta K_S^2]/(2K_L^2K_S^2)+1$, where $\epsilon_\beta=\epsilon_\gamma=K_L+K_S-m\omega^2$, $\epsilon_\alpha=2K_L-m\omega^2$, $\epsilon_\delta=2K_S-m\omega^2$, (ii) for on-site model: $a_1=(\epsilon_A\epsilon_B-2K^2)/(2K^2)$ and $a_2=[\epsilon_A^2\epsilon_B^2-K^2(\epsilon_A+\epsilon_B)^2]/(2K^4)+1$, where $\epsilon_A=2K-m_A\omega^2$, $\epsilon_B=2K-m_B\omega^2$, and (iii) for mixed model: $a_1=(\epsilon_\gamma\epsilon_\beta-K_S^2-K_L^2)/(2K_LK_S)$ and $a_2=[\epsilon_\alpha\epsilon_\beta\epsilon_\gamma\epsilon_\delta-(\epsilon_\beta\epsilon_\delta+\epsilon_\gamma\epsilon_\delta)K_L^2-(\epsilon_\alpha\epsilon_\beta+\epsilon_\alpha\epsilon_\gamma)K_S^2]/(2K_L^2K_S^2)+1$, where $\epsilon_\alpha=2K_L-m_A\omega^2$, $\epsilon_\beta=K_L+K_S-m_B\omega^2$, $\epsilon_\gamma=K_L+K_S-m_A\omega^2$, $\epsilon_\delta=2K_S-m_B\omega^2$. The equation $a_2-1=0$ actually determines the global band edges. For some specific choice of the parameters, the global band edges are situated at (i) $\omega^2=0, 2.438\,45, 3.0$, and $6.561\,55$ for transfer model with parameters $m_A=m_B=1$, $K_L=1$, $K_S=2$, (ii) $\omega^2=0, 1.219\,22, 1.5$, and $3.280\,78$ for on-site model with $m_A=2$, $m_B=1$, $K_L=K_S=1$, and (iii) $\omega^2=0, 1.379\,66, 2.205\,91$, and 5.91443 for mixed model with $m_A=2$, $m_B=1$, $K_L=1$, $K_S=2$. It is apparent from Eqs. (13) that apart from the global band edges, all other eigenfrequencies are doubly degenerate. The hierarchical nature of the trace-map relation Eq. (3) also suggests that the eigenfrequencies of the nth generation chain remain as eigenfrequencies in all the succeeding higher generation chains, and consequently they also belong to the spectrum of the infinite TM lattice. In Figs. 2(a), 2(b) and 2(c), we have plotted the allowed frequencies for transfer, on-site, and mixed models, respectively, for various generations of the TM lattice. These figures clearly show that for any given model, the positions of the global band edges remain unaltered with system size, and also higher generation chains contain all the frequencies of every lower generation chains.

The above kind of analysis about the frequency spectrum is not possible for more general model of the TM lattice having nonzero pseudoinvariant. The allowed frequencies can be found numerically by solving the eigenvalue condition $W_n=2$, and the presence of non-trivial term I_{n+1} in the trace map Eq. (10) indicates that the positions of the global band edges for any arbitrary generation chain are different from those of other generation chains. Also there is in general no normal mode frequency that is common to every generation TM lattice. The spectrum for the general model do not contain any degenerate level. To illustrate all these behaviors of the phonon spectrum of general model, we take the parameters as $m_\alpha=2$, $m_\beta=1$, $m_\gamma=1.77$, $m_\delta=1.33$, $K_L=1$, and $K_S=1.7$, in which case $J_n\neq 0$, and in Fig. 2(d) we plot the allowed frequencies with generation index n. Thus we see that the nature of the phonon spectrum for the general model of the TM lattice is quite different from the spectra for transfer, on-site, and mixed models. In fact, the spectral behavior of the general model of the TM lattice is somewhat similar to those of other quasiperiodic systems, like the Fibonacci chain.

B. Phonon density of states

We now calculate the density of phonon modes for the TM lattice using RSRG scheme presented in Sec. III. For a system corresponding to Eq. (1), the equations of motion for the single-particle Green's functions are given by

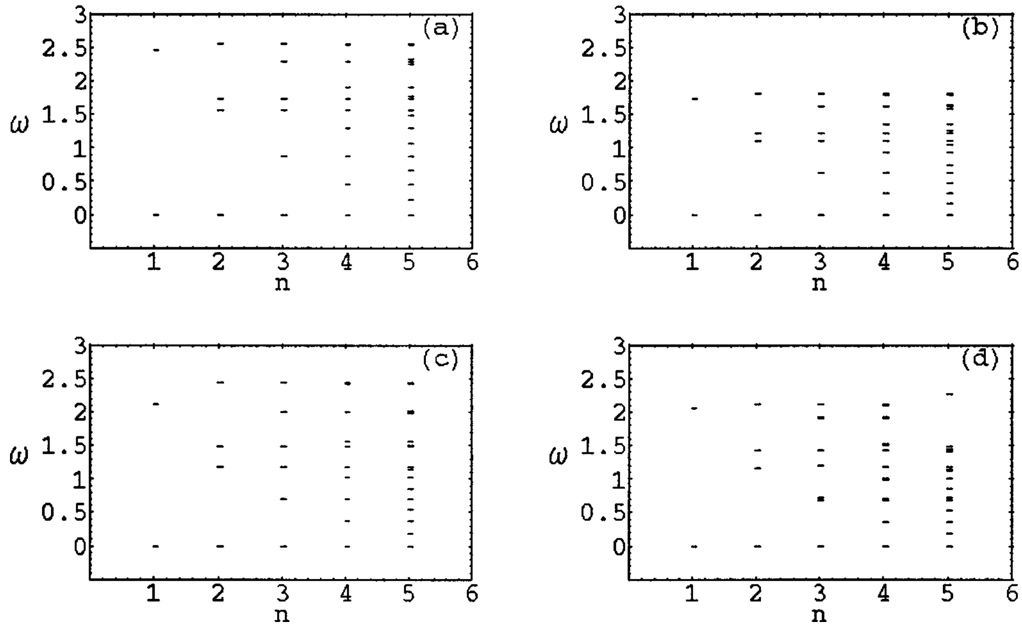

FIG. 2. Plot of allowed frequencies ω for various generations n for (a) transfer model, $m_\alpha = m_\beta = m_\gamma = m_\delta = 1$, $K_S/K_L = 2$, (b) on-site model, $m_\alpha = m_\gamma = 2$, $m_\beta = m_\delta = 1$, $K_L = K_S = 1$, (c) mixed model, $m_\alpha = m_\gamma = 2$, $m_\beta = m_\delta = 1$, $K_S/K_L = 2$, and (d) general model, $m_\alpha = 2$, $m_\beta = 1$, $m_\gamma = 1.77$, $m_\delta = 1.33$, $K_L = 1$, $K_S = 1.7$.

$$\epsilon_i G_{ij}(\omega) = -\delta_{ij} + K_{i,i+1} G_{i+1j}(\omega) + K_{i,i-1} G_{i-1j}(\omega), \tag{14}$$

where $\epsilon_i = K_{i,i+1} + K_{i,i-1} - m_i \omega^{+2}$ and $\omega^+ = \omega + i0^+$. The local density of states can be obtained from the relation

$$\rho_i(\omega) = -\frac{1}{\pi}\mathrm{Im}[G_{ii}(\omega^+)]. \tag{15}$$

If we renormalize the set of Eqs. (14) using the RSRG scheme of Sec. III, the recursion relations for the parameters again satisfy Eqs. (8) provided we replace $\omega \to \omega^+$. The imaginary part of ω^+ ensures that the coupling constants K_L and K_S flow to zero under renormalization and ϵ's attain fixed point values ϵ^*'s. Then the site-diagonal Green's functions can be easily computed from Eq. (14) and the average density of states can be expressed as

$$\rho(\omega) = \frac{1}{\pi}\mathrm{Im}\left[\frac{x_\alpha}{\epsilon_\alpha^*} + \frac{x_\beta}{\epsilon_\beta^*} + \frac{x_\gamma}{\epsilon_\gamma^*} + \frac{x_\delta}{\epsilon_\delta^*}\right], \tag{16}$$

where x_μ is concentration of μth-type site in the TM lattice, μ being either α, β, γ or δ.

In Figs. 3(a), 3(b), 3(c), and 3(d), we have plotted $\rho(\omega)$ as a function of ω, respectively, for transfer, on-site, mixed and general models of the TM lattice. For numerical calculations, we choose the parameter as those in Fig. 2. It is apparent from Figs. 3(a), 3(b), and 3(c) that the global bands for transfer, on-site, and mixed models are confined within the region as determined by the condition $a_2 = 1$. We see from Figs. 3(a), 3(b), 3(c), and 3(d) that the low-frequency regions of these curves are almost identical. This is due to the fact that the low-frequency region corresponds to long-wavelength continuum limit, and in this region phonon density of states becomes a smooth function of the frequency ω. For the sake of comparison, we have also plotted the phonon density of states (dotted curve) for periodic system $m_\alpha = m_\beta = m_\gamma = m_\delta = 1$, $K_L = K_S = 1$. However, in other frequency regions, the curves have very spiky structures, and the spectra are highly fragmented. Thus the vibrational properties of the TM lattice are similar to other quasiperiodic systems, and in this sense the aperiodic TM lattice behaves normally. On the other hand, we see that the eigenmodes are extended rather than critical for transfer, on-site, and mixed models, while in case of general model with nonvanishing pseudoinvariant the eigenmodes are critical.

V. NATURE OF THE EIGENMODES FOR TRANSFER, ON-SITE, AND MIXED MODELS

In order to study the nature of the eigenmodes for transfer, on-site, and mixed models of the TM lattice in details, let us first start from the global transfer matrices M_n and $\bar{M}_n$, and the auxiliary matrices N_n and $\bar{N}_n$. These matrices can be written as

$$N_n = \alpha_n \Pi + \beta_n \sigma_x + \gamma_n \sigma_y + \delta_n \sigma_z,$$

$$\bar{N}_n = \bar{\alpha}_n \Pi + \bar{\beta}_n \sigma_x + \bar{\gamma}_n \sigma_y + \bar{\delta}_n \sigma_z,$$

$$M_n = a_n \Pi + b_n \sigma_x + c_n \sigma_y + d_n \sigma_z,$$

$$\bar{M}_n = \bar{a}_n \Pi + \bar{b}_n \sigma_x + \bar{c}_n \sigma_y + \bar{d}_n \sigma_z, \tag{17}$$

where σ_x, σ_y, σ_z are 2×2 Pauli matrices, Π is a 2×2 identity matrix. The parameters O_n's ($O = \alpha, \beta, \gamma, \delta, a, b, c$, and d) satisfy, respectively, the following recursion relations:

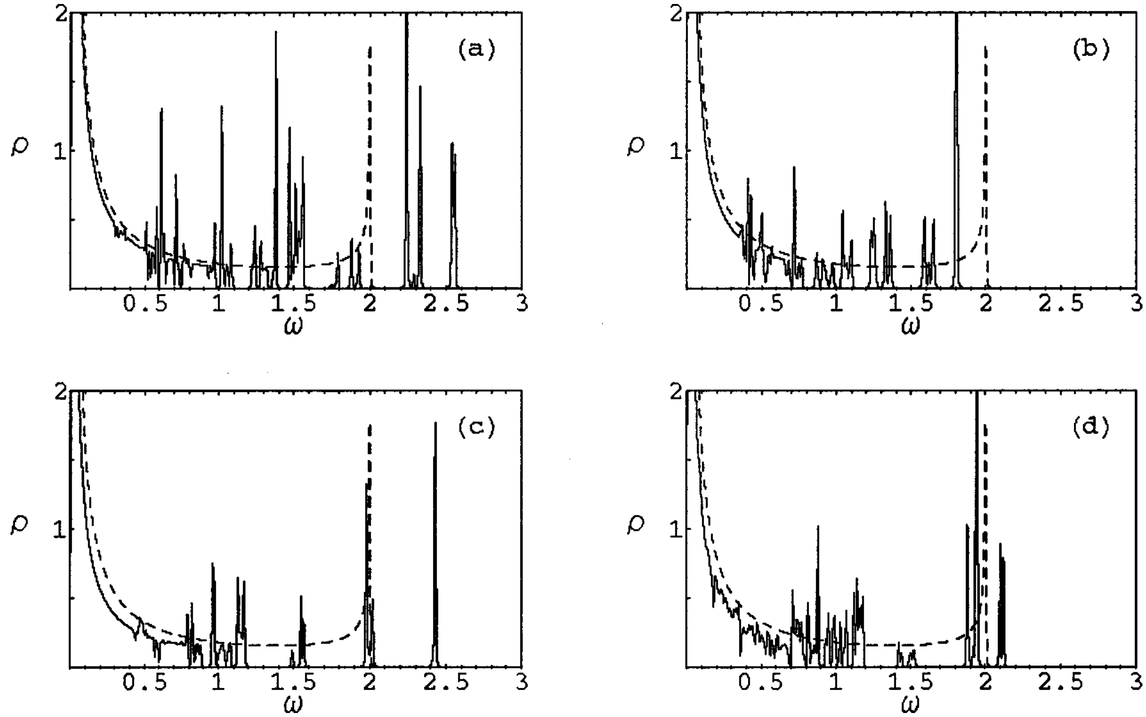

FIG. 3. Plot of $\rho(\omega)$ vs ω for (a) transfer, (b) on-site, (c) mixed, and (d) general models with parameters as those in Fig. 2.

$$\alpha_{n+1}=\overline{a}_n\alpha_n+\overline{d}_n\delta_n+\overline{b}_n\beta_n+\overline{c}_n\gamma_n,$$

$$\beta_{n+1}=\overline{b}_n\alpha_n+\overline{a}_n\beta_n+i(\overline{c}_n\delta_n-\overline{d}_n\gamma_n),$$

$$\gamma_{n+1}=\overline{a}_n\gamma_n+\overline{c}_n\alpha_n+i(\overline{d}_n\beta_n-\overline{b}_n\delta_n),$$

$$\delta_{n+1}=\overline{a}_n\delta_n+\overline{d}_n\alpha_n+i(\overline{b}_n\gamma_n-\overline{c}_n\beta_n),$$

$$a_{n+1}=\overline{\alpha}_n\alpha_n+\overline{\delta}_n\delta_n+\overline{\beta}_n\beta_n+\overline{\gamma}_n\gamma_n,$$

$$b_{n+1}=\beta_n\overline{\alpha}_n+\overline{\beta}_n\alpha_n+i(\overline{\gamma}_n\delta_n-\gamma_n\overline{\delta}_n),$$

$$c_{n+1}=\gamma_n\overline{\alpha}_n+\overline{\gamma}_n\alpha_n+i(\beta_n\overline{\delta}_n-\overline{\beta}_n\delta_n),$$

$$d_{n+1}=\overline{\alpha}_n\delta_n+\overline{\delta}_n\alpha_n+i(\overline{\beta}_n\gamma_n-\overline{\gamma}_n\beta_n), \tag{18}$$

with

$$\alpha_0(\overline{\alpha_0})=\delta_0(\overline{\delta_0})=\epsilon_\beta/2K_S(\epsilon_\gamma/2K_L),$$

$$\beta_0(\overline{\beta_0})=(K_S-K_L)/2K_S[(K_L-K_S)/2K_L],$$

$$\gamma_0(\overline{\gamma_0})=-(i/2)(K_L+K_S)/K_S[-(i/2)(K_L+K_S)/K_L],$$

$$a_0(\overline{a_0})=d_0(\overline{d_0})=\epsilon_\alpha/2K_L(\epsilon_\delta/2K_S),$$

$$b_0(\overline{b_0})=0 \quad \text{and} \quad c_0(\overline{c_0})=-i.$$

The recursion relations for the parameters $\overline{O}_n$'s can be obtained from Eqs. (18) by replacing $O\rightarrow\overline{O}$ and $\overline{O}\rightarrow O$ in these equations.

The recursion relations for the parameters have a quite complex structure for the general case. Interestingly, we observe that these relations get simplified when we impose the restrictions on the parameters corresponding to transfer, on-site, or mixed models of the TM lattices. These restrictions are (i) $m_\alpha=m_\gamma=m_A$, $m_\beta=m_\delta=m_B$, and $K_L=K_S$ for on-site model, (ii) $m_\alpha=m_\beta=m_\gamma=m_\delta$ and $K_L\neq K_S$ for transfer model, and (iii) $m_\alpha=m_\gamma=m_A$, $m_\beta=m_\delta=m_B$, and $K_L\neq K_S$ for mixed model. Then we can treat these three cases on a common footing, and the recursion relations for the parameters of the global transfer matrices M_n and $\overline{M}_n$ become identical in form. After some lengthy algebra, we can express them into the following compact form:

$$a_{n+2}=1+a_n^2f_n^{(a)},$$

$$\overline{a}_{n+2}=1+\overline{a}_n^2\overline{f}_n^{(a)},$$

$$b_{n+2}=a_nf_n^{(b)},$$

$$\overline{b}_{n+2}=\overline{a}_n\overline{f}_n^{(b)},$$

$$c_{n+2}=a_nf_n^{(c)},$$

$$\overline{c}_{n+2}=\overline{a}_n\overline{f}_n^{(c)},$$

$$d_{n+2}=a_nf_n^{(d)},$$

$$\overline{d}_{n+2}=\overline{a}_n\overline{f}_n^{(d)} \qquad \text{for} \qquad n\geqslant 1, \tag{19}$$

where $f_n^{(a)}(\overline{f}_n^{(a)})$, $f_n^{(b)}(\overline{f}_n^{(b)})$, $f_n^{(c)}(\overline{f}_n^{(c)})$, and $f_n^{(d)}(\overline{f}_n^{(d)})$ are functions of O_n's and $\overline{O}_n$'s ($O=\alpha,\beta,\gamma,\delta,a,b,c,$ and d). The explicit expression for $f_n^{(a)}$ and $\overline{f}_n^{(a)}$ are $f_n^{(a)}=4(a_{n+1}-1)$ and $\overline{f}_n^{(a)}=4(\overline{a}_{n+1}-1)$, and the analytic expression for other f's can be easily calculated. Now we can identify the parameters a_n and $\overline{a}_n$ in Eq. (19) as the traces $a_n=\frac{1}{2}\mathrm{Tr}M_n$

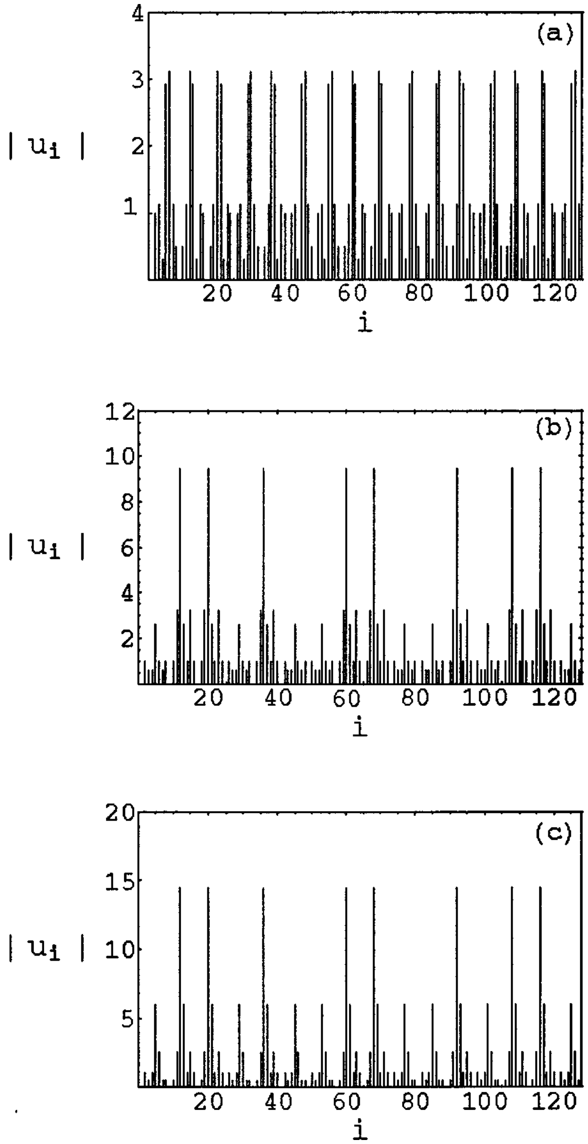

FIG. 4. Plot of $|u_i|$ vs i at (a) $\omega=2.288\,25$ for transfer, (b) $\omega=1.618\,03$ for on-site, and (c) $\omega=2.0$ for mixed models with parameters as those in Figs. 2(a), 2(b), and 2(c), respectively.

and $\overline{a}_n=\frac{1}{2}\mathrm{Tr}\overline{M}_n$ and we have the equality $a_n=\overline{a}_n$ (since $\mathrm{Tr}M_n=\mathrm{Tr}\overline{M}_n$ for $n\geqslant 1$). So we can insert the eigenvalue conditions $a_1^2(\overline{a_1^2})=a_2^2(\overline{a_2^2})=\cdots=a_n^2(\overline{a_n^2})=0$ [see Eqs. (13)] into the Eq. (19), and get $a_{n+2}=\overline{a}_{n+2}=1$ and $b_{n+2}(\overline{b}_{n+2})=c_{n+2}(\overline{c}_{n+2})=d_{n+2}(\overline{d}_{n+2})=0$, giving $M_{n+2}=\overline{M}_{n+2}=\Pi$ for all $n\geqslant 1$. The transfer matrices M_n and $\overline{M}_n$ correspond to the sequences S_n and $\overline{S}_n$, and we can consider S_n and $\overline{S}_n$ as the building blocks for the infinite TM lattice. Thus the global transfer matrix for the infinite TM lattice becomes identity at the frequencies obtained from the roots of the equations $a_1^2(\overline{a_1^2})=a_2^2(\overline{a_2^2})=\cdots=a_n^2(\overline{a_n^2})=0$, and consequently the systems support delocalized eigenmodes. In Fig. 4 we have plotted the amplitudes of the phonon modes as a function of the site index i for (a) transfer model, $m_\alpha=m_\beta=m_\gamma=m_\delta=1$ and $K_L=1$, $K_S=2$ at $\omega=2.288\,25$, (b) on-site model, $m_A=2$, $m_B=1$, and $K_L=K_S=1$ at $\omega=1.618\,03$, and (c) mixed model, $m_A=2$, $m_B=1$, $K_L=1$, $K_S=2$ at $\omega=2$. These figures clearly indicate the delocalized nature of the vibrational modes for the transfer, on-site, and mixed models of the TM lattice. But at the global band edges we have $a_2-1=0$, and at these frequencies the matrices M_n and $\overline{M}_n$ no longer become identity matrix. We observe numerically that at the global band edges, the amplitudes u_N behaves as $\sim N$ (N being the system size).

Alternatively, the study of the localization behavior of the modes also gives information about the nature of the states. The Lyapunov exponent $\gamma(\omega)$, being the inverse of the localization length $\xi(\omega)$, can be easily calculated from our RSRG scheme, and it can be expressed as[20]

$$\gamma(\omega)=\mathrm{Lt}_{n\to\infty}\left[\frac{1}{2^n}\ln\left|K_S^{(n)}\right|\right], \tag{20}$$

where $K_S^{(n)}$ is the nth renormalized value of the spring-constant K_S. It is to be noted that the value of $\gamma(\omega)$ is quite independent of the choice of $K_L^{(n)}$ or $K_S^{(n)}$, since both of them attain fixed point values in the limit $n\to\infty$ and hence they carry the same information about the system.

We notice that the Lyapunov exponent always vanishes precisely at all allowed normal mode frequencies of the system corresponding to any model of the TM lattice. So the localization length is infinity for any arbitrary model of the TM lattice. It means that the vibrations are not confined within any finite region of the lattice, and the modes should have extended character. However, a careful study of the flow pattern of the effective coupling constants with renormalization shows that the models with zero pseudoinvariant behave quite differently from those having nonzero pseudoinvariant. We see that the effective coupling constants always flow to zero under renormalization for systems with nonzero pseudoinvariant. But from a physical point of view, the effective coupling constants should never flow to zero on renormalization for delocalized modes. This clearly shows that the states are neither localized nor extended for models with nonzero pseudoinvariant, and obviously the eigenmodes are critical in these cases. On the other hand, when the pseudoinvariant vanishes identically as in the case of transfer, on-site, or mixed models, the effective coupling constants never flow to zero with renormalization at all allowed frequencies of the system. It implies that the models of the TM lattice having zero pseudoinvariant support delocalized eigenmodes. From the above analysis we see that the vanishing of the pseudoinvariant has an important role on the nature of the eigenmodes of the TM lattice.

At this point we would like to make the following comments. There are several well-established approaches for characterizing the critical nature of eigenstates in quasiperiodic systems. One way of understanding the critical wave functions is the demonstration that their amplitudes do not tend to zero at infinity, but are bounded below through the system[21]. There are some approaches for characterizing the extend critical eigenstates.[19,22] The multifractal method provides another tool for characterizing critical eigenfunctions.[11] Now the crucial point is that in these methods, we need a prior knowledge about the amplitudes of the wave function. But for TM lattice we have a four-dimensional nonlinear trace-map relation when pseudoinvariant does not vanish, and we have to determine the normal mode frequencies numerically from this trace-map relation. This introduces error in the computation of normal mode frequencies, and consequently the normal mode amplitudes cannot be calculated with sufficient accuracy. Actually the calculations of the amplitudes become quite unstable due to the Cantor-set nature of the spectrum, and also due to the fact that the error magnifies very rapidly in the case of TM lattice as its trace map has higher dimensionality than that of the Fibonacci lattice. So it is not possible to characterize the critical nature of the states of TM lattice using the above-mentioned approaches. For this reason we have characterized the critical nature of the modes of TM lattice in an alternative way as discussed in the previous paragraph on the basis RSRG method.

The absence of a well-suited mathematical framework to obtain analytical results on the behavior of random, quasiperiodic, and incommensurate systems has led to the introduction of what has been referred to as diagnostic tools by Sanchez *et al.*[23] These include transmission coefficient, Landauer resistance, Lyapunov coefficient, integrated density of states, inverse participation ratio, and the multifractal analysis of the wave-function measure. Although the information that any one of these tools can provide isolately is not conclusive as rigorous proof, when grouped together they can produce quite compelling evidence about the nature of the considered states. In this context our method provides another such diagnostic tool, namely, the study of the recurrent properties of the pseudoinvariant. In this sense, the present method is in line with the recent work by Naumis,[6] where the study of Lyapunov exponents is introduced as a suitable tool to classify the corresponding eigenstates as extended, localized, or critical ones.

VI. CONCLUSIONS

In this paper, we study in details the vibrational properties of the aperiodic TM lattice using various models for the system. Using RSRG method we determine the trace-map relation for a general model of the TM chain, and show that this dynamical map has a pseudoinvariant. We observe that the pseudoinvariant plays a key role in characterizing the nature of the normal modes of the system. When pseudoinvariant vanishes identically as in transfer, on-site, and mixed models, all eigenmodes except those corresponding to the global band edges have delocalized character. While for models with nonzero pseudoinvariant, the eigenmodes are all critical in nature. Interestingly, we observe that the transfer, on-site, and mixed models satisfy the same trace-map relation, and analysis of the trace-map relation shows that for these systems, all eigenfrequencies are doubly degenerate except those corresponding to the global band edges. Using the present RSRG procedure, the phonon density of states and the Lyapunov exponents can also be calculated easily.

*Electronic address: anath@cmp.saha.ernet.in
†Electronic address: sachin@cmp.saha.ernet.in

[1] D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).
[2] R. Merlin, K. Bajema, Roy Clarke, F.-Y. Juang, and P. K. Bhattacharya, Phys. Rev. Lett. **55**, 1768 (1985).
[3] M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).
[4] Kazumoto Iguchi, Phys. Rev. B **43**, 5915 (1991); **43**, 5919 (1991); M. Kohmoto, Bill Sutherland, and K. Iguchi, Phys. Rev. Lett. **58**, 2436 (1987); Kazumoto Iguchi, Mater. Sci. Eng. B **15**, L13 (1992); Kazumoto Iguchi, Int. J. Mod. Phys. B **11**, 2157 (1997).
[5] X. Huang and C. Gong, Phys. Rev. B **58**, 739 (1998).
[6] G. G. Naumis, Phys. Rev. B **59**, 11 315 (1999).
[7] J. M. Luck, Phys. Rev. B **39**, 5834 (1989).
[8] C. S. Ryu, G. Y. Oh, and M. H. Lee, Phys. Rev. B **46**, 5162 (1992); **48**, 132 (1993).
[9] A. Chakabarti, S. N. Karmakar, and R. K. Moitra, Phys. Rev. Lett. **74**, 1403 (1995); Lewen Fan and Zhifang Lin, *ibid.* **75**, 2903 (1995).
[10] Anathnath Ghosh and S. N. Karmakar, Phys. Rev. B **58**, 2586 (1998).
[11] M. Kohmoto, Bill Sutherland, and C. Tang, Phys. Rev. B **35**, 1020 (1986).
[12] M. Quilichini and T. Janssen, Rev. Mod. Phys. **69**, 277 (1997).
[13] M. Kohmoto, Bill Sutherland, and K. Iguchi, Phys. Rev. Lett. **58**, 2436 (1987).
[14] M. Kolář and M. K. Ali, Phys. Rev. A **39**, 6538 (1989).
[15] H. Hiramoto and M. Kohmoto, J. Phys. Soc. Jpn. **65**, 3915 (1996).
[16] F. Axel and J. Peyriére, J. Stat. Phys. **56**, 1013 (1989).
[17] Anathnath Ghosh and S. N. Karmakar, Phys. Rev. B **57**, 2834 (1998).
[18] F. Axel, J. P. Allouche, M. Kléman, M. Mendés-France, and J. Peyriére, J. Phys. (Paris), Colloq. **47**, C3-181 (1986).
[19] V. Kumar, J. Phys.: Condens. Matter **2**, 1349 (1990); A. Chakrabarti, S. N. Karmakar, and R. K. Moitra, Phys. Lett. A **168**, 301 (1992).
[20] Riccardo Farchioni and Giuseppe Grosso, Phys. Rev. B **51**, 17 348 (1995).
[21] B. Iochum and D. Testard, J. Stat. Phys. **65**, 715 (1991).
[22] E. Macia and F. Dominguez-Adame, Phys. Rev. Lett. **76**, 2957 (1996).
[23] A. Sanchez, E. Macia, and F. Dominguez-Adame, Phys. Rev. B **49**, 147 (1994).