

Renormalization-Group Study of One-Dimensional Quasiperiodic Systems

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We report a new approach to the study of electron spectral clustering and wave-function scaling in several one-dimensional quasiperiodic systems. The approach is based on renormalization-group ideas. We introduce a novel decimation technique which generates a simple physical picture of the electron spectral behavior and the nature of the wave functions. Our renormalization-group scheme is verified by the numerical computation of the probability density summed over the states belonging to the clusters and subclusters of the spectrum.

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Recently, there have been a number of studies of phonon and tight-binding electron models on one-dimensional (1D) quasiperiodic (QP) lattices, motivated by the discovery^{1,2} of the quasicrystal phase. Now, such studies become directly relevant to experiments because of the actual construction of a Fibonacci superlattice of GaAs-AlAs by Merlin *et al.*³

In this Letter, we report a new approach to the study of spectral clustering and wave-function scaling in several 1D QP systems. The approach is based on renormalization-group (RG) ideas. A main virtue of it lies in the introduction of a novel decimation technique which generates a very simple and intuitive physical picture of the spectral behavior and the nature of the wave functions.

We will concentrate our attention on the tight-binding electron model defined by $t_{n,n+1}\psi_{n+1} + t_{n,n-1}\psi_{n-1} + \epsilon_n\psi_n = E\psi_n$, where ϵ_n and ψ_n are respectively the site energy and the probability amplitude at the n th site, while $t_{n,n+1} = t_{n+1,n} \equiv T_n$ is the hopping transition amplitude associated with the bond between site n and site $n+1$. Three simpler cases will be considered. In case (A), the site energies ϵ_n are constant (which will be absorbed into the eigenenergy E), and the bonds take two values, T_s (strong) and T_w (weak), arranged in a Fibonacci sequence. This sequence is generated² by repeated applications of the substitution rule $T_w \rightarrow T_w T_s$ and $T_s \rightarrow T_w$, starting from the initial sequence $S_1 = T_w$. Therefore, $S_2 = T_w T_s$, $S_3 = T_w T_s T_w$, $S_4 = T_w T_s T_w T_w T_s$, and so on. Case (B) is the same as (A), but with the interchange $T_w \leftrightarrow T_s$. In case (C), the bonds are constant, $T_n = T$, but the site energies take two values, V_1 and V_2 , arranged in a Fibonacci sequence.

The above models were recently proposed and studied by several groups.^{4,5} They found self-similar structures in the spectrum and the wave functions. In this work, we introduce a RG analysis, which directly

relates the self-similarity of the spectrum and the wave functions to that of the underlying lattice. In addition, the behavior of each wave function can be simply related to the position of its energy in the hierarchical structure of the spectrum. The theoretical prediction, made in Ref. 4, of the existence of many localized states located in gaps has been experimentally confirmed.⁶ The scaling behavior of the localization length of these states can also be analyzed by our RG approach, but this will be presented in future publications.⁷

Consider first the case (A), for which Fig. 1(a) is a typical plot of the energy spectrum. One of the goals of our RG, as described below, is to explain the trifurcating pattern exhibited in the spectrum.

In the following, we describe the RG procedure for this case. In the absence of the weak bonds ($T_w = 0$), the Fibonacci lattice is broken into isolated sites (atoms) and double sites (molecules). The spectrum then consists of three infinitely degenerate levels: $E = 0$ for the atomic states and $E = \pm T_s$ for the bonding and antibonding molecular states. As we take the weak bonds into account, these states are coupled together. However, the dominant effect is the resonant coupling among the states of the same energy.

We can construct an effective Hamiltonian⁷ within a given degenerate level. The elimination of states outside this level produces effective couplings among the degenerate states. As an approximation we will only keep the first two leading terms. Energy shifts of the same order as the smaller term kept in the effective couplings can occur and can be taken into account. However, they will be ignored here in order to simplify the description of our RG.

For the level $E = 0$, the renormalized lattice consists of the atomic sites in the original lattice. These sites are connected by the effective bonds $-T_w^2/T_s$ and T_w^3/T_s^2 . The former is for atoms separated by one

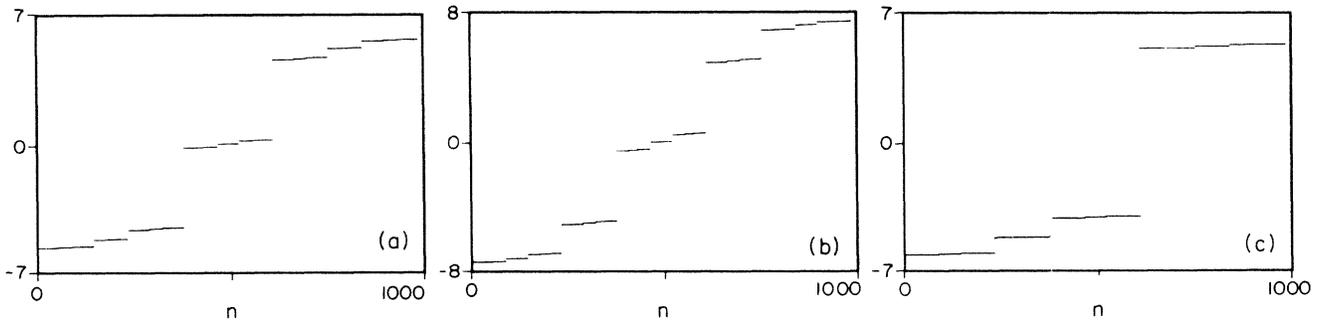


FIG. 1. Energy spectrum of our model in the three cases, (A), (B), and (C), specified in the text. The eigenenergies are plotted from left to right in increasing order. The lattice has 987 sites and fixed-end boundary conditions. (a) Case (A), with $T_w = 1$ and $T_s = 5$; (b) case (B), with $T_w = 1$ and $T_s = 5$; (c) case (C), with $T = 1$, $V_1 = -5$, and $V_2 = 5$.

molecule in the original lattice, while the latter is for atoms separated by two neighboring molecules. These bonds are arranged in a Fibonacci sequence, so that the structure of the new lattice is the same as its mother lattice (see Fig. 2). The associated probability densities, defined below, are shown in Fig. 3. For the level $E = T_s$, the basic units of the renormalized lattice are the bonding molecular states in the unperturbed original lattice. These units are connected by the effective bonds $T_w/2$ and $T_w^2/2T_s$. The former is between the bonding states of neighboring molecules in the original lattice, while the latter is for the bonding states of molecules mediated by an atomic site. Again, the arrangement of the bonds is a Fibonacci sequence, which gives the new lattice the same structure as the original one (see Fig. 4). Finally, for the level $E = -T_s$, we have a new lattice of antibonding molecules. The bonds are $-T_w/2$ and $T_w^2/2T_w$ arranged in a Fibonacci sequence. This completes the first step of our RG analysis.

In the second step of our RG analysis, we first remove the weaker bonds in the new lattices obtained in the first step. We are then left with the isolated units (superatoms) and bonding and antibonding double units (supermolecules). The three levels $E = 0, \pm T_s$ are then each split into three sublevels. For each of

these sublevels we can construct a Fibonacci lattice, using the method of resonant coupling.

This procedure continues on and on, and eventually we obtain a spectral pattern of three main clusters (bands), each of which consists of three subclusters (subbands), and so on. In general, the middle cluster (or subcluster) is narrower than the side clusters by a ratio of order $|T_w/T_s|$. This explains the trifurcating structure of the spectrum found by Nori and Rodriguez⁴ [also see Fig. 1(a)].

It must be emphasized that our RG approach is only exact in the limit of $|T_w/T_s| \ll 1$ [in cases (A) and (B)] or $|T/(V_1 - V_2)| \ll 1$ [in case (C)]. However, as can be verified from the numerical results of Ref. 4,

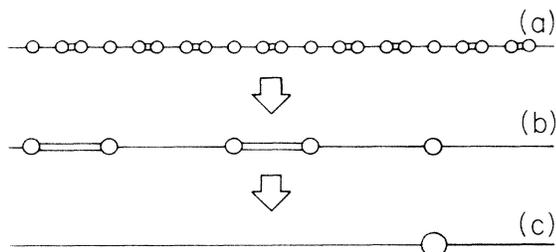


FIG. 2. Schematic representation of the decimation procedure favoring the atomic sites. The double (single) lines denote the strong (weak) effective bonds. The molecules in (a) are eliminated, producing the renormalized chain in (b). Eliminating the new molecules, we obtain the renormalized chain in (c).

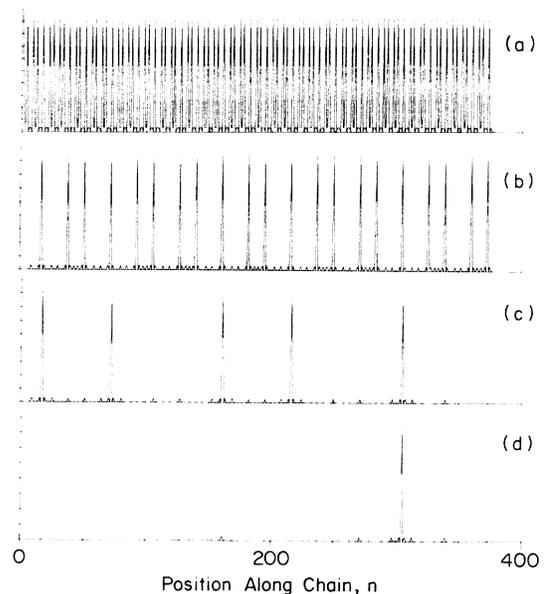


FIG. 3. Probability density, P_n , vs site position, n , along the chain. In (a)–(d) the probability densities have contributions from the states belonging respectively to (a'), (b'), (c'), and (d'), where (a') denotes the central main cluster of states around $E = 0$ in Fig. 1(a), (b') the central subcluster of (a'), (c') the central subcluster of (b'), and (d') the central subcluster of (c').

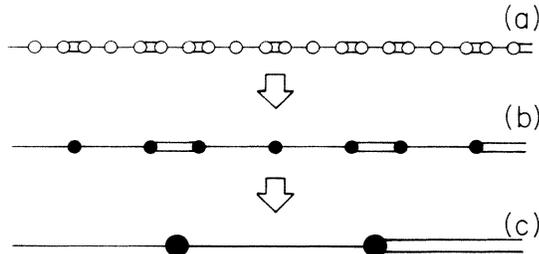


FIG. 4. Schematic representation of the decimation procedure favoring the bonding molecular states. The double (single) lines denote the strong (weak) effective bonds. The isolated atoms in (a) are eliminated, producing the renormalized chain in (b). Eliminating the isolated atoms again obtain the renormalized chain in (c).

even $|T_w/T_s|=0.5$ can be regarded as $\ll 1$, for the purpose of giving qualitative predictions. When $|T_w/T_s| \leq 0.2$, predictions about the widths of the clusters become very accurate [see Fig. 1(a)]. Also, as the energy shifts due to renormalizations are included, even the positions of the clusters can be determined fairly well.⁷

In order to verify the results of our RG approach further, we plotted the probability density (PD), $P_n = \sum_s |\psi_n^{(s)}|^2$, summed over the states belonging to certain clusters and subclusters in the spectrum; n represents the site position along the chain. In Fig. 3(a), the PD over the central cluster is plotted as a function of n . The PD is uniformly peaked on the isolated sites, which corresponds to the renormalized lattice obtained in the first step of our RG analysis for the $E=0$ level. The PD over the central subcluster of the central cluster [Fig. 3(b)] is uniformly peaked on the sites corresponding to the superisolated atomic states in the second step of our RG analysis. As we narrow the range of the spectrum towards the center, we see a very clear hierarchical structure in the successive PD's [Figs. 3(c) and 3(d)], exactly corresponding to what the RG suggests. On the other hand, as we plot the PD's over the top cluster [Fig. 5(a)], top subcluster of the top cluster [Fig. 5(b)], etc. [Figs. 5(c)–5(e)], we see another type of hierarchical structure corresponding to the bonding molecular states, bonding supermolecular states, and so on. *It is important to note that the lattices of Figs. 2(a), 2(b), and 2(c) correspond to the PD's of Figs. 3(b), 3(c), and 3(d), respectively. Also, the lattices of Figs. 4(a), 4(b), and 4(c) correspond to the PD's of Figs. 5(c), 5(d), and 5(e), respectively.* The exact correspondence between them is remarkable.

The scaling behavior⁸ of the wave function at $E=0$ can be readily obtained from our RG analysis. First, this state belongs to the central cluster of the spectrum, so that the wave function should be primarily peaked on the isolated atoms. The strength of the

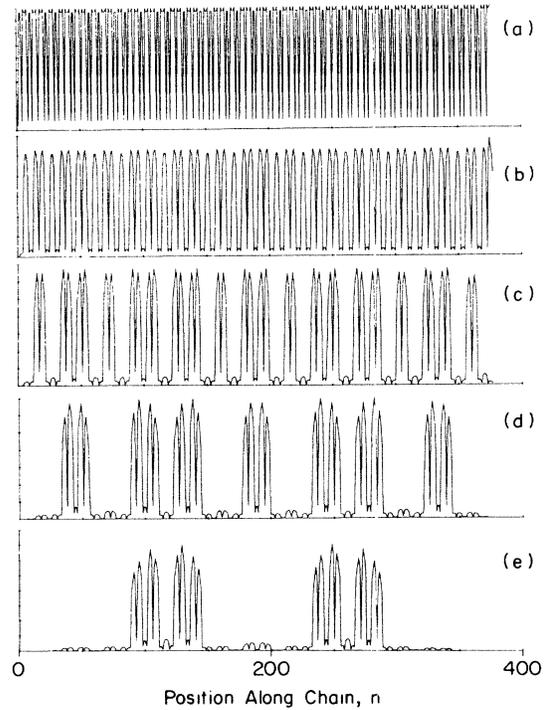


FIG. 5. Probability density, P_n , vs site position, n , along the chain. In (a)–(e) the probability densities have contributions from the states belonging to (a''), . . . , (e'') respectively, where (a'') denotes the top main cluster of Fig. 1(a), (b'') the top subcluster of (a''), (c'') the top subcluster of (b''), and so on.

wave function on the isolated atoms should be $|T_s/T_w|$ times the strength on the molecules. Second, this state also belongs to the central subcluster of the central cluster; therefore the strength on the superisolated, i.e., more isolated, atoms should be $|T_s/T_w|$ times the strength on other isolated atoms. If we continue this analysis, we see that on the m th-order superisolated atoms, the wave function has a relative strength of order $|T_s/T_w|^m$. Since an m th-order superisolated atom first appears at a distance of order τ^m away (to the right) from the origin, the envelope of the wave function scales in distance as a *power law*, with the power given by $\ln|T_s/T_w|/\ln\tau$. This result is equivalent to the one obtained by Kohmoto and Banavar⁵ on the basis of a three-iteration map.

A similar scaling behavior of the wave function can be obtained for the state at the top or bottom of the spectrum.⁷ In general, for any given state we can associate with it a *string*, $p_1 p_2 p_3 \dots$, from our RG analysis. The p_i 's take values of t , c , and b , meaning top, central, and bottom, respectively. For instance, if the energy belongs to the central cluster, the top subcluster of the central cluster, etc., then we associate with it a string $ct \dots$. If the string has a periodic tail, then we call the state a rational state. It is not difficult to see

that for a rational state, the wave function should have a self-similar behavior.⁷ Chaotic behavior of the wave functions may appear for irrational states.

So far, we have only considered case (A) of our model. In case (B), the Fibonacci lattice breaks into biatomic molecules and triatomic molecules, if we ignore the weaker bonds. There are five levels in the first approximation: $E = \pm T_s$ for the bonding and antibonding biatomic molecules, and $E = 0, \pm\sqrt{2}T_s$ for the three normal modes of the triatomic molecules. An effective Hamiltonian can be constructed within each of the degenerate levels. But the resultant sublattices have only isolated units and double-unit molecules in a further approximation. Therefore, the previous arguments apply for the subsequent analysis. So the spectrum should consist of five main clusters, each of which trifurcates indefinitely as in case (A) [see Fig. 1(b)].

In case (C), the first approximation of ignoring the bonds results in two degenerate levels. An effective Hamiltonian can be constructed for each of the levels. It can be shown that the resultant sublattices have the same structure as the Fibonacci lattice in case (A). Thus, the whole spectrum should consist of two main clusters, each of which trifurcates indefinitely [see Fig. 1(c)].

Our RG approach should be useful for other self-similar lattices, of which our model, with the three cases considered, is merely the simplest example. It might be possible to apply this approach to higher-dimensional lattices. Currently, we are exploring such possibilities.⁷

An important point should be emphasized. In the present work, we initially constructed a RG theory, which is then numerically verified by plotting the probability density over the clusters, subclusters, etc. For a general quasiperiodic system, it is not easy to find a RG theory beforehand. Thus, in a numerical approach, one is strongly advised not just to find the energy spectrum, but also to find the probability density

over the clusters, subclusters, and so on. There should be an intimate relationship between the behavior of the densities and the energy ranges of the clusters. By doing so, one can gain deeper insight into the problem. With luck, one may even be able to find a RG theory afterwards. The probability densities may also be plotted in momentum space, which could be useful for nearly free QP systems. In this case, the wave function peaks in momentum space but not in real space.

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¹D. Schechtman *et al.*, Phys. Rev. Lett. **53**, 1951 (1984).

²D. Levine and P. J. Steinhardt, Phys. Rev. Lett. **53**, 2477 (1984).

³R. Merlin *et al.* Phys. Rev. Lett. **55**, 1768 (1985).

⁴F. Nori and J. P. Rodriguez, Phys. Rev. B **34**, 2207 (1986).

⁵J. M. Luck and D. Petritis, J. Stat. Phys. **42**, 289 (1986); M. Kohmoto and J. Banavar, Phys. Rev. B **34**, 563 (1986).

⁶R. Merlin *et al.*, Bull. Am. Phys. Soc. **31**, 348 (1985), and to be published.

⁷F. Nori, Q. Niu, E. Fradkin, and J. P. Rodriguez, to be published; Q. Niu and F. Nori, to be published.

⁸D. Thouless and Q. Niu [J. Phys. A **16**, 1911 (1983)], on the basis of a renormalization-group analysis, have discussed the qualitative features of the wave function for the diagonal QP case. The scaling of the spectrum for this case has been studied, through a transfer-matrix approach, by Kohmoto *et al.*, Phys. Rev. Lett. **50**, 1870 (1983); S. Ostlund *et al.*, Phys. Rev. Lett. **50**, 1873 (1983); M. Kohmoto and Y. Oono, Phys. Lett. **102A**, 745 (1985).