Renormalization group of random Fibonacci chains

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A renormalization method is proposed to analyze the electronic band structure of disordered Fibonacci chains. The perfect (quasiperiodic) chain is contemplated as a particular case. Both bond and on-site problems are considered. The method is computationally efficient and suitable to deal with large chains in real space. It can be useful for the study of electronic properties of random tilings.

I. INTRODUCTION

The electronic properties of Fibonacci and generalized Fibonacci chains have been exhaustively studied. One effective method is the renormalization-group technique, which was developed to study the physical properties of periodic and quasiperiodic systems[1,2] even before the discovery of the first quasicrystalline alloy in 1984.[3] It has been proven that the spectrum of a Fibonacci chain is a Cantor set of zero Lebesgue measure[4,5] and it is believed that all the eigenstates are neither localized nor extended, but critical.[4–6] A similar situation holds for a class of generalized Fibonacci chains, but here there is the possibility of the spectrum being locally smooth and that extended states exist.[7] The renormalization-group method has also been applied to two-dimensional quasiperiodic lattices[8,9] where singular continuous spectra and critical eigenstates are also found (for a review see Ref. 10).

Fibonacci chains provide a simplified tool for examining the effects of quasiperiodicity,[4,11] and their study has been strongly motivated by molecular-beam epitaxy experiments yielding the first experimental realization of a Fibonacci system.[12] Less attention, however, has been paid to random systems in the sense of a random tiling. The one-dimensional realization of a perfect quasicrystal is the Fibonacci chain whose Fourier-transform consists of a dense set of delta peaks, although it must be borne in mind that there is still controversy about the true nature of quasicrystallinity. In addition to the perfect quasicrystal model, there exists the random tiling model which has successfully explained most features of quasicrystalline alloys (for a review see Ref. 13). The Fourier transform of a random tiling structure consists of delta peaks plus diffuse scattering and their one-dimensional realization is a disordered Fibonacci chain preserving the same reciprocal space properties.

The main purpose of this paper is to provide a renormalization-group procedure which is useful to study the local electronic properties of large random Fibonacci chains in a simple and efficient computational way. This method was previously implemented to tackle the localization problem in Fibonacci chains,[14] and was also applied to two-dimensional Penrose tilings.[15] Here, we present a generalization where the Fibonacci chain is only a particular case, and has the advantage of being extendible to treat the case of random Penrose tilings. Since no experiment has yet been devised to tell which of the major competing quasicrystal models (quasiperiodic vs random tiling) is correct to describe real quasicrystals, the method proposed here can shine some light onto this matter by describing the effect of phason disorder on electronic spectra of quasiperiodic structures.

The outline of the paper is as follows. In Sec. II we describe the construction of random Fibonacci chains and derive their renormalization-group equations. In Secs. II A and II B we apply the derived transformations to calculate the local density of states (LDOS) at a central site in random Fibonacci chains with varying degrees of disorder. Section III is devoted to results and discussion.

II. RENORMALIZATION GROUP

The Fibonacci sequence describes the alternation of "words" L and S, with lengths l_L and l_S. Let us call F_n the sequence obtained according to the following concatenation rule:

$$F_n = F_{n-1} * F_{n-2}, \quad F_0 = S, \quad F_1 = L \ , \tag{1}$$

where the asterisk denotes string concatenation. The words F_n converge to an infinite word F_∞ called the Fibonacci sequence which is related to the golden mean $\tau=(1+\sqrt{5})/2$ by $F_{n+1}/F_n \to \tau$ when $n \to \infty$. F_{n+1} can also be obtained from F_n by applying the following substitution rule:

$$L \to LS, \quad S \to L \ .$$

The Fibonacci chain is built by putting atoms on positions x_n in such a way that the bond lengths, $x_n - x_{n-1}$, take two values, namely, l_L and l_S. It is well known that the deterministic chain constructed in this way is neither periodic nor random, but quasiperiodic, and constitutes the one-dimensional realization of a perfect quasicrystal.

The one-dimensional case of a random tiling is a ran-

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dom Fibonacci chain, which can be constructed as follows. Let us consider the same words L and S with the following random concatenation rule:

$$R_n = \begin{cases} R_{n-1} * R_{n-2} & \text{with probability } p \\ R_{n-2} * R_{n-1} & \text{with probability } q = 1-p \end{cases} . \quad (2)$$

$R_0 = S$, $R_1 = L$, and $0 \le p \le 1$ is a fixed probability. So, for instance,

$$R_2 = \begin{cases} LS & \text{with probability } p \\ SL & \text{with probability } q \end{cases}$$

and

$$R_3 = \begin{cases} LSL & \text{with probability } p^2+q^2 \\ SLL & \text{with probability } pq \\ LLS & \text{with probability } pq \end{cases} .$$

In this way, the infinite R_∞ can be viewed as a random reshuffling of words L and S in F_∞. We shall consider the linear random Fibonacci chain built by associating a bond of length l_L to L and l_S to S in R_∞.

The so constructed random Fibonacci chain can be described by the one-electron tight-binding Hamiltonian:

$$H = \sum_i |i\rangle \epsilon_i \langle i| + \sum_{i,j} |i\rangle t_{ij} \langle j| ,$$

where $|i\rangle$ is the Wannier state associated with the ith vertex of the chain and t_{ij} is the nearest-neighbor hopping integral. In the bond problem (nondiagonal disorder) the hopping integrals take two values t_l and t_s. For the case of on-site problem (diagonal disorder) the site energies consist of ϵ_A and ϵ_B arranged in Fibonacci sequence. The matrix elements of the Green's function $G_{ij} = \langle i|G(Z)|j\rangle$ satisfy the following set of equations:

$$(Z-\epsilon_i)G_{ij} = \delta_{ij} + \sum_k t_{ik} G_{kj}, \quad i = 0,1,2,\ldots , \quad (3)$$

where $Z = E + i\eta$, $\eta \to 0$.

A. Bond problem

Following Barrio and Wang,[14] the renormalization procedure consists of eliminating the coordinates of the central site from the equations of motion for the Green's function (3) in each iteration. This allows us to handle only the atoms at the boundaries of the bonds in order to construct the next generation. The first three iterations are shown schematically in Fig. 1.

The chain in the second iteration consists of three atoms with self-energies: $\epsilon_L^{(1)}$, $\epsilon_C^{(2)} = \epsilon_R^{(1)} + \epsilon_L^{(0)}$, and $\epsilon_R^{(0)}$, respectively (subscripts L, C, and R stand for left, center, and right sites and the number in parenthesis labels the iteration), and hopping integrals $\tau^{(1)}$ and $\tau^{(0)}$. The coordinates of the central site can be eliminated from equation (3), and one gets a single effective bond with two effective atoms. The renormalization-group equations for this iteration are

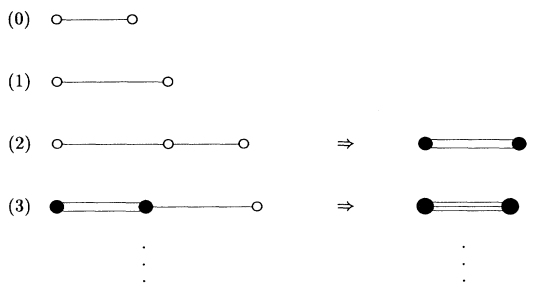

FIG. 1. Scheme showing the renormalization procedure for eliminating the coordinates of the central site in the second and third iteration of the concatenation process for growing the Fibonacci chain. The three atoms and the two bonds of the chain are replaced by two effective atoms with a single effective bond.

$$E_L^{(2)} = \epsilon_L^{(1)} + \frac{\tau^{(1)}\tau^{(1)}}{Z-(\epsilon_R^{(1)}+\epsilon_L^{(0)})} ,$$

$$E_R^{(2)} = \epsilon_R^{(0)} + \frac{\tau^{(0)}\tau^{(0)}}{Z-(\epsilon_R^{(1)}+\epsilon_L^{(0)})} , \quad (4)$$

$$t^{(2)} = \frac{\tau^{(1)}\tau^{(0)}}{Z-(\epsilon_R^{(1)}+\epsilon_L^{(0)})} ,$$

where E and t are used for renormalized ϵ and τ parameters. In the third iteration we have $\epsilon_L^{(2)} = E_L^{(2)}$, and the equations for the nth step can be written in terms only of renormalized variables as

$$E_L^{(n)} = E_L^{(n-1)} + \frac{t^{(n-1)}t^{(n-1)}}{Z-(E_R^{(n-1)}+E_L^{(n-2)})} ,$$

$$E_R^{(n)} = E_R^{(n-2)} + \frac{t^{(n-2)}t^{(n-2)}}{Z-(E_R^{(n-1)}+E_L^{(n-2)})} ,$$

$$t^{(n)} = \frac{t^{(n-1)}t^{(n-2)}}{Z-(E_R^{(n-1)}+E_L^{(n-2)})} ,$$

with the initial values

$$E_L^{(0)} = E_L^{(1)} = E_R^{(0)} = E_R^{(1)} = 0$$

and (5)

$$t^{(0)} = t_l, \quad t^{(1)} = t_s .$$

This renormalization procedure in a deterministic Fibonacci chain can be extended to the random concatenation rule given in (2). Figure 2(a) shows how the second iteration of Fig. 1 looks in the random case. By renormalizing the two possible configurations of the chain and averaging self-energies and hopping integrals; these configurations can also be replaced by a single effective bond with two effective atoms. The renormalized (and averaged) self-energies and hopping integrals of the single chain are now

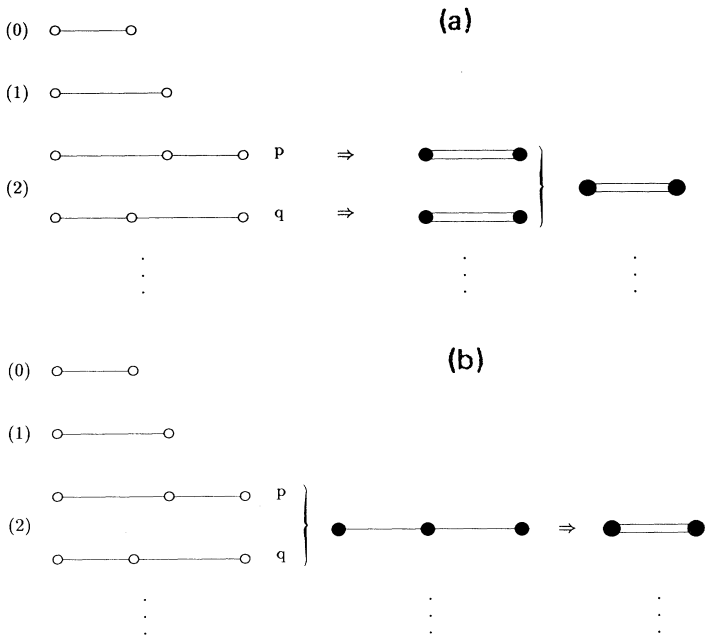

FIG. 2. Scheme of the renormalization procedure of the random Fibonacci chain according to the concatenation rule (2). Two kinds of defects are introduced. (a) For type I disorder the renormalization of the two possible configurations is carried out prior to average. (b) Type II disorder arises when the two possible configurations are averaged prior to renormalization.

$$E_L^{(2)}=p\epsilon_L^{(1)}+q\epsilon_L^{(0)}+p\frac{\tau^{(1)}\tau^{(1)}}{Z-(\epsilon_R^{(1)}+\epsilon_L^{(0)})}+q\frac{\tau^{(0)}\tau^{(0)}}{Z-(\epsilon_R^{(0)}+\epsilon_L^{(1)})},$$

$$E_R^{(2)}=p\epsilon_R^{(0)}+q\epsilon_R^{(1)}+p\frac{\tau^{(0)}\tau^{(0)}}{Z-(\epsilon_R^{(1)}+\epsilon_L^{(0)})}+q\frac{\tau^{(1)}\tau^{(1)}}{Z-(\epsilon_R^{(0)}+\epsilon_L^{(1)})},$$

$$t^{(2)}=\tau^{(1)}\tau^{(0)}\left[\frac{p}{Z-(\epsilon_R^{(1)}+\epsilon_L^{(0)})}+\frac{q}{Z-(\epsilon_R^{(0)}+\epsilon_L^{(1)})}\right].$$

In terms of the renormalized parameters, the general formulas for the nth iteration read

$$E_L^{(n)}=pE_L^{(n-1)}+qE_L^{(n-2)}+p\frac{t^{(n-1)}t^{(n-1)}}{Z-(E_R^{(n-1)}+E_L^{(n-2)})}+q\frac{t^{(n-2)}t^{(n-2)}}{Z-(E_R^{(n-2)}+E_L^{(n-1)})},$$

$$E_R^{(n)}=pE_R^{(n-2)}+qE_R^{(n-1)}+p\frac{t^{(n-2)}t^{(n-2)}}{Z-(E_R^{(n-1)}+E_L^{(n-2)})}+q\frac{t^{(n-1)}t^{(n-1)}}{Z-(E_R^{(n-2)}+E_L^{(n-1)})},\tag{6}$$

$$t^{(n)}=t^{(n-1)}t^{(n-2)}\left[\frac{p}{Z-(E_R^{(n-1)}+E_L^{(n-2)})}+\frac{q}{Z-(E_R^{(n-2)}+E_L^{(n-1)})}\right],$$

with the initial condition (5).

The above procedure yields the self-energies and hopping integrals of disordered chains constructed according to the concatenation rule given in (2), whose properties in reciprocal space are those of a random tiling.[16,17] Observe, however, that a different kind of disorder can be introduced if the two possible configurations are averaged prior to renormalization, as depicted in Fig. 2(b). Note that in this iteration there is a finite probability of getting LL and SS configurations. Consequently, in larger chains, one is actually averaging arbitrarily large crystalline regions, yielding random chains that have lost the random tiling reciprocal space properties. These two kinds of disorder will be alluded to as type I [Fig. 2(a)] and type II [Fig. 2(b)]. We shall consider type II disorder for comparison purposes only.

The corresponding recurrence formulas for type II disorder are

$$E_L^{(n)}=pE_L^{(n-1)}+qE_L^{(n-2)}+\frac{(pt^{(n-1)}+qt^{(n-2)})^2}{Z-E_C^{(n)}},$$

$$E_R^{(n)}=pE_R^{(n-2)}+qE_R^{(n-1)}+\frac{(pt^{(n-2)}+qt^{(n-1)})^2}{Z-E_C^{(n)}},\tag{7}$$

$$t^{(n)}=\frac{(pt^{(n-1)}+qt^{(n-2)})(pt^{(n-1)}+qt^{(n-2)})}{Z-E_C^{(n)}},$$

where

$$E_C^{(n)}=p(E_R^{(n-1)}+E_L^{(n-2)})+q(E_R^{(n-2)}+E_L^{(n-1)}).\tag{8}$$

Since each diagonal matrix element of the Green's function gives the LDOS at the corresponding site, the LDOS at the central site of the Fibonacci chain is given by[18]

$$\rho_i(E)=-\frac{1}{\pi}\lim_{\eta\to 0}\mathrm{Im}G_{ii}(Z),\tag{9}$$

where Im stands for the imaginary part. It is straightforward to obtain the renormalized equation for the Green's function at the central site, which reads

$$G_{CC}=\left[Z-E_C^{(n)}-\frac{t^{(n-1)}t^{(n-1)}}{Z-E_L^{(n-1)}}-\frac{t^{(n-2)}t^{(n-2)}}{Z-E_R^{(n-2)}}\right]^{-1}, \tag{10}$$

where the self-energies and hopping integrals at step n are given by (6) and (7) for disorder types I and II, respectively, and $E_C^{(n)}$ is given by (8) for both types of disorder.

B. On-site problem

The above renormalization procedure can be implemented to solve the on-site problem in an analogous way. In this case, we have two different site energies, ϵ_A and ϵ_B, and a real bond T which must link chains $n-1$ and $n-2$. This makes a difference to the renormalization procedure of the precedent section since now, for disorder type I, the two renormalized chains are joined by a bond T in the proper (with probability p) or reverse (with probability q) way. These two possible configurations are renormalized separately by eliminating the coordinates of the two central sites to get a single effective bond with two effective atoms. Finally, the two resulting possibilities are averaged.

The general nth step formulas for the on-site problem with the type I disorder are

$$\begin{aligned}
E_L^{(n)}&=pE_L^{(n-1)}+qE_L^{(n-2)}+p\frac{t^{(n-1)}t^{(n-1)}(Z-E_L^{(n-2)})}{(Z-E_R^{(n-1)})(Z-E_L^{(n-2)})-T^2}\\
&\quad+q\frac{t^{(n-2)}t^{(n-2)}(Z-E_L^{(n-1)})}{(Z-E_R^{(n-2)})(Z-E_L^{(n-1)})-T^2},\\
E_R^{(n)}&=pE_R^{(n-2)}+qE_R^{(n-1)}+p\frac{t^{(n-2)}t^{(n-2)}(Z-E_R^{(n-1)})}{(Z-E_R^{(n-1)})(Z-E_L^{(n-2)})-T^2}\\
&\quad+q\frac{t^{(n-1)}t^{(n-1)}(Z-E_R^{(n-2)})}{(Z-E_R^{(n-2)})(Z-E_L^{(n-1)})-T^2},\\
t^{(n)}&=Tt^{(n-1)}t^{(n-2)}\times\left[\frac{p}{(Z-E_R^{(n-1)})(Z-E_L^{(n-2)})-T^2}+\frac{q}{(Z-E_R^{(n-2)})(Z-E_L^{(n-1)})-T^2}\right],
\end{aligned} \tag{11}$$

with the initial conditions

$$E_L^{(2)}=\epsilon_A,\quad E_R^{(2)}=\epsilon_B,\quad t^{(2)}=T,$$
$$E_L^{(3)}=E_R^{(3)}=\epsilon_A+\frac{T^2}{Z-\epsilon_B},\quad t^{(3)}=\frac{T^2}{Z-\epsilon_B}.$$

The corresponding recurrence formulas for the type II disorder are

$$\begin{aligned}
E_L^{(n)}&=pE_L^{(n-1)}+qE_L^{(n-2)}+\frac{(pt^{(n-1)}+qt^{(n-2)})^2[Z-(pE_L^{(n-2)}+qE_L^{(n-1)})]}{S^{(n)}},\\
E_R^{(n)}&=pE_R^{(n-2)}+qE_R^{(n-1)}+\frac{(pt^{(n-2)}+qt^{(n-1)})^2[Z-(pE_R^{(n-1)}+qE_R^{(n-2)})]}{S^{(n)}},\\
t^{(n)}&=\frac{(pt^{(n-2)}+qt^{(n-1)})(pt^{(n-1)}+qt^{(n-2)})T}{S^{(n)}},
\end{aligned} \tag{12}$$

where

$$S^{(n)}=[Z-(pE_L^{(n-2)}+qE_L^{(n-1)})][Z-(pE_R^{(n-1)}+qE_R^{(n-2)})]-T^2.$$

Given that now one has to retain two central sites in the last renormalization step, the LDOS must be evaluated in one of the two central sites. The Green's function at the central site nearest to the left atom is given by

$$G_{aa}=\left[Z-E_R^{(n-1)}-\frac{t^{(n-1)}t^{(n-1)}}{Z-E_L^{(n-1)}}-\frac{T^2}{Z-E_L^{(n-2)}-t^{(n-2)}t^{(n-2)}/(Z-E_R^{(n-2)})}\right]^{-1}.$$

The self-energies and hopping integrals at step n are given by (11) and (12) for disorder types I and II, respectively.

III. RESULTS AND DISCUSSION

As discussed above, the local Green's functions of random Fibonacci chains can be calculated, in a given step n, in terms of the renormalization-group equations (6) or (7) for the bond, and (11) or (12) for the on-site problems. The site energy ϵ in the bond problem was initially set to zero for all sites with $t_l=-1.0$ and $t_s=-1.5$. Regarding the on-site problem we selected $\epsilon_A=1$, $\epsilon_B=-1$ and $T=-1$. The following calculations were made for 100

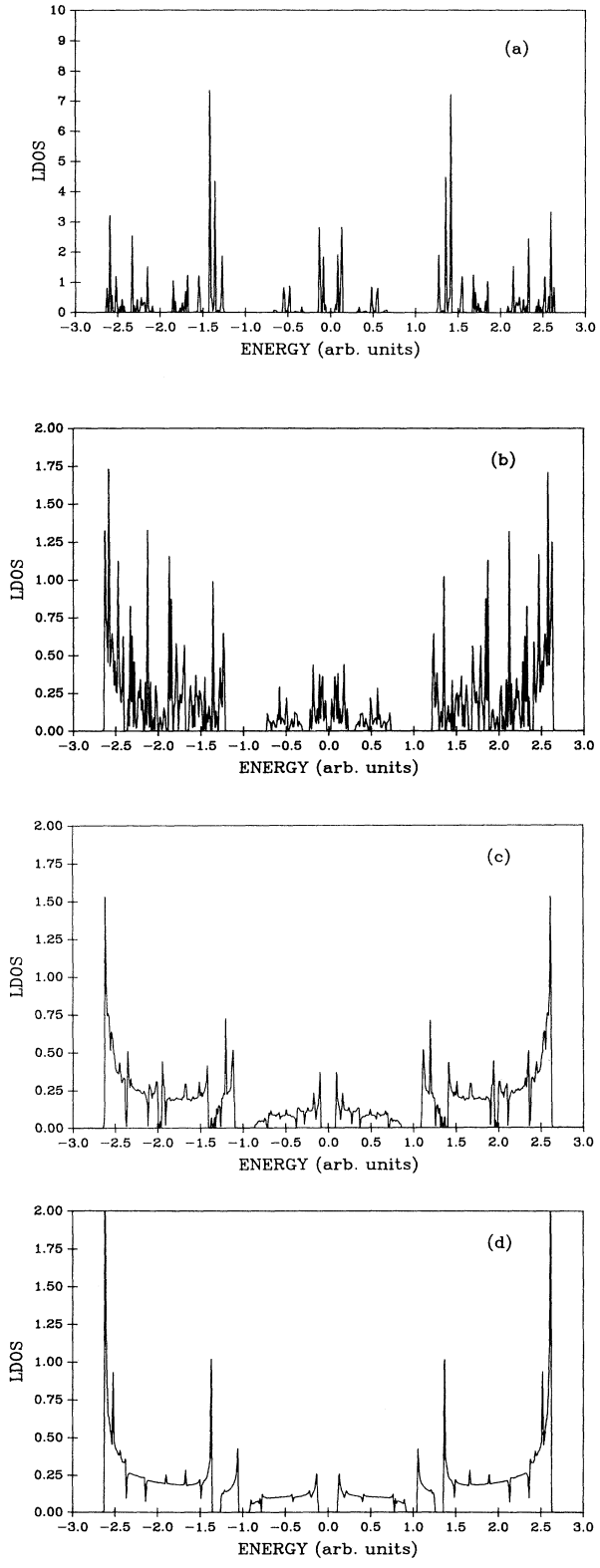

FIG. 3. LDOS, in arbitrary units, for different values of p, for the bond problem with type I disorder. (a) $p=1$ (Fibonacci chain), (b) $p=0.95$, (c) $p=0.75$, and (d) $p=0.5$. Note that the gross features of the Fibonacci chain of the spectrum are preserved, and the spectrum is smoothed.

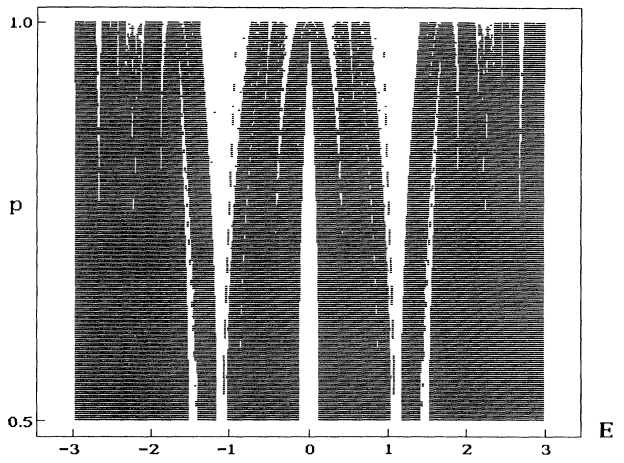

FIG. 4. Band structure as function of p for the bond problem with type I disorder.

iteration chains ($\sim 10^{20}$ sites).

Figure 3 shows typical examples of LDOS for the bond problem at the central site of a chain with the type I disorder for $p=1$ (perfect Fibonacci chain), 0.95, 0.75, and 0.5, respectively. The spectrum at $p=1$ is the same obtained using other approaches and found to be a Cantor set.[1,4–6] As p decreases, the gross features of the spectrum are preserved and the spectrum is smoothed. Many of the characteristics of the underlying Fibonacci chain survive even for $p=0.5$. The features of the smoothed spectrum have a close resemblance with the spectrum of rational approximants of the Fibonacci chains,[19] it is also interesting to observe that the phonon spectrum of a 3D Penrose tiling is also smoothed when randomized.[20] The band structure of the spectra at different values of p can be better appreciated in Fig. 4, where energy is plotted vs p. Observe that the gap at $E=0$ (absent in a Fibonacci chain) opens up as p decreases. In contrast with type I, when the type II disorder is introduced, slight deviations from $p=1$ change the main features of the spectrum.

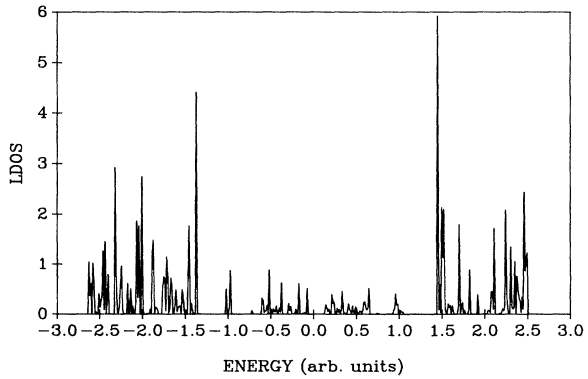

FIG. 5. LDOS, in arbitrary units, at $p=0.95$ for the bond problem with type II disorder. The features of the spectrum are changed severely with respect to the Fibonacci one.

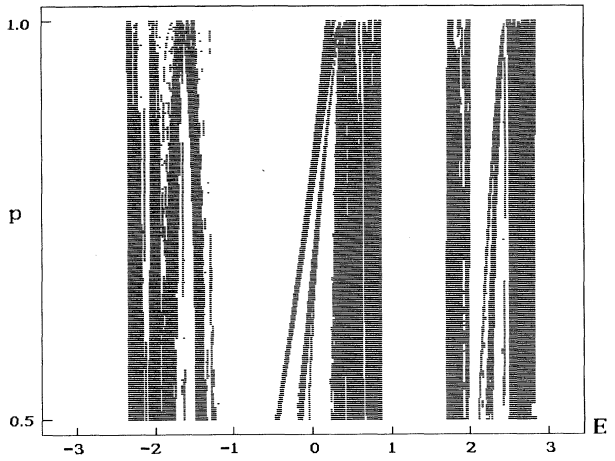

FIG. 6. Band structure as function of p for the on-site problem with type I disorder.

Figure 5 shows the case at $p=0.95$.

For the on-site problem, the LDOS obtained when $p=1$ with formulas (11) or (12) coincides with previous calculations.[21,22] Figure 6 shows the bands of the spectra as a function of p for type I disorder. As in the bond problem, in this case the gross structure of the spectrum preserves the characteristics of the underlying Fibonacci chain. Also, for the type II disorder, small variations of p change the structure of the spectrum, in a similar fashion to that reported in Ref. [21], where the authors consider random site energy fluctuations in Fibonacci chains.

Summarizing, we have introduced a renormalization-group scheme to calculate the electronic spectrum of random Fibonacci chains, with the following characteristics.

(1) The method is computationally simple and efficient, enabling it to treat long chains with minimum effort.

(2) The Fibonacci chain is treated as a particular case; disorder is introduced dynamically during chain growth, and consists of phason defects which preserve the random tiling properties of the chain.

(3) Although the LDOS was calculated at the central site, it is not difficult to obtain equations for any other chain site. In fact, one can, in principle, obtain the total trace of the Green's function as in the case of a perfect chain,[14] but in this case the accuracy and computation time is heavily dependent of the number of sites.

(4) The method can be extended to two dimensions and can be useful to study still unknown random tiling effects on the localization problem.

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