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Global scaling properties of the spectrum for the Fibonacci chains

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By means of the approximate renormalization approach of Niu and Nori [Phys. Rev. Lett. **57**, 2057 (1986)] the widths of subband segments in the spectrum and the occupation probabilities on subbands are obtained to the lowest order for the two-value Fibonacci chains. The global scaling properties of the spectrum are then analytically calculated.

Quasiperiodic or incommensurate crystals represent a natural intermediate case between periodicity and randomness. Since Shechtman, Blech, Gratias, and Cahn observed surprising crystallographic properties[1] much attention has been focused on studies of such quasicrystals.[2] Amongst the models studied three types of the tight-binding Fibonacci chains are rather commonly discussed. They are described by the equation

$$t_{n+1}\psi_{n+1}+t_n\psi_{n-1}=E_n\psi_n \ , \tag{1}$$

where ψ_n is the probability amplitude at site n. When the site energies are constant and the hopping integrals or bonds take two values, T_s (strong) and T_w (weak), arranged in a Fibonacci sequence, we have the Fibonacci chains of types S and W with the majority in the sequence being T_s and T_w, respectively. The third kind of Fibonacci chain is type E in which the bonds are constant, but the site energies, hence E_n, take two values, arranged in a Fibonacci sequence.

The self-similarity in the spectra and the wave functions for the Fibonacci chains have been studied by several groups.[3-6] Recently, Niu and Nori[7] have developed a new approximate renormalization approach to the study of electron spectral clustering and wave function scaling in the Fibonacci chains. Their decimation technique generates a clear and simple physical picture of the electronic spectral behavior and the nature of the wave functions. The knowledge drawn from this renormalization procedure allows us to calculate analytically the global scaling properties of the spectrum fractal by means of the algorithm proposed by Halsey *et al.* in Ref. 8.

The renormalization-group approach of Niu and Nori is based on the weak bond approximation. At first we briefly explain the main ideas in a somewhat different way which is more appropriate to our purpose here. From the property of the Fibonacci sequence a Fibonacci chain of type W can be viewed as a chain of type E consisting of dimers and monomers (step $W\rightarrow E$, see Fig. 1). The dimer consists of two atoms bonded or antibonded with a strong bond. Dimers and monomers are then connected with weak bonds. Similarly, a chain of type S can be viewed as a chain of type E consisting of trimers and dimers. On the other hand, a chain of type E can be viewed as a chain of type W consisting of all "white" or all "black" sites (step $E\rightarrow W$, see Fig. 2). By combining these two steps an original chain of type W can be renormalized into a new W chain with new sites and new weak and strong bonds. The chain of type E is convenient for calculation of the density of states. If we neglect the weak bonds in Fig. 2(0), then the spectrum consists of two degenerate levels: $E=E_w$ and $E=E_b$. To the lowest order, the occupation probabilities on these two levels are equal to $\omega=\frac{1}{2}(\sqrt{5}-1)$ and ω^2, respectively. On the other hand, the chain of type W is convenient for calculation of the "energy band" widths. If we neglect weak bonds in Fig. 1(0), then the spectrum of a W chain consists of three degenerate levels: $E=0$ and $E=\pm T_s$. The width of the "coarse-grained energy band" is equal to $2T_s$.

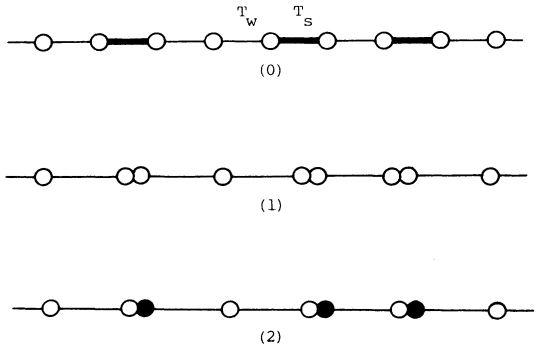

FIG. 1. A chain of type W (0) can be viewed as a chain of type E consisting of binding (1) or antibinding (2) dimers.

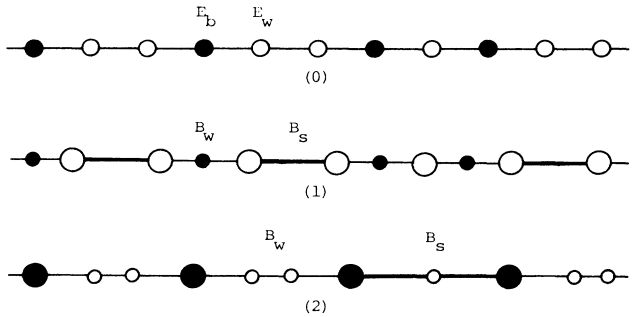

FIG. 2. A chain of type E (0) can be viewed as a chain of type W consisting of (1) all "white" or (2) all "black" sites.

Let us describe a W chain with the word $W(P,B_s,B_w)$, where the three numbers P, B_s, and B_w are the occupation probability and the absolute values of the strength of strong bonds and weak bonds, respectively. In the above we have mentioned that two successive steps $W \rightarrow E \rightarrow W$ renormalize a W chain to a new W chain. The bonds in the new W chain have been given in Ref. 7 based on perturbation theory.[9] The results can be represented as

$$W(1,T_s,T_w) \begin{cases} E \begin{cases} W(\omega^2, \frac{1}{2}T_w, \frac{1}{2}T_w t) \\ W_0(\omega^3, tT_w, t^2T_w) \end{cases} \\ \bar{E} \quad \bar{W}(\omega^2, \frac{1}{2}T_w, \frac{1}{2}T_w t) \end{cases},$$

where $t \equiv T_w/T_s \ll 1$, and the bar indicates antibinding. Here in the derivation of occupation probabilities for three daughter W chains we have viewed the spectrum of the mother W chain as two overlapping spectra of daughter E chains. The widths of subbands are given by $2B_s$. From any member $W_i(P,s,ts)$ of a given generation of a W chain the next generation can be created in the following way:

$$W_i(P,s,ts) \begin{cases} W(P\omega^2, \frac{1}{2}ts, \frac{1}{2}t^2 s) \\ W_0(P\omega^3, t^2 s, t^3 s) \\ \bar{W}(P\omega^2, \frac{1}{2}ts, \frac{1}{2}t^2 s) \end{cases}.$$

This procedure gives us the information about the splitting of subbands, their widths, and their occupation probabilities.

We now analyze the global scaling properties of the spectrum for a W chain from the partition function defined in Ref. 8,

$$\Gamma(q,\tau,\{S_i\},l) = \sum_{i=1}^{N} \frac{p_i^q}{l_i^\tau} . \tag{2}$$

In our case each l_i is the width of a subband and p_i the occupation probability on that subband. From the above discussion we have

$$\Gamma^{(n)} = \left(\frac{\omega^{3q}}{(2tT_w)^\tau} + \frac{2\omega^{2q}}{T_w^\tau} \right) \left(\frac{\omega^{3q}}{t^{2\tau}} + \frac{2\omega^{2q}}{(\frac{1}{2}t)^\tau} \right)^n . \tag{3}$$

The calculation from this point on is parallel to that for the two-scale Cantor set in Ref. 8. For large n, at a given q, the partition function is of the order unity only when τ is chosen at a definite value.[8] When n is very large the partition function $\Gamma^{(n)}$ can be estimated with just a single term, the maximal term in the binomial expension for $\Gamma^{(n)}$. Suppose that this term is the one proportional to $\binom{n}{m}$. The condition determining the maximal term in the expansion of $\Gamma^{(n)}$ then gives

$$\tau = \frac{\ln[\frac{1}{2}(n/m-1)] + q\ln\omega}{\ln(2t)} . \tag{4}$$

The condition $\Gamma^{(n)} = 1$ leads to an equation for n/m:

$$q\ln\omega(\ln t + 3\ln 2) - 2\ln t \ln[\tfrac{1}{2}(n/m-1)] + \ln(n/m)\ln(2t) = 0 . \tag{5}$$

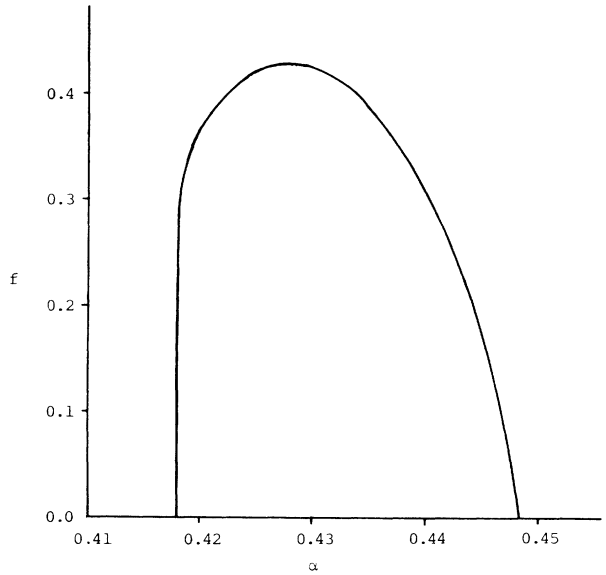

FIG. 3. The plot of f vs α for the spectrum of a W chain with $t = 0.2$.

The density exponent f of a set of $2^{n-m}\binom{n}{m}$ segments with the same size $\sigma \equiv 2^{m-n+1}t^{n+m+1}T_w^2$ is determined by

$$2^{n-m}\binom{n}{m}\sigma^f = 1 , \tag{6}$$

which gives

$$f = \frac{(n/m-1)\ln[\frac{1}{2}(n/m-1)] - (n/m)\ln(n/m)}{(n/m+1)\ln t - (n/m-1)\ln 2} . \tag{7}$$

The exponent determining the singularity in the measure α is determined by

$$\omega^{3m}\omega^{2(n-m)} = \sigma^\alpha , \tag{8}$$

which gives

$$\alpha = \frac{(2n/m+1)\ln\omega}{(n/m+1)\ln t - (n/m-1)\ln 2} . \tag{9}$$

The relation $\tau = q\alpha - f$ can be verified from Eqs. (4), (5), (7), and (9). The functional relations between $f(\alpha)$ and α are given by Eqs. (7) and (9) in a parametric form through the parameter $\xi \equiv n/m$. In Fig. 3 we display the curve $f(\alpha)$ for $t = 0.2$.

The "kneading sequences" can be assigned to subband segments. Only the infinite "tail" of the sequence determines the asymptotic scaling behavior. Because of this the same results can be deduced for an S chain or E chain. We have derived the global scaling properties of the spectrum for the Fibonacci chains from the approximate renormalization procedure. It would be interesting to compare the analytical results with numerical calculations in the future.

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