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LETTER TO THE EDITOR

Number of scaling factors in incommensurate systems

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Abstract. We study the scaling properties of an incommensurate system which obeys simple clustering rules, the one-dimensional tight-binding Schrödinger equation with a Fibonacci sequence potential. We find that the clustering rules do not guarantee a finite number of scaling factors. We find the energy spectrum by recursion. The clustering rules and recursion relations suggest *different* descriptions of the *same* spectrum. Based on the thermodynamic formalism, we compare these descriptions, calculate their associated scaling functions, and construct the mapping between them.

How many scaling factors fully characterise incommensurate systems? This question has received considerable attention in recent years [1-7]. Much of this attention has focused on the one-dimensional discrete Schrödinger equation with a periodic hull function $V(x) = V(x+1)$:

$$\psi_{n+1} + \psi_{n-1} + V(n\phi)\psi_n = \varepsilon\psi_n \tag{1}$$

where n is a lattice site label. One important example is Harper's equation [8] where

$$V(x) = \lambda \cos(2\pi x). \tag{2}$$

This has been adopted to describe non-interacting electrons in a two-dimensional crystal in a magnetic field with ϕ being the number of flux quanta through a unit cell. At $\lambda = 2$ the states change from being extended to being localised for almost all values of ϕ, leaving a *fractal* spectrum of allowed energies ε.

The spectrum was observed by Hofstadter [1] to obey hierarchical 'clustering rules': at a field ϕ the spectrum divides into three regions separated by two gaps, one central region which is a copy of the spectrum at $\phi' = \{\phi/(1-2\phi)\}$, and two side regions which are copies of the spectrum at $\phi'' = \{1/\phi\}$. (If $\phi > \frac{1}{2}$ then first replace ϕ with $1-\phi$.) Here $\{x\}$ denotes the fractional part of x. The clustering rules impose a natural division of the energy bands, defining a tree structure (figure 1(a)) where a band at one level of the tree branches into two side bands and a central band at the next level. We note, however, that neither the relative positions of the subbands nor their sizes relative to the separating gaps follow from the above rules.

Recently, the spectrum has been perceived to be multifractal for any irrational value of ϕ [2, 7], meaning that it is not fully characterised by one exponent (for example, the fractal dimension) but by a whole *distribution* of exponents. However, based on a proof of Hofstadter's clustering rules [1], which imply self-similarity, Stinchcombe and Bell [6] suggested that this distribution of exponents could be

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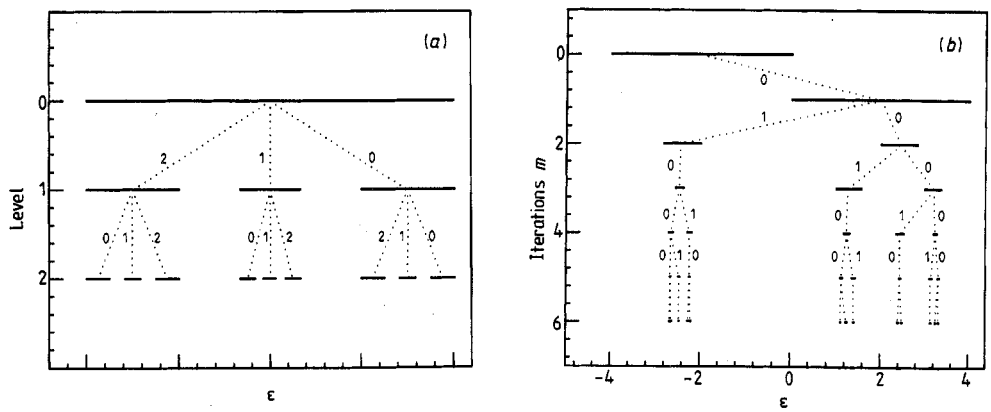

Figure 1. Tree structures and associated labelling for (*a*) the three-scale tree and (*b*) the 'Fibonacci' tree in the plot of iterations m against allowed energies ε.

extracted from a *finite* number of scaling factors when ϕ is a quadratic irrational†. For the golden mean, $\phi = \phi_g = \frac{1}{2}(\sqrt{5}-1) = 0.618\,033\,9\ldots$ where $\phi' = \phi'' = \phi$, the spectrum was conjectured to be determined solely by two scaling factors, one for the central band and one for the two side bands. This result would seem to imply an immense simplification in the description of incommensurate systems.

In this letter we examine critically the idea of scaling governed by a finite number of scaling factors. In order to simplify the problem and increase the numerical accuracy in evaluating the allowed states, we use the square-well potential at $\phi = \phi_g$, with

$$V(x) = \begin{cases} -\lambda & \text{if } -\phi_g < x \leqslant 1-2\phi_g \\ \lambda & \text{if } 1-2\phi_g < x \leqslant 1-\phi_g \end{cases} \tag{3}$$

first considered by Kohmoto *et al* [3] and Ostlund *et al* [4]. The potential $V(n\phi_g)$ is equivalent to the Fibonacci chain $+-++-+-++-++-\ldots$ in the two step heights $+\lambda$ and $-\lambda$. To generate this chain recursively, consider it as the limit of a sequence of partial chains $+, +-, \ldots$ where the nth chain is the concatenation of the $(n-1)$th and $(n-2)$th chains.

The main advantage of the potential (3) is that it yields to an exact renormalisation-group analysis [3, 4]. The transfer matrices expressing (1) can be multiplied to form chains of matrices analogous to the above chains of $\pm\lambda$. Accordingly, the nth product matrix is itself the product of the two previous product matrices. Thus the transfer-matrix equations can be reduced to a polynomial recursion relation on the traces of these matrix products. As a result, the energy spectrum can be calculated from the simple recursion relation

$$u_{i+1} = 2u_i u_{i-1} - u_{i-2} \tag{4a}$$

with initial conditions

$$u_{-1} = 1 \qquad u_0 = \tfrac{1}{2}(\varepsilon + \lambda) \qquad u_1 = \tfrac{1}{2}(\varepsilon - \lambda) \tag{4b}$$

where u_i is half the trace of the ith product matrix. The allowed energies ε are those that put u_∞ between -1 and 1. Here the potential strength λ is chosen to be 2. The

† Irrational roots of quadratic polynomials with integer coefficients. For this kind of irrational, iteration of ϕ'' (as well as ϕ') cycles through a finite number of irrationals.

choice is largely arbitrary since the wavefunctions are known to be critical, i.e. neither localised nor extended, for all non-zero step sizes. By contrast, Harper's potential is critical only at the special value $\lambda = 2$.

The recursion relation (4*a*) defines a natural tree structure on the allowed energy bands after a given number of iterations m (figure 1(*b*)). According to (4*a*), the number of bands at level m is given by the Fibonacci number F_m, where $F_{m+1} = F_m + F_{m-1}$, $F_0 = F_1 = 1$. At each level, every band is restricted to lie within the edges of either its 'parent' band or its 'grandparent' band. Hence, the *same* energy spectrum is described by two distinct trees. Involing the thermodynamical formalism [10] we demonstrate below how these two structures are related. In particular, we find the appropriate scaling functions, and show that the clustering rules do not imply the existence of a finite number of scaling factors.

From the tree structures presented in figure 1, a natural 'thermodynamics' [9] is defined. Every path through a tree can be labelled by a sequence $\boldsymbol{j} = (j_0, j_1, \ldots)$. For the 'Fibonacci' tree (figure 1(*b*)), $j_0 = 0$, and $j_i = 0, 1$, with the constraint that a one must be followed by a zero, i.e. $j_i = 1$ implies $j_{i+1} = 0$. For the 'three-scale' tree (figure 1(*b*)), $j_i = 0, 1, 2$. Denote the sizes of the intervals at level m by $\Delta_m(\boldsymbol{j}_m)$, where $\boldsymbol{j}_m \equiv (j_0, \ldots, j_m)$. A partition function $Z_m(\beta)$ is defined by

$$Z_m(\beta) \equiv \sum_{\boldsymbol{j}_m} \Delta_m(\boldsymbol{j}_m)^\beta. \tag{5}$$

In the limit of large m, 'the thermodynamic limit', $Z_m(\beta)$ scales according to exponents given by the 'free energy' $F(\beta)$

$$F(\beta) \equiv -\lim_{m\to\infty} (\ln Z_m(\beta)/\ln N_m) \tag{6}$$

where N_m is the number of intervals at level m, i.e. $N_m = F_m$ for the Fibonacci tree, and $N_m = 3^m$ for the three-scale tree. We note that $F(0) = -1$, and that the fractal (Hausdorff) dimension D_f is the value of β at which $F(\beta) = 0$.

The Legendre transform of $F(\beta)$, the 'entropy' $S(E)$

$$S(E) = \beta E - F(\beta) \qquad E = F'(\beta) \tag{7}$$

gives the density of exponents E, i.e. for every exponent

$$E = E(\boldsymbol{j}) \equiv \lim_{m\to\infty} E_m \equiv -\lim_{m\to\infty} (\ln \Delta_m(\boldsymbol{j}_m)/\ln N_m) \tag{8}$$

$S(E)$ yields the degeneracy

$$S(E) \equiv \lim_{\delta E\to 0} \lim_{m\to\infty} [\ln(\mathcal{N}_m(E)\delta E)/\ln N_m] \tag{9}$$

where $\mathcal{N}_m(E)\delta E$ denotes the number of times the exponent E_m occurs between $E_m - \frac{1}{2}\delta E$ and $E_m + \frac{1}{2}\delta E$. Since $S'(E) = \beta$, the maximal value of $S(E)$ is one. Moreover, according to (8) and (9), $D(E) = S(E)/E$ is the fractal dimension of the subfractal characterised by the exponent E. In particular, the (total) fractal dimension D_f is the maximal value of $D(E)$, as is also clear from (7).

For the three-scale tree the two side-band scales are supposed to be equal [6]. Call the two equivalent scaling factors a and the other scaling factor b. At level m this set (consisting of 3^m intervals) is divided into subsets, each containing $2^k\binom{m}{k}$ intervals of size $a^k b^{m-k}$. This immediately enables us to write down the entropy in the large-m limit where Stirling's formula is valid:

$$S(E) = y(E)\frac{|\ln y(E)|}{\ln 3} + (1-y(E))\frac{\ln 2 + |\ln(1-y(E))|}{\ln 3} \tag{10a}$$

where

$$y(E)=\frac{E\ln 3-|\ln a|}{|\ln b|-|\ln a|}. \tag{10b}$$

The bounds on the exponents are, assuming $1>a>b$,

$$E_{\min}=|\ln a|/\ln 3 \qquad E_{\max}=|\ln b|/\ln 3. \tag{11}$$

From (10*a*) and (10*b*) we note that the two coinciding scaling factors give rise to a finite entropy $S(E_{\min})=\ln 2/\ln 3$ at $E=E_{\min}$.

Also the form of the free energy is very simple for the three-scale set:

$$\begin{aligned}F(\beta)&=-\lim_{m\to\infty}\ln\left(\sum_{j_m}\Delta_m(j_m)^\beta\right)[\ln(3^m)]^{-1}\\&=-\lim_{m\to\infty}\ln\left[\sum_{k=0}^{m}2^k\binom{m}{k}(a^kb^{m-k})^\beta\right](m\ln 3)^{-1}\\&=-\lim_{m\to\infty}\ln\left[\sum_{k=0}^{m}\binom{m}{k}(2\alpha^\beta)^k(b^\beta)^{m-k}\right](m\ln 3)^{-1}\\&=-\ln(2a^\beta+b^\beta)/\ln 3.\end{aligned} \tag{12}$$

Hence, D_f is found as the value of β for which $2a^\beta+b^\beta=1$.

To estimate the free energy for the Fibonacci tree from finite-level calculations, one must consider the possibility of an amplitude multiplying $Z_m(\beta)$ in (6), as well as its variation. In figure 2 we show the behaviour of the partition function $Z_m(\beta)$ for

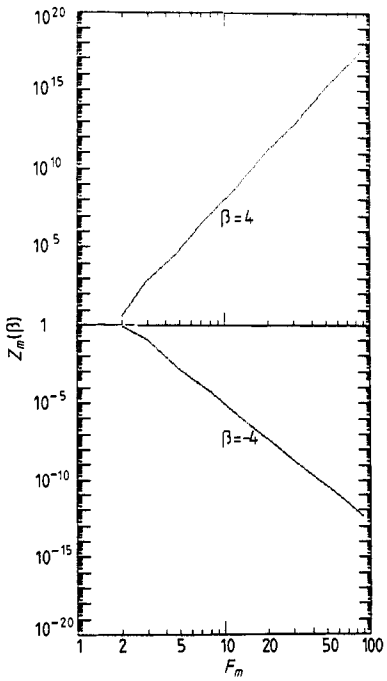

Figure 2. Partition function $Z_m(\beta)$ plotted against Fibonacci number F_m (log-log plot). The free energy $F(\beta)$ is the negative of the limiting slope. Note that the curves are not linear, but show a slight oscillation of period $\sim\phi_g^{-2}$.

$\beta = \pm 4$ as m, and thereby F_m, increases. The free energy $F(\pm 4)$ is the negative of the limiting slope. The oscillations seen in figure 2 have a period corresponding to a factor $\sim \phi_g^{-2} = 2 + \phi_g$. Figure 3($a$) shows two entropy curves obtained by (i) calculating the partition function $Z_m(\beta)$ (equation (5)) at two levels, (ii) determining an approximate value of the free energy $F(\beta)$, assuming $Z_m(\beta) \propto F_m^{-F(\beta)}$, and (iii) calculating the Legendre transform. To diminish the effect of the oscillations (figure 2) the two entropy curves are evaluated from levels 7, 9 and levels 8, 10, respectively. Although the variation is clear, there is no sign of the emergence of a finite entropy at the lower bound $E_{\min}$. From the related dimension curves (figure 3(b)) the fractal dimension D_f is estimated to be $D_f = 0.4545 \pm 0.0002$.

The spectrum can be studied further by means of the scaling function $\sigma(t)$

$$\sigma(t) \equiv \lim_{m\to\infty} \frac{\Delta_{m+1}(j_{m+1})}{\Delta_m(j_m)} \tag{13a}$$

where

$$t = \lim_{m\to\infty} F_{m+1}^{-1} \sum_{i=0}^{m} j_i F_i \tag{13b}$$

for the Fibonacci tree, and

$$t = \lim_{m\to\infty} 3^{-(m+1)} \sum_{i=0}^{m} j_i 3^i \tag{13c}$$

for the three-scale tree. For the latter, we immediately obtain (figure 4(a))

$$\sigma(t) = \begin{cases} a & \text{if } 0 \leqslant t < \frac{1}{3} \text{ or } \frac{2}{3} \leqslant t < 1 \\ b & \text{if } \frac{1}{3} \leqslant t < \frac{2}{3}. \end{cases} \tag{14}$$

We find that the scaling function obtained from (13a) and (13b) is much more complicated. In figure 4(b) we have plotted the approximation determined from levels

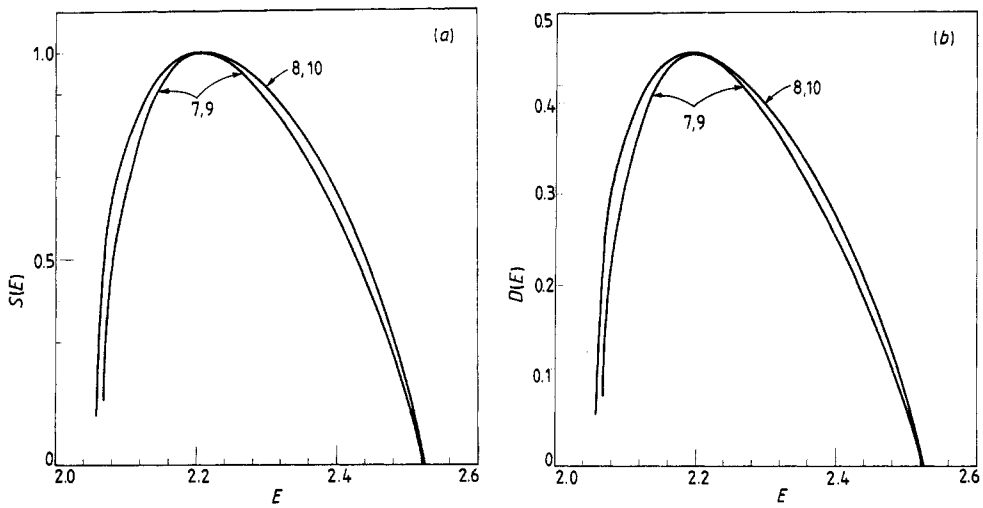

Figure 3. (a) Entropy functions $S(E)$ obtained from the Fibonacci tree structure with intervals found from equation (4). (b) The associated dimension functions $D(E)$. The maximum value of $D(E)$ equals the fractal dimension. The labels 7, 9 and 8, 10 refer to the levels from which the curves are calculated (see text).

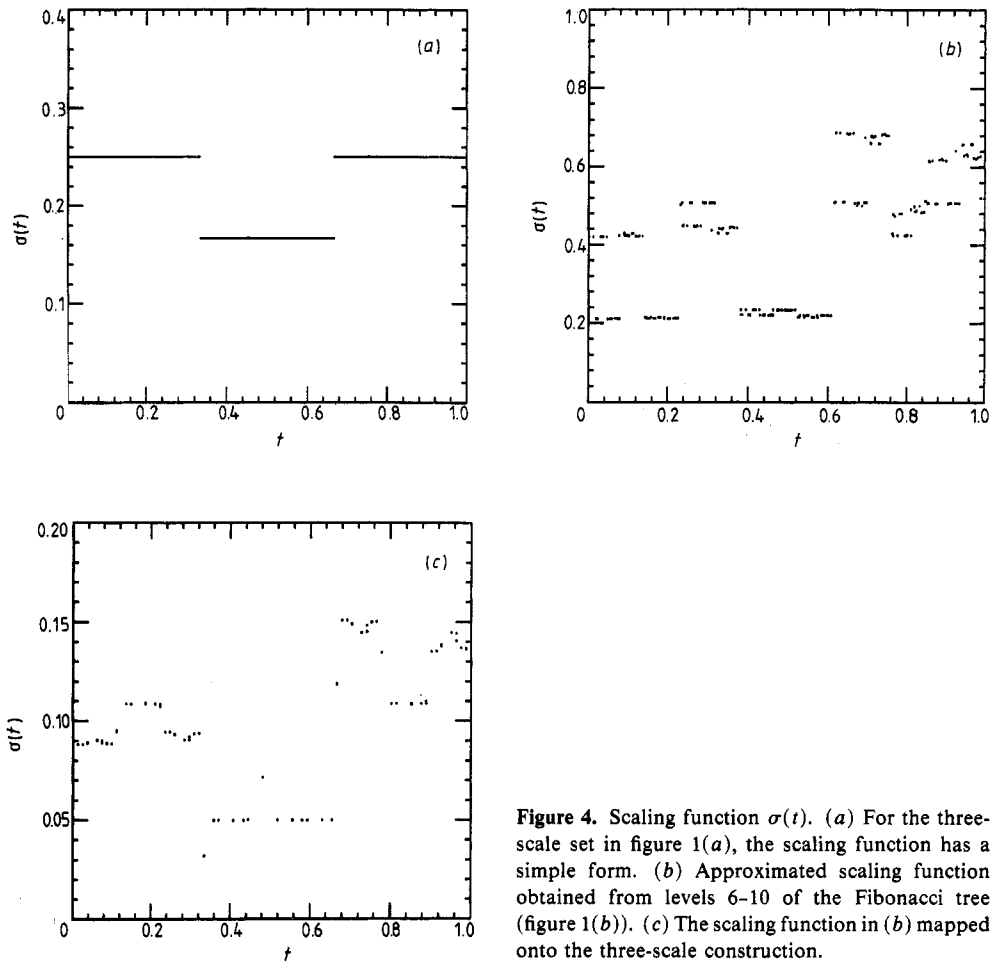

Figure 4. Scaling function $\sigma(t)$. (a) For the three-scale set in figure 1(a), the scaling function has a simple form. (b) Approximated scaling function obtained from levels 6–10 of the Fibonacci tree (figure 1(b)). (c) The scaling function in (b) mapped onto the three-scale construction.

6–10. However, to compare the two scaling functions we must first find the mapping between them. We do this by finding a translation between the paths in the form of a short dictionary from one j sequence to the other. From the Fibonacci tree to the three-scale tree this mapping is given by

$$0,0\rightarrow 0 \qquad 0,1,0\rightarrow 1 \qquad 1,0\rightarrow 2 \tag{15}$$

starting at j_1. Using (15) the scaling function in figure 4(b) is mapped to the function shown in figure 4(c). Unlike the simple step function of figure 4(a), this new scaling function manifests many distinct scales. Two scales predominate, but a great deal of fine structure is evident and indications of self-similarity are clearly visible. The fractal nature of figure 4(c) implies that $\sigma(t)$ assumes an infinite number of distinct values. However, since the deviations seem to decay quickly, the three-scale set is not a bad approximation. A similar situation arises in studies of the logistic map. There the tree structure is well approximated by a *two-scale* set, with a central-band scale α^{-1} and a side-band scale α^{-2} [10]. Although this provides a useful estimate of the fractal dimension, it does not capture the full scaling behaviour.

In summary, we have considered the one-dimensional tight-binding model with a Fibonacci sequence potential. For this system the energy spectrum is found by recursion. The clustering rules and recursion relations suggest *different* descriptions of the *same* spectrum. Based on the thermodynamic formalism, we have compared these descriptions, calculated their associated scaling functions, and constructed the mapping between them. Our analysis shows that incommensurate systems which obey simple clustering rules do not, in general, have a finite number of scaling factors.

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