# Multifractal spectral and wave-function properties of the quasiperiodic modulated-spring model

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A method is discussed to analyze multifractal properties of spectra and wave functions by means of an entropy function. The method is exemplified on a model for lattice vibrations in an incommensurate crystal phase. It is shown that the model has a spectrum with scaling properties. Moreover, it is probably singular continuous, which is a rather exceptional case. This is even true when the spectrum becomes a fat fractal. The scaling properties of the mode wave functions are discussed.

## I. INTRODUCTION

It is well known that systems with a quasiperiodic structure may show an interesting behavior in the spectra of their elementary excitations and in their electron spectra. These properties have been studied on a number of models. Most of them are linear-chain models, either tight-binding models of the form

$$t_j c_{j-1}+t_{j+1}c_{j+1}+\varepsilon_j c_j = E c_j \ , \tag{1.1}$$

or Schrödinger equations of the type

$$\left[-\frac{\hbar}{2m}\frac{d^2}{dx^2}+V(x)\right]\Psi(x)=E\Psi(x) \ , \tag{1.2}$$

where $t_j$ are hopping matrix elements, $\varepsilon_j$ site energies, and $V(x)$ a quasiperiodic potential.

One of the best studied examples is the Harper or almost-Mathieu equation which is of type (1) with $t$'s that do not depend on the site ($t_j=1$) and on-site potentials

$$\varepsilon_j=\lambda\cos(2\pi Qj+\theta) \ , \tag{1.3}$$

which give a quasiperiodic problem if $Q$ is irrational. For this model Hofstadter[1] has calculated numerically the spectrum for commensurate approximations to an incommensurate $Q$. The model is self-dual, which means that its Fourier transform has the same form, only with a different value for the coupling parameter $\lambda$. This allowed statements about the spectrum (some of them rigorous) to be proved by Aubry and André,[2] Avron and Simon,[3] Bellissard, Lima, and Scoppola,[4] and Gordon.[5] For almost all incommensurate values of $Q$ (with the exception of the set of Liouville numbers which is of measure zero) the spectrum is absolutely continuous and the states are extended for $\lambda<\lambda_c=2$, one has a point spectrum and localized states for $\lambda>\lambda_c$, and for $\lambda=\lambda_c$ the spectrum is singular continuous and the states are critical.[6,7] So the last case is an exception. Also the model is exceptional in the sense that the sharp transition disappears if one changes the cosine into another periodic function.[6]

Another exceptional model is proposed by Kohmoto, Kadanoff, and Tang[8] and Ostlund *et al.*[9] in which $\varepsilon_n$ is a Fibonacci sequence of two values. The model behaves very similarly to the almost-Mathieu model at $\lambda=\lambda_c$, but has different scaling indices which vary continuously with respect to the coupling constant (difference between the two values for $\varepsilon_n$).

In general there are for a given value of $Q$ both extended and localized states, but generally no critical states. This has been found, for example in the modulated Kronig-Penney (KP) model[10] which is of type (2) with

$$V(x)=\sum_j \delta(x-ja-f\cos(2\pi Qj+\theta)) \ , \tag{1.4}$$

By numerical methods de Lange and Janssen have shown that for given $Q$ the character of the states depends on the energy and that one may have simultaneously extended and localized states. This behavior may well be seen in a two-dimensional superspace description.[11] The same properties are not found in the mass-modulated KP model with

$$V(x)=\sum_j [1-\lambda\cos(2\pi Qj+\theta)]\delta(x-ja) \ , \tag{1.5}$$

since Bellissard *et al.*[12] have shown that this model may be mapped on the almost-Mathieu equation.

A tight-binding model may be regarded as a lattice-vibration model with nearest-neighbor coupling. If $u_n$ are the displacements from an equilibrium array, and if only nearest-neighbor interactions are taken into account, the potential energy may be written as

$$V=\tfrac{1}{2}\sum_j [k_j(u_j-u_{j-1})^2+k_{j+1}(u_j-u_{j+1})^2+s_j u_j^2] \ . \tag{1.6}$$

If we take all the masses to be identical and set to unity, the equations of motion are given by

$$\omega^2 u_j=k_j(u_j-u_{j-1})+k_{j+1}(u_j-u_{j+1})+s_j u_j \ . \tag{1.7}$$

For the choice $k_j=1$ and $s_j=\lambda\cos(2\pi Qj+\theta)-2$ one obtains the almost-Mathieu equation.

Another lattice-vibration model is the modulated-spring model, which has

$$k_j=g(Qj), \quad s_j=0; \quad g(x)=g(x+1) \ . \tag{1.8}$$

 

The potential energy in this model depends only on differences of $u$'s and the model has, consequently, a zero-frequency mode. For the choice

$$g(x)=1-\Delta\cos(2\pi x+\theta) \tag{1.9}$$

this model has been analyzed by de Lange and Janssen.[13] They find that the spectrum behaves like a Cantor set and that the spectra have scaling behavior as a function of $q$ and $\omega$. Numerical calculations showed that the spectrum has a very intricate structure, which may be described in terms of the continued-fraction expression of $Q$. This result was similar to that of Hofstadter for the almost-Mathieu model.

A version of the modulated-spring model with a discontinuous modulation function,

$$g(x)=\begin{cases} A & \text{for } -\phi<x<1-2\phi \\ B & \text{for } 1-2\phi<x<1-\phi \end{cases}. \tag{1.10}$$

was studied.[14–16]. Here $\phi=(\sqrt{5}-1)/2$ is the inverse of the golden ratio. The sequence of spring constants forms then a Fibonacci sequence. It can be shown[15,16] that this model has the renormalization-group type equation which is analogous to that of the electronic tight-binding model on the Fibonacci chain.[8,9] Therefore again it shows a singular continuous spectrum and critical states.

The spectra and wave functions or eigenvectors of the various models show a large variety in behavior. The problem is to characterize this numerically. For a spectrum with scaling properties one number that gives a certain characterization is its Hausdorff dimension. For the degree of localization several ways have been proposed for that purpose. A method which generalizes all these approaches and which uses the full information contained in the multifractals is by means of a spectrum of scaling indices which is a function of the scale exponents present in the problem. Usually this function is denoted by $f(\alpha)$. A generalization of this concept has been given by Halsey *et al.*[17] Kohmoto[18] has introduced a formulation analogous to the formalism of statistical mechanics with an entropy function and a free energy with which the scaling properties of multifractals fully may be described. In the latter formalism the $f(\alpha)$ function has a natural interpretation. There are previous papers which try to use the multifractal analysis to the incommensurate electronic problem,[19–22] but an interpretation of the spectrum of scaling indices in terms of the entropy function is not given.

In the present paper we discuss a particular model, the modulated-spring model, because of its interesting properties and to study the application of the entropy function method to the scaling properties of a physical system.

The organization of the paper is as follows. In Sec. II, the formalism and its application to spectra and wave functions (or vibration eigenvectors) are discussed. In Sec. III we discuss the spectra of the modulated-spring model, for the case that the wave vector of the modulation is the inverse of the golden mean and that the amplitude of the modulation is maximal (i.e., $\Delta=1$). In Sec. IV the eigenvectors of the same system are studied, in Sec. V the spectra for $\Delta<1$, and in Sec. VI the eigenvectors for the latter case. In Sec. VII, a nonsinusoidal modulation is considered. Final remarks are given in Sec. VIII.

As discussed above there is a direct relation between electron models in the tight-binding approximation and vibration models. In the former case wave functions are given by the numbers $c_j$, in the latter displacements are given by $u_j\exp(i\omega t)+\text{c.c.}$, where for a periodic system with period $N$ one has $u_{j+mN}=\exp(ikm)u_j$ $(0<n<N+1)$ and $u_j$ is an eigenvector of the dynamical matrix. Because our discussion applies equally well to the electron as to the phonon problem we shall always talk about wave functions instead of wave functions or eigenvectors.

## II. SCALING ANALYSIS OF THE SPECTRUM AND WAVE FUNCTIONS

In a scaling analysis of a fractal set with measure (multifractal), we consider a systematic partition of the set. The $n$th level of the partition consists of a number of bars with length $l_i$. A scaling index for $l_i$ is given by $l_i\sim e^{-n\varepsilon_i}$. We consider a situation where a probability measure $p_i$ is associated with each bar. The scaling index of singularity is given by $p_i\sim l_i^{\alpha_i}$. Now distributions of $\varepsilon$ and $\alpha$ specify the scaling properties of the multifractal. Here one can use a formalism equivalent to statistical mechanics to obtain the distributions. The analysis of the spectrum is a special case where we have a distribution of $l_i$, but where $p_i$ is constant. On the other hand, the wave function has a distribution of $p_i$, but $l_i$ is constant. For a more detailed discussion on the statistical-mechanics of multifractals, see Ref. 18.

### A. Spectrum

In order to understand the scaling of the spectrum, we need to define appropriate scaling indices and the entropy function for them. It is convenient then to consider systematic approximations or finite partitions of the Cantor-set spectrum. This can be done by replacing the irrational number $Q$ by a series of rational numbers which are obtained by truncating the continued-fraction expansion of $Q$. For example, the inverse of the golden mean $[\phi=(\sqrt{5}-1)/2]$ is approximated by a series of rational numbers $F_{n-1}/F_n=\{\frac{1}{2},\frac{2}{3},\frac{3}{5},\frac{5}{8},\frac{8}{13},\ldots\}$ where $F_n$ is a Fibonacci number defined recursively as $F_{-1}=F_0=1$ and $F_{n+1}=F_n+F_{n-1}$. At the $n$th level of approximation of the Cantor-set spectrum, we have $N$ bands whose widths are denoted by $\Delta_i$ $(i=1,\ldots,N)$. The number of bands grows exponentially with respect to $n$ as $N\sim a^n$ (in the example above $N=F_n$ and $a=\tau=\phi^{-1}$).

Let us define a scaling index for $\Delta_i$ by

$$\varepsilon_i=-\frac{1}{n}\ln\Delta_i\ . \tag{2.1}$$

We also define an entropy function $S(\varepsilon)$ by

$$S(\varepsilon)=\frac{1}{n}\ln\Omega(\varepsilon)\ , \tag{2.2}$$

where $\Omega(\varepsilon)d\varepsilon$ is the number of bands whose scaling index lies between $\varepsilon$ and $\varepsilon+d\varepsilon$. Here it is important to notice

that $\Delta_i$ and $\Omega(\varepsilon)$ depend exponentially on $n$. A band at the $n$th level splits into many bands at a higher level and may thus yield a number of different values of the scaling indices $\varepsilon$. However, we expect that the entropy function which represents the distribution of $\varepsilon$ will converge to a smooth limiting form as $n$ tends to infinity, and give the complete information about the scaling behavior.

As in the formalism of statistical mechanics, it is convenient to introduce a "partition function" and a "free energy," which are defined by

$$Z_n(\beta)=\sum_{i=1}^{N}\Delta_i^{\beta} \tag{2.3}$$

and

$$F(\beta)=\lim_{n\to\infty}\frac{1}{n}\ln Z_n(\beta)\ . \tag{2.4}$$

Once the free energy is calculated (see Fig. 1, for example), the entropy function is obtained by a Legendre transformation,

$$S(\varepsilon)=F(\beta)+\beta\varepsilon\ , \tag{2.5}$$

$$\varepsilon=-\frac{dF(\beta)}{d\beta}\ . \tag{2.6}$$

Thus by changing "temperature" $\beta$ one can pick a value of $\varepsilon$ and then the corresponding $S(\varepsilon)$ is calculated. On the other hand, $\beta$ can be written in terms of $\varepsilon$ as

$$\beta=\frac{dS(\varepsilon)}{d\varepsilon}\ . \tag{2.7}$$

Usually $S(\varepsilon)$ is defined on an interval $[\varepsilon_{\min},\varepsilon_{\max}]$ and there is no scaling behavior corresponding to $\varepsilon$ which is outside the interval and $S(\varepsilon)=0$. However, $F(\beta)$ is still defined there and from (2.5) it is given by $F(\beta)=-\varepsilon_{\max}\beta$ for $\beta>\beta_{\min}$ and $F(\beta)=-\varepsilon_{\min}\beta$ for $\beta<\beta_{\max}$. Thus useful information is only contained in $F(\beta)$ for the region between $\beta_{\min}$ and $\beta_{\max}$ where it is not linear.

The Hausdorff $D_H$ is the zero $\beta_c$ of the free energy [see (2.3) and (2.4)], i.e.,

$$F(D_H)=0\ . \tag{2.8}$$

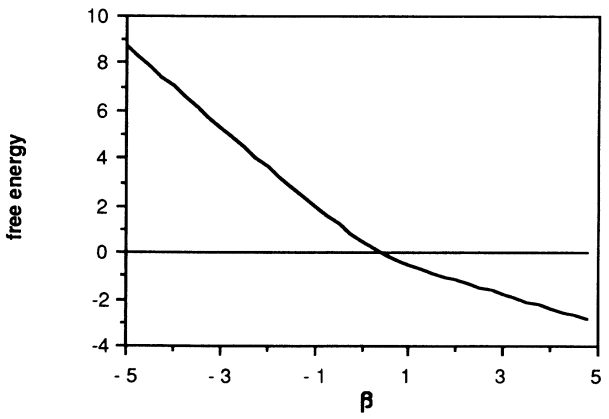


FIG. 1. The free energy for a spectrum (period 89, $\Delta=1$).

From (2.5), (2.7), and (2.8) we have

$$\beta_c=\frac{S(\varepsilon)}{\varepsilon}=\frac{dS(\varepsilon)}{d\varepsilon}\ . \tag{2.9}$$

Thus the Hausdorff dimension $D_H=\beta_c$ has a geometrical interpretation in $\varepsilon-S(\varepsilon)$ plot: it is a slope of the line through the origin tangent to $S(\varepsilon)$.

The index $\varepsilon$ which represents scaling of the Lebesgue measure of the energy spectrum can actually be related to the singular behavior of the density of states. At the $n$th level of approximation, each band carries the same number of states: $p_i=1/N=a^{-n}$ (the total number of states is normalized to unity, i.e., $\sum_i p_i=1$). An index $\alpha_i$ which represents the singular behavior of the density of states is defined as

$$p_i\sim\Delta_i^{\alpha_i}\ . \tag{2.10}$$

Since $p_i=1/N=a^{-n}$ and $\Delta_i\sim e^{-n\varepsilon_i}$ [see (2.1)], it is related to $\varepsilon$ by

$$\alpha\varepsilon=\ln a\ . \tag{2.11}$$

The spectrum of singularity introduced by Halsey *et al.*[17] is given by

$$\Omega'(\alpha)\sim\langle\Delta\rangle^{f(\alpha)}\ , \tag{2.12}$$

where $\Omega'(\alpha)d\alpha$ is a number of bands whose scaling index $\alpha$ lies between $\alpha$ and $\alpha+d\alpha$, namely $\Omega'(\alpha)=\Omega(\varepsilon)\,|\,d\varepsilon/d\alpha\,|$, and $\langle\Delta\rangle$ is a representative value of $\Delta$ which was not specified clearly in Ref. 17. If one identifies $\langle\Delta\rangle=\exp(-n\varepsilon)$ [see (2.1)], $f(\alpha)$ can be related to the entropy function by

$$f(\alpha)=\frac{S(\varepsilon)}{\varepsilon}\ . \tag{2.13}$$

This simple relation between $f(\alpha)$ and $S(\varepsilon)$ holds since the measure $p_i$ is constant in this case. In general the measure has its own scaling behavior and we do not have a simple relation like (2.13).

An absolute continuous spectrum, for which the states are extended, has a nonsingular density of states (apart from possible Van Hove singularities) and $\alpha$ is given by 1 [see (2.10)]. On the other hand, a point spectrum, which corresponds to localized states, would give $\alpha=0$. If $\alpha$ is different from 0 or 1, the spectrum has a nontrivial scaling and probably one can expect a singular continuous spectrum. The corresponding wave functions are neither localized nor extended in the standard way and are called "critical." Thus the entropy functions $S(\varepsilon)$ and $f(\alpha)$ give the essential information on the spectral type and the nature of the wave functions.

### B. Wave functions

A wave function is defined on lattice sites which are regular. Therefore the wave function is not singular nor fractal as it is. However, for the incommensurate problem there is a consistent way to take a scaling limit of the lattice which is a continuous interval [0,1]. Then the wave function defined on the interval can have singularities and scaling which we shall analyze.

In the $n$th approximation the system is periodic with period $N$. Consider now the square of the wave function at site $i$ as a probability measure, namely,

$$p_i = |u_i|^2 . \tag{2.14}$$

Here the summation is restricted to sites $i$ with nonvanishing $u_i$. We normalize $p_i$ to unity by

$$\sum_{i=1}^{N} p_i = \sum_{i=1}^{N} |u_i|^2 = 1 \tag{2.15}$$

for a finite system with $N$ sites. Assign a uniform Lebesgue measure $l = N^{-1}$ to all the sites. Then the size of the system is normalized to unity. In the limit of $n$ tending to infinity, the probability measure is defined on the interval [0,1] and one can discuss singularities and scaling. Here the support of the probability measure is nonfractal, but the distribution of the measure can have scaling. Note the difference from the previous case of the spectrum in which the probability measure is uniformly assigned but the support may be a Cantor set or a fractal.

The scaling index for the Lebesgue measure is given by $l = \exp(-n\varepsilon)$ and is constant:

$$\varepsilon = \ln a . \tag{2.16}$$

The scaling index for the probability measure is defined as

$$p_i = l_i^{\alpha} \tag{2.17}$$

and the entropy for $\alpha$ is defined as

$$S'(\alpha) = \frac{1}{n} \ln \Omega(\alpha) , \tag{2.18}$$

where $\Omega(\alpha)d\alpha$ is the number of sites which have index between $\alpha$ and $\alpha + d\alpha$. As $n$ is increased a single site becomes many sites and it is not possible in general to follow a single scaling index. However we expect that the entropy function $S'(\alpha)$ which represents the distribution of $\alpha$ converges to a smooth limiting form as $n$ tends to infinity. Thus the scaling behavior of the wave function is well represented by $S'(\alpha)$.

As in the previous case of the spectrum, it is convenient to introduce a partition function

$$Z'(q) = \sum_i p_i^q , \tag{2.19}$$

and a free energy

$$G(q) = \frac{1}{n} \ln Z'(q) . \tag{2.20}$$

The entropy function is given by the Legendre transformation

$$S'(\alpha) = G(q) + q\alpha\varepsilon , \tag{2.21}$$

and

$$\alpha\varepsilon = -\frac{dG(q)}{dq} . \tag{2.22}$$

The function $f(\alpha)$ in this case is defined as[17]

$$\Omega(\alpha) \sim l^{f(\alpha)} , \tag{2.23}$$

and relates to the entropy function by [see (2.18)]

$$S'(\alpha) = \varepsilon f(\alpha) . \tag{2.24}$$

For an extended wave function we should have $\alpha = 1$, and a localized wave function has $f(\alpha)$ consisting of two points: $f = 0$ at $\alpha = 0$ and $f = 1$ at $\alpha$ going to infinity. The point $\alpha = 0$ corresponds to the sites with nonzero $u$ and the point $\alpha$ at infinity all the other sites. For a scaling wave function with one exponent $\alpha_0$, $f$ again consists of two points: $f(0) = 0$ and $f(\alpha_0) = 1$ (an example is given in the Appendix and illustrated in Fig. 2). For a critical wave function with a distribution of scaling indices we expect to have a smooth $f(\alpha)$ defined in a finite region $[\alpha_{\min}, \alpha_{\max}]$.

## III. SPECTRA OF THE MODULATED-SPRING MODEL, $\Delta = 1$

The modulated-spring model was proposed as a simple model to mimic the behavior of the lattice vibrations in an incommensurate system, with the idea that the force constants would not be constant in the crystal but would experience an influence of the period of the incommensu-

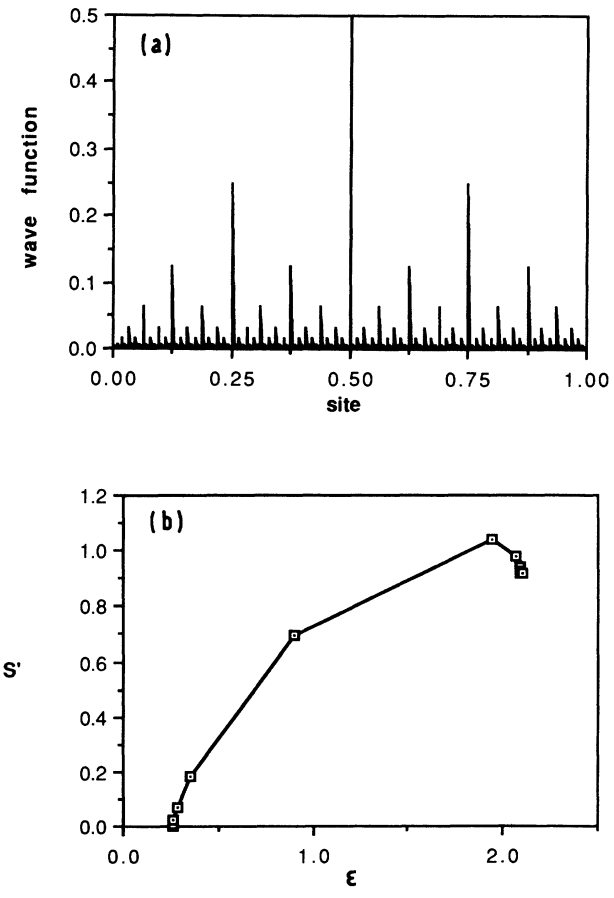


FIG. 2. (a) The function $u(x)$ for an approximant to a scaling function: $N = 2^m$, $u(2^{m-j} + z2^{m-j+1}) = 2^{m-j}$ for $j = 1, \ldots, m$, $z = 1, \ldots, 2^{m-1}$. This function has only one scaling exponent: $\alpha_0 = 2$. (b) The entropy function $S'(\varepsilon)$ for this wave function.

rate modulation. For small amplitude the modulation function is almost sinusoidal which leads to the equations of motion

$$\omega^2 u_j = k_j(u_j - u_{j-1}) + k_{j+1}(u_j - u_{j+1}) , \tag{3.1}$$

with spring constants

$$k_j = 1 - \Delta \cos(2\pi Q j + \theta) . \tag{3.2}$$

For $\Delta = 1$ this leads to a physically extreme situation that for incommensurate values of $Q$ the spring constants become arbitrarily small. They do not vanish, however, as long as $\theta$ is not a multiple of $Q$ modulo $2\pi$. The way to study the spectrum here for an incommensurate value of $Q$ is to use the continued-fraction expansion for $Q$. As the simplest case we take $Q$ to be $\phi$ the inverse of the golden ratio. Approximants for $Q$ are then the rational numbers $F_{n-1}/F_n$, the ratio of two consecutive Fibonacci numbers. We then determine numerically the eigenvalues of the dynamical matrix for given wave vector $k$. Because for a commensurate structure and $\theta = 0$ springs become zero, we take the case $\theta = \pi/N$ which corresponds to bands of maximal width for the given $Q$ and $\Delta$. For a commensurate approximation there are $F_n$ bands for which the boundaries are found for $k = 0$ and $k = \pi$. When $n$ tends to infinity not only the number of bands tends to infinity and consequently their widths to zero, but also the total Lebesgue measure of the spectrum $B$ ends to zero as $B \sim N^{-\delta}$ with $\delta = 0.67$ (see Fig. 3). This behavior of the total Lebesgue measure was also found in the almost-Mathieu equation at $\lambda = \lambda_c$.[6] From the spectra the self-similar properties are conspicuous (see Fig. 4). If one considers the width of the highest band for increasing values of $n$, this scales down according to

$$\Delta_{\text{top}} \sim \exp(-n\varepsilon) \tag{3.3}$$

with $\varepsilon$ approximately equal to 0.7 (Fig. 5). Here we want to analyze these scaling properties in more detail using the technique formulated in Sec. II.

Therefore, we calculate for increasing values of $n$ the free energy,

$$F(\beta) = \frac{1}{n} \ln \left[ \sum_i \Delta_i^{\beta} \right] , \tag{3.4}$$

and the values of $\varepsilon$ and the entropy $S(\varepsilon)$ as a function of $\beta$. As discussed in Sec. II A the Hausdorff dimension of the spectrum is given by $\beta_c$ for which $F(\beta_c) = 0$. Results for the entropy function for $F_n = 34$, 89, and 144 are given in Fig. 6. From this it is clear that we are already in the limiting region, the results do no longer depend on the size. The Hausdorff dimension is estimated to be 0.38. However, Fig. 6 is an indication that there is more than one scaling exponent. It proves that the spectrum in this case is singular continuous. A model with an absolutely continuous spectrum like the almost-Mathieu model for $\lambda < \lambda_c$ behaves in a completely different way.[20] In our opinion the present result is a strong support for the conjecture that the spectrum is singular continuous.

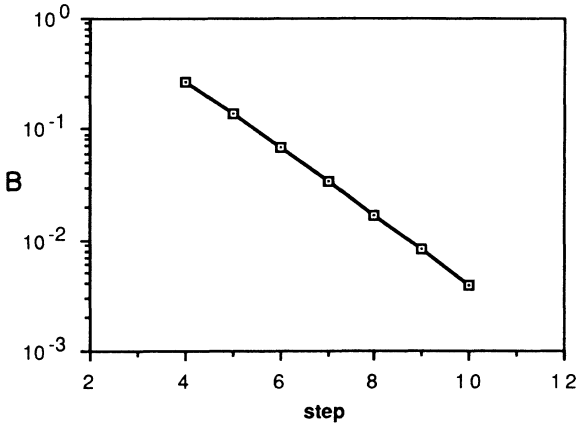


FIG. 3. The Lebesgue measure $B$ of the spectrum against $n$. The size of the system at step $n$ is $F_n$.

## IV. EIGENVECTORS OF THE MODULATED-SPRING MODEL, $\Delta = 1$

To analyze the corresponding wave functions we calculate for the same commensurate approximants the eigenvectors of the dynamical matrix and apply to them to analysis of Sec. II B. So first we calculate for every wave function the quantity

$$G(q) = \frac{1}{n} \ln \left[ \sum_{i=1}^{F_n} |u_i|^{2q} \right] , \tag{4.1}$$

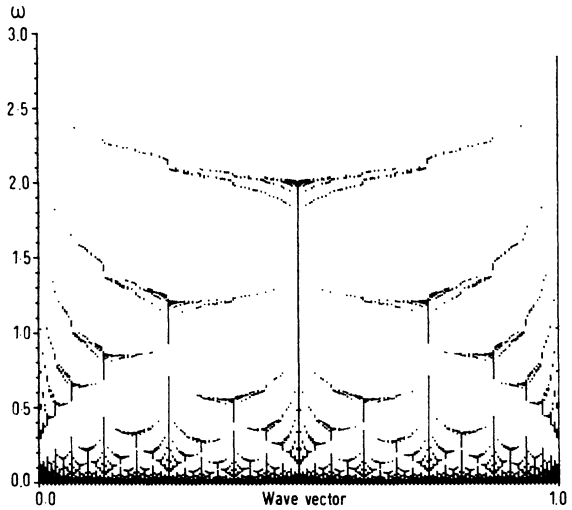


FIG. 4. Spectra of the modulated spring model with $\Delta = 1$ for a selection of commensurate modulation wave vectors (Ref. 23). These are chosen as consecutive Farey numbers $Q(n,j)$, where $n = 1,2,3,\ldots,7$ and $j = 1,\ldots,2^m$. These are defined as follows. $Q(1,1) = 0/1$, $Q(1,2) = 1/1$. A Farey number at level $m$ is obtained from two consecutive ones $p/q$ and $p'/q'$ at level $m-1$ as $(p+p')/(q+q')$.

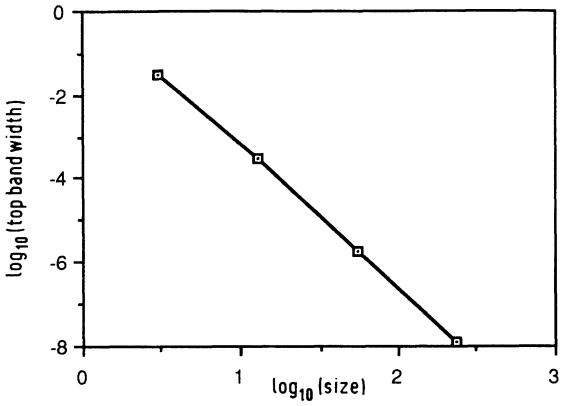


FIG. 5. The log of the width of the top band for $\Delta=1$ against the log of the size $F_{n+1}$ of the system.

where the sum is restricted to non-vanishing values of $u_i$. Then the scaling exponent entropy function is obtained as

$$S'(\alpha)=G(q)=q\varepsilon\alpha \tag{4.2}$$

with

$$\alpha=-\frac{1}{\varepsilon}\frac{dG(q)}{dq} \tag{4.3}$$

and

$$\varepsilon=\ln\phi\ . \tag{4.4}$$

The spectrum of singularity is given by

$$f(\alpha)=S'(\alpha)/\varepsilon\ . \tag{4.5}$$

The wave function at $\omega^2=0$, which always exists because the system is translational invariant, has $\alpha=1$, $f(\alpha)=1$ [see Eq. (2.23)], and clearly is an extended state. The other wave functions, however, are neither localized nor extended.

In Fig. 7, the wave functions are given for some modes with $k=0$ (which is equivalent to the periodic boundary condition) for systems with period 55 and 233. For $N=55$ the modes 50 and 51 are given, and for $N=233$, the mode 89 is given. The characters of the corresponding modes in the incommensurate limit are not clear from these pictures. However, the spectra of scaling index for the two cases are quite different. In Fig. 8 the functions $f(\alpha)$ are given for the two $N=55$ modes. These do not change much for higher $N$, and we consider that they are

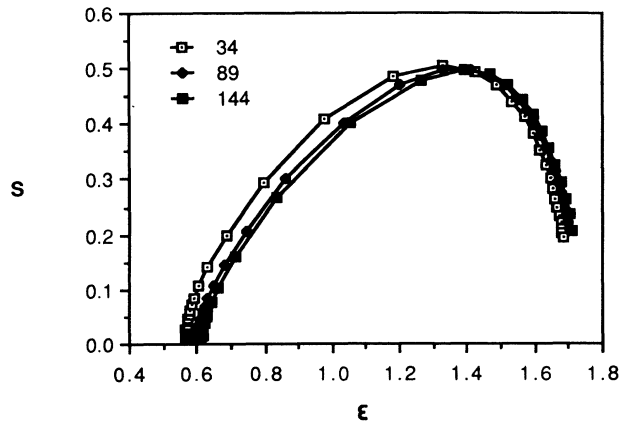


FIG. 6. The entropy function $S(\varepsilon)$ for the spectra for various values of $n$. (Size $F_n$, $\Delta=1$.)

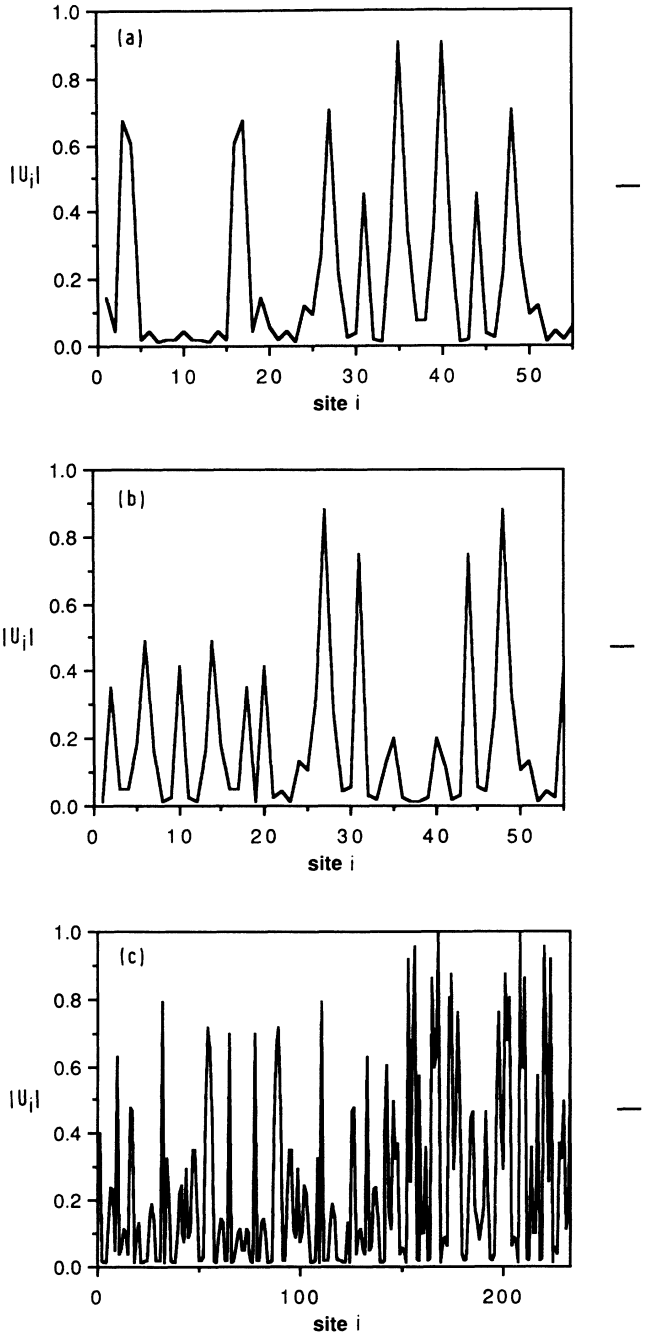


FIG. 7. Wave functions for a number of modes in periodic systems with $N=55$ [vectors 50(a) and 51(b)] and $N=233$ [vector 89(c)].

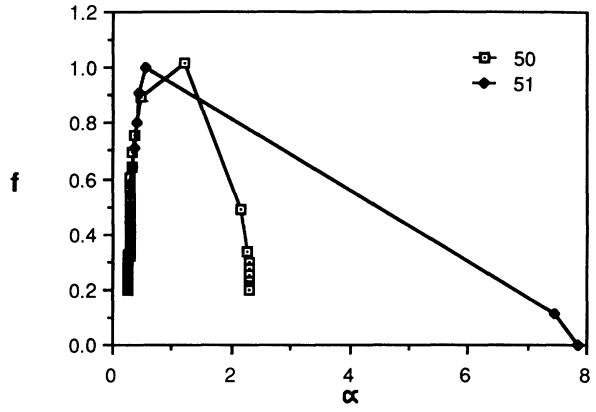


FIG. 8. Functions $f(\alpha)$ for the $N=55$ wave functions in Fig. 7.

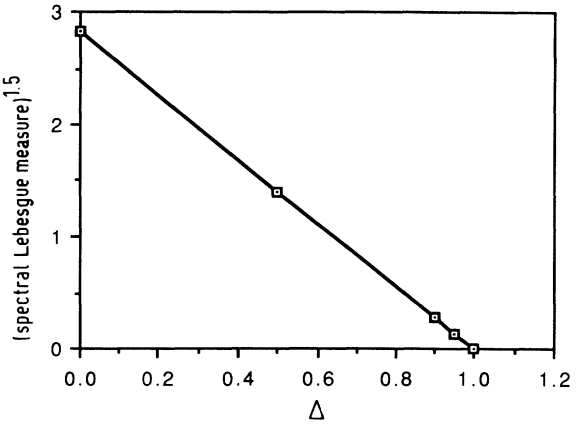


FIG. 9. The measure of the spectrum as a function of the modulation parameter Δ.

already close to limiting forms. There is a clear difference between the odd modes, which are at the bottom of a band, and the even modes, which are at the top. The points in the picture correspond to equidistant values of $q$. Negative values of $q$ correspond to larger values of $\alpha$. For wave functions at the bottom of the band the low-$q$ points go to $f=0$ for a large value of $\alpha$ and the high-$q$ points accumulate at a finite value of both $\alpha$ and $S'$. The limiting value of $\alpha$ is between 0 and 1 which implies that the wave function should be called critical. For wave functions at the top of the band there are cumulation points for finite values of $\alpha$ and $S'$ at both ends of the $q$ scale. So although the wave functions look rather similar, their scaling behavior is different. This difference is not well described by the fractal dimension which is for both cases almost the same.

The highest point of the wave function corresponds to the smallest $\alpha$. The fact that the entropy functions $S'(\alpha)$ or $f(\alpha)$ has nonzero value has a significant consequence. The wave function does not decay at all and could be considered to be extended. However it is not a standard extended wave function since it has scaling and is critical. Note that some critical wave functions of the Fibonacci lattice to decay algebraically, and $f(\alpha)$ vanishes for the smallest $\alpha$.[15,22]

Sometimes the degree of localization of a wave function is given by the partition ratio,

$$\frac{\sum_i u_i^4}{\left[\sum_i u_i^2\right]^2} \tag{4.6}$$

which is just the value of $Z'(q)$ at $q=2$ and thus only gives very limited information on scaling and localization of the wave function.

## V. SPECTRA FOR $\Delta<1$

When the coefficient Δ in (3.2) is not unity, the spectrum has in the incommensurate limit a finite Lebesgue measure: the spectrum becomes fat (see Fig. 9). For Δ tending to zero the measure goes to 2. Empirically the Lebesgue measure of the spectrum behaves as

$$B=2(1-\Delta)^{2/3} . \tag{5.1}$$

To see whether the fact that the spring constants may become arbitrarily small is determining for the singular continuous spectrum, or that such a spectrum may occur for a fat fractal as well, we have analyzed the spectrum for Δ between 0 and 1.

With the same method as in Sec. III we determined the entropy function for various approximants to $\phi$ and for various values of the modulation parameter Δ. The result for a number of values of Δ is shown in Fig. 10. Care has been taken to be sure that the result does no longer depend strongly on the size: the limiting curves for $n$ tending to infinity do not differ significantly from the ones shown here. As soon as Δ differs from unity the function $S(\varepsilon)$ starts to shift but its support remains restricted to a finite interval and is not just $\varepsilon=1$ as one would have for extended states. Only in the limit for

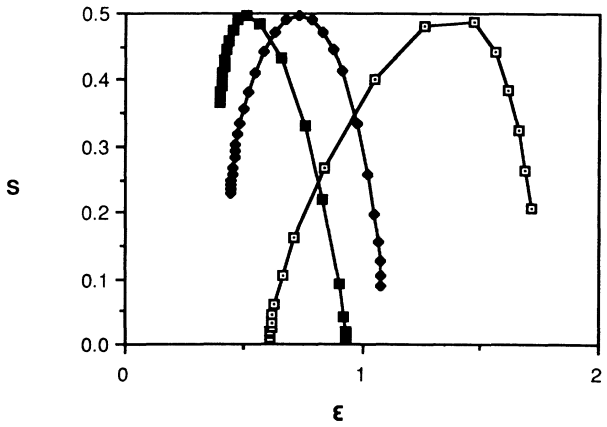


FIG. 10. The entropy function $S(\varepsilon)$ of the spectrum for three different values of the modulation parameter Δ: □, Δ=1.0; ◆, Δ=0.95; ■, Δ=0.5.

$\Delta=0$ the interval shrinks to a point. The conclusion is that also the spectrum in this case has scaling properties and is, therefore, a fat fractal. The higher-order gaps, however, tend rapidly to zero.

## VI. EIGENVECTORS FOR $\Delta < 1$

Because the spectra for the case $\Delta < 1$ still show scaling behavior it is interesting to look at the character of the

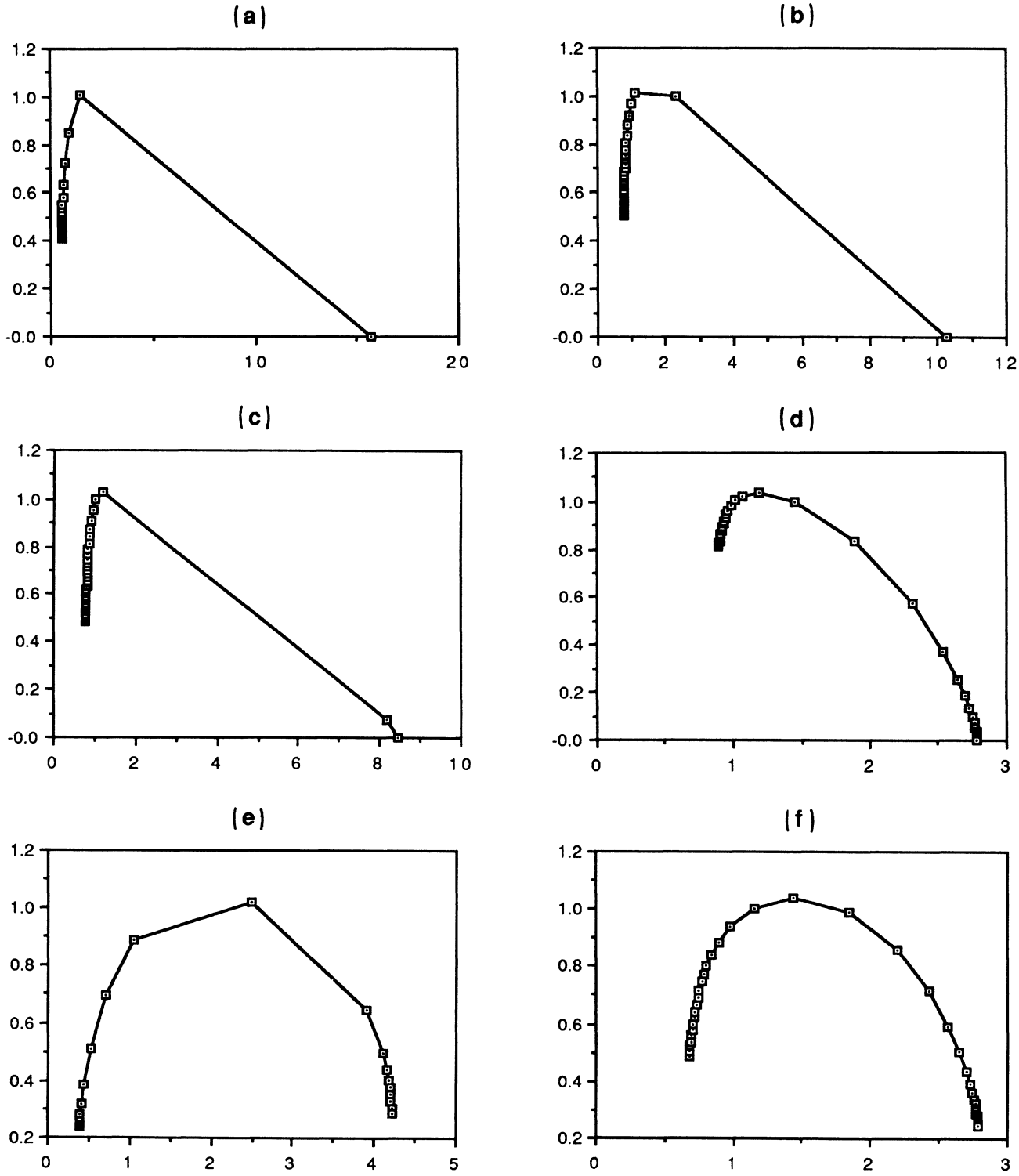


FIG. 11. The entropy function for a number of eigenvectors at $N=89$ for various values of the modulation parameter $\Delta$. (a)–(d), a wave function at the bottom of the band; $\Delta=1.0$, 0.95, 0.9, and 0.5, respectively. (e)–(h), a wave function at the top of the band; $\Delta=1.0$, 0.95, 0.9, and 0.5, respectively.

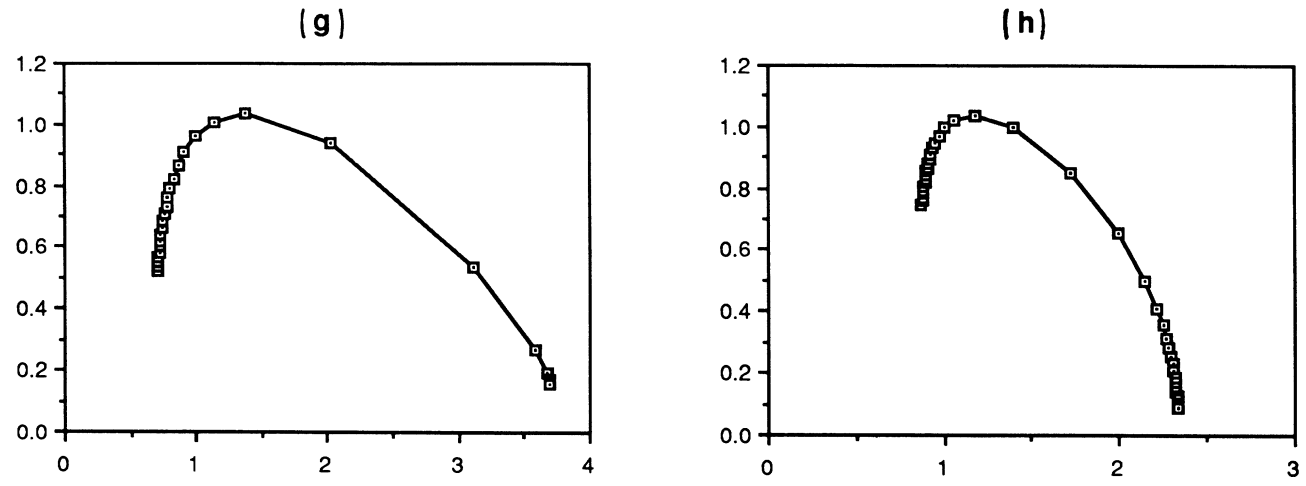


FIG. 11. (*Continued*).

wave functions. Therefore, we made a preliminary investigation, using the same techniques as in Sec. IV. We did this for a number of values of $\Delta$: 1.0, 0.95, 0.9, and 0.5.

In Fig. 11 the results are given for two wave functions for these four values of $\Delta$. It turns out the same difference exists between wave functions at the top of a band and those at the bottom as in the case $\Delta=1$. The 14th eigenvector for $k=0$ is at the bottom of the band and has a support of $S'$ that is much smaller than that for the 13th which is at the bottom. A careful analysis of this change and of the character of wave functions in the middle of a band still has to be done. The bottom wave function has points with entropy zero for large values of $\alpha$. These values increase to infinity when $\Delta$ tends to unity. On the other hand the support $[\alpha_{\min},\alpha_{\max}]$ shrinks to zero when $\Delta$ goes to zero, in agreement with the fact that in that case all wave functions are certainly extended.

The preliminary investigation points to the expectation that the critical states are not restricted to certain energy ranges. So, if there is a mobility edge, this probably also has a fractal character.

## VII. NONSINUSOIDAL MODULATION

The modulation function $g(x)$ in the preceding sections was chosen as the most simple, sinusoidal, one. If one changes this into a function with higher harmonics, the simple description of the spectrum in terms of the continued-fraction expansion of the modulation wave vector breaks down.[13] The sinusoidal function has the special property that in $k$ space one has again a discrete problem with nearest-neighbor interaction only. For a special choice of the Hamiltonian this even leads to the almost-Mathieu equation which is a self-dual model.

To see whether the sinusoidal form of the modulation is at the origin of the special spectral properties we investigated the modulated-spring model with

$$g(x)=1-\Delta\tanh[\mu\cos(2\pi x+\theta)]/\tanh(\mu)\ . \qquad (7.1)$$

When $\mu$ goes to zero this gives the sinusoidal form (1.9), when $\mu$ goes to infinity, one obtains a discrete function similar to (1.10). To see the properties of the spectrum, we calculated the spectral Lebesgue measure for a number of approximants to the inverse golden mean, in the case $\Delta=1$. The results are shown in Fig. 12. Again, the limit of the spectral measure is zero, but, what is more, the scaling exponent is independent of the value of $\mu$. Asymptotically, (this region is reached already for small values of $n$) the curves run parallel. This is an indication that the spectrum will be a fractal for all values of $\mu$. The sinusoidal form of the modulation, therefore, is not important for having a singular continuous spectrum.

## VIII. FINAL REMARKS

We have presented a method to characterize the scaling and fractal properties of a spectrum or of wave functions by means of an entropy function. It uses the full information and may distinguish therefore better between different situations than often used quantities as the Hausdorff dimension or the participation ratio. These

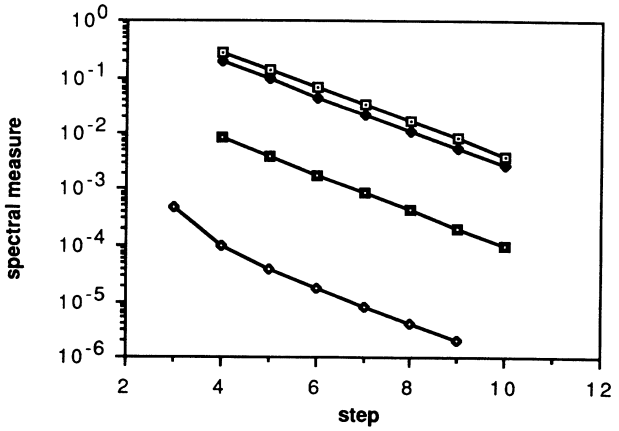


FIG. 12. Spectral Lebesgue measure for the modulated-spring model with modulation function (7.1), for values $\mu=0.01$ (⊡), 1.0 (♦), 5.0 (□), and 10.0 (◇), respectively.

two numbers are contained in the information given by the entropy function.

We have applied the method to a model for lattice vibrations in an incommensurate (or quasiperiodic) crystal phase, the modulated-spring model. This model has very interesting properties. We have examined the special case that the modulation wave vector is the golden ratio.

For the maximal modulation amplitude, $\Delta=1$ which corresponds to the situation that the spring constants become arbitrarily small, the entropy function behaves as that of a fractal, supporting the conjecture that the spectrum is singular continuous, which is one of the few known examples of such a spectrum.

This situation remains when $\Delta<1$. In this case there are fractal properties and the spectrum is a fat fractal. The wave functions in the case $\Delta=1$ are neither extended (except for the single $\omega=0$ mode) nor localized. They should be considered as critical, in agreement with the character of the spectrum. For $\Delta<1$ one still has critical states and probably a mobility edge with fractal properties. The character of the wave functions depends on their position in the band. This situation requires a further analysis.

Only the spectra and wave functions for wave vector equal to the golden mean have been considered. Scaling behavior for other wave vectors can in principle be investigated by the same technique. This does, however, not explain the special scaling properties in the $Q$-$\omega$ plane, i.e., if one compares different wave vectors.[23]

## ACKNOWLEDGMENTS

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## APPENDIX

An exact calculation of the entropy function can be made for a simple model for the wave function. Consider a chain with length normalized to one. Then $u(\frac{1}{2})=1$, $u(\frac{1}{4})=u(\frac{3}{4})=p$, $u(\frac{1}{8})=u(\frac{3}{8})=u(\frac{5}{8})=u(\frac{7}{8})=p^2$, etc. For the $n$th step in the approximation there are $2^n-1$ sites. The function $Z_n'$ is

$$Z_n'(q)=\sum_{i=1}^{N} u_i^{2q}=\frac{1-(2p^{2q})^n}{1-2p^{2q}} \ . \tag{A1}$$

Here $p^{2q}$ is supposed to be unequal to $\frac{1}{2}$. Then for $p^{2q}>\frac{1}{2}$ mainly the sites with small values of $u$ contribute and one has

$$G\sim\frac{1}{n}\ln(2p^{2q})^n=\ln 2+2q\ln p \ , \tag{A2}$$

which gives $\alpha=-2\ln p/\ln 2$ and $S'=1$. For $p^{2q}>\frac{1}{2}$ one has

$$G\sim\frac{-1}{n}\ln(\,|\,1-2p^{2q}\,|\,) \ , \tag{A3}$$

which goes to zero, implying a value zero for both $\alpha$ and $S'$. In this case the support of $S'$ consists of two points. The sites with small function values $u_i$ determine the scaling exponent, which is 2 if $p=\frac{1}{2}$.

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