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LETTER TO THE EDITOR

Phase transitions on strange sets: the Ising quasicrystal

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Abstract. A quantum Ising spin chain with nearest-neighbour couplings arranged in a quasiperiodic sequence is considered. The Cantor set structure of the energy spectrum is analysed in terms of the thermodynamic description of multifractals. Evidence is given that the spectrum of scales develops a singular behaviour: this is associated with a first-order phase transition of a new type. It is argued that this effect involves, not only quantum spins, but the whole class of phonon-like propagation problems on quasiperiodic chains.

Propagation along aperiodic chains generated by inflation rules is characterized by critical states (neither extended nor localized) and Cantor set energy spectra.

The associated scaling properties can be explored within a renormalization group (RG) scheme, based on the underlying hierarchical order of the chains.

In a wide variety of cases, including the Schrödinger problem with potentials assigned in the Fibonacci way, the RG exponents are model dependent.

As pointed out in [1], while, for example, in tight binding models of electron propagation the exponents depend on the values of the potential, in phonon propagation they further depend on the specific value of energy: this implies energy spectra with inhomogeneous scaling behaviour (see also [2], where the discrete Laplace operator is considered). In this letter we try to further specify the effects of this dependence on the Cantor structure of the spectra: we consider a quantum Ising spin chain with two-valued nearest-neighbour (NN) couplings ordered according to a Fibonacci sequence, and prove that its energy spectrum is a multifractal characterized by a first-order phase transition in the spectrum of singularities.

As will be clarified in the following, quantum spin chains do indeed belong to the mentioned class of phonon-like problems, so that our results holds for the whole class.

The interest of this model is twofold: on the one hand it mimics the behaviour of quasiperiodic superlattices generated by magnetic constituents, on the other hand it conjugates the critical properties of the spectrum with the occurrence of a phase transition.

The model has been numerically studied in [3]; in [4] it was analytically shown that it undergoes a phase transition and the corresponding critical exponents were determined; furthermore, by means of a RG analysis, the scaling exponents of the spectrum were obtained.

The Hamiltonian has the form:

$$H = -h \sum_n \sigma_n^{(3)} - \sum_n J_n \sigma_n^{(1)} \sigma_{n+1}^{(1)} \tag{1}$$

where the $\sigma_n^{(i)}$ $(i=1,2,3)$ are spin-$\frac{1}{2}$ operators, h is a magnetic field in the 3 direction, and the coupling constants J_n assume two values J_0 and J_1, ordered according to the Fibonacci sequence, generated by iterating the substitution rule $J_0 \to J_0J_1$, $J_1 \to J_0$.

It is well known [5] that the eigenvalues Λ of the Hamiltonian operator H can be obtained from the equation:

$$h\varepsilon_k\psi_{k+1} + h\varepsilon_{k-1}\psi_{k-1} + (h^2+\varepsilon_k^2)\psi_k = \Lambda^2\psi_k \tag{2}$$

where $\varepsilon_i = J_i/2$ and ψ is a classical field.

The eigenvalue problem (2) is reminiscent of a discrete Laplacian problem [2] and can be associated [4] with the study of the following map [6], characteristic of the Fibonacci substitution rule:

$$x_{n+1} = 2x_nx_{n-1} - x_{n-2}. \tag{3}$$

Performing the fixed-point analysis of (3) one defines scaling exponents $\bar{\Delta}$ as $\Delta\Sigma \approx (\Delta\Lambda^2)^{\bar{\Delta}}$ where $\Delta\Sigma$ denotes the fraction of states associated with a band having width $\Delta\Lambda^2$. One verifies (see e.g. [7]) that

$$I = x_{n+1}^2 + x_n^2 + x_{n-1}^2 - 2x_{n+1}x_nx_{n-1} - 1$$

is conserved under the map. As a consequence, the mentioned exponents depend on I, which in the present case has the form [4]:

$$I = \left[\left(\frac{\varepsilon_0}{\varepsilon_1} - \frac{\varepsilon_1}{\varepsilon_0}\right)\frac{\Lambda}{2h}\right]^2 \qquad \varepsilon_i = \frac{J_i}{2}.$$

It has been established in various numerical studies of the map (3) that two cycles mainly contribute to the scaling, with different exponents $\bar{\Delta}$ (see e.g. [1] and [8]).

A 2-cycle gives an exponent:

$$\bar{\Delta}_{(2)} = \frac{2\log\sigma}{\log\rho_{(2)}}$$

$$\rho_{(2)} = \rho_{(2)}(I) = \tfrac{1}{2}[2+\gamma^{1/2} + (\gamma + 4\gamma^{1/2})^{1/2}]$$

where $\gamma = 25 + 16I$ ($\rho_2(0) = \sigma^4$, $\sigma = (1+\sqrt{5})/2$).

A 6-cycle gives an exponent:

$$\bar{\Delta}_{(6)} = \frac{6\log\sigma}{\log\rho_{(6)}}$$

$$\rho_{(6)} = \rho_{(6)}(I) = [1 + 4(1+I)^{1/2} + 2(1+I)]^2 \qquad \rho_{(6)}(0) = \sigma^6.$$

The scaling exponents of the Λ and of the Λ^2 spectra coincide everywhere but at $\Lambda = 0$: there the exponent $\bar{\Delta}_{(2)} = \frac{1}{2}$ for the Λ^2 spectrum implies $\Delta\Sigma \approx \Delta\Lambda$.

We directly verified from the scaling of the lowest-energy band that at the Ising critical point of the model, where $\Lambda = 0$ is attained [4], this is indeed the case, while elsewhere this band consistently scales as $\Delta\Sigma \approx (\Delta\Lambda)^{\bar{\Delta}_{(2)}}$.

We perform the global analysis in terms of the thermodynamic formalism for multifractals as introduced in [9]. Upon denoting with $\Lambda_{i,n}$ the width of the ith band at the nth iteration of the map, one defines the 'partition function' $Z(\tau)$ as the limit of the sequence $Z_n(\tau)$:

$$Z_n(\tau) = \Sigma_i \Lambda_{i,n}^{-\tau} \approx (F_{n+1})^{q_n(\tau)}. \tag{4}$$

Here Z_n refers to the nth periodic approximant of the spectrum, which in the present case has F_{n+1} bands, F_n being the Fibonacci numbers ($F_{n+1}=F_n+F_{n-1}$, $F_0=F_1=1$).

The limit of the sequence $q_n(\tau)$ is the 'free energy' $q(\tau)$.

If one assumes a local scaling exponent μ_i:

$$\Lambda_{i,n} \approx (F_{n+1})^{-\mu_i}$$

the average scaling exponent μ at the 'inverse temperature' τ is given by:

$$\mu=\mu(\tau)=\frac{\mathrm{d}q(\tau)}{\mathrm{d}\tau}.$$

The entropic measure is given by the so-called scaling spectrum $S(\mu)$, related to the free energy in the following way:

$$q(\tau)=S(\mu)+\tau\mu.$$

In an alternative approach [10] one defines a function $f(\alpha)$ from the inverse $\tau(q)$ of the free energy:

$$\tau(q)=-f(\alpha)+q\alpha$$

whence $\alpha=1/\mu$; the value of f at α is the dimension of the subset with scaling exponent α.

Recalling our definition of $\bar{\Delta}$, we expect to recover such exponents, in connection with unmixed scaling, at the extrema of the support of $f(\alpha)$. One could actually go further, noticing that the map (3) admits a symbolic representation (see [11]), so that each energy band $\Lambda_{i,n}$ is associated with a string of symbols identifying a path along a tree.

By suitably generalizing the procedure applied to a binary tree for the two-scale Cantor set, e.g. in [10], one is tempted to recover the local scaling μ_i at each band from the corresponding path along the tree.

This program is far from being completed even for homogeneous scaling, i.e. when the quantity I depends on the potential only, but a further obstacle here is that the exponents $\bar{\Delta}$ are Λ dependent.

We now discuss how this dependence influences the thermodynamic functions.

One can verify that when Λ is in the spectrum, the following inequality holds: $\bar{\Delta}_{(2)}(\Lambda)<\bar{\Delta}_{(6)}(\Lambda)$. Both exponents are decreasing functions of Λ, so that we expect:

$$\bar{\Delta}_{(2)}(\Lambda_{\max}) \leqslant \alpha \leqslant \bar{\Delta}_{(6)}(\Lambda_{\min}). \tag{5}$$

We always verified (5) to hold within numerical error.

In the periodic case $\varepsilon_0=\varepsilon_1$ implies $I=0$, and one merely gets $\bar{\Delta}_{(2)}=\frac{1}{2}$ and $\bar{\Delta}_{(6)}=1$. The two scales do not mix, so that the support of $f(\alpha)$ reduces to the two points $\alpha=\frac{1}{2}$ ($f(\frac{1}{2})=0$) and $\alpha=1$ ($f(1)=1$). Correspondingly, the function $\mu(\tau)$ is equal to 1 at $\tau<0$ (continuous spectrum) and equal to 2 (Van Hove singularity) at $\tau>0$.

For every $r=\varepsilon_1/\varepsilon_0$ different from 1 the scales mix: e.g., in figure 1 we display $\mu(\tau)$ for $r=0.99$.

Multifractality is 'fully developed' in the case of figures 2(a), (b), referring to $f(\alpha)$ and $\mu(\tau)$ respectively at $\varepsilon_0=0.5$, $r=0.5$. Recalling [4] that the Ising critical point of the model is at $\varepsilon_0=\varepsilon_{0,c}=r^{-1/\sigma^2}$ ($h=1$) we are in the weak coupling regime, corresponding to the paramagnetic phase.

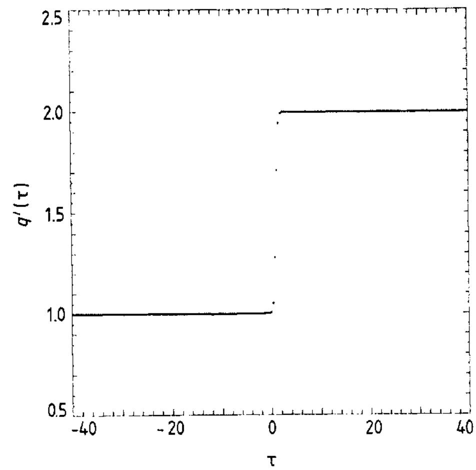

Figure 1. Average scaling exponent $\mu(\tau) = q'(\tau)$ at $\varepsilon_0 = 1.3$, $r = 0.99$; all figures are obtained from approximants up to the 14th order.

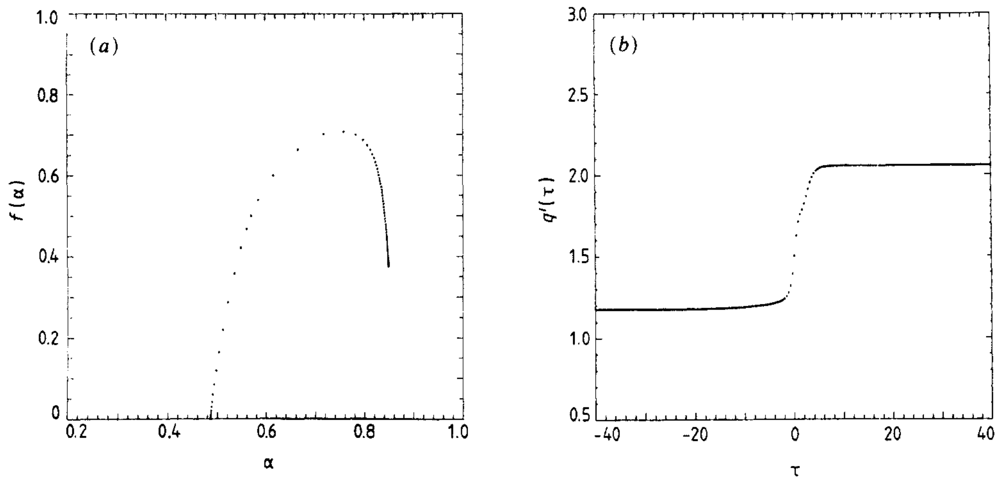

Figure 2. $\varepsilon_0 = 0.5$, $r = 0.5$; (a): scaling function $f(\alpha)$; (b): $\mu(\tau) = q'(\tau)$.

Let us now split the F_{n+1} bands of the nth approximant in two clusters (down and up), made of the first F_{n-1} low-energy bands and of the remaining F_n respectively, and separately compute the thermodynamic functions for the two clusters. Were it not for the Λ dependence, one should obviously obtain the same $f(\alpha)$. The actual result is exhibited in figure 3(a), where, in order to have better resolution, we consider $\varepsilon_0 = 2.5$ and $r = 0.5$. One can verify that the supports of the two $f(\alpha)$ separately satisfy (6), with $\Lambda_{\min}$ and $\Lambda_{\max}$ referring to the corresponding (up and down) cluster; at the same time, the free energies $q(\tau)$ intersect at $\tau = 0$ (see figure 4).

Note that the free energy of the total spectrum is given by the upper boundary of the two branches [9], as one easily realizes upon writing (4) as:

$$Z_n(\tau) = Z_{n,\mathrm{U}}(\tau) + Z_{n,\mathrm{D}}(\tau) \tag{6}$$

and keeping the leading contribution for large n.

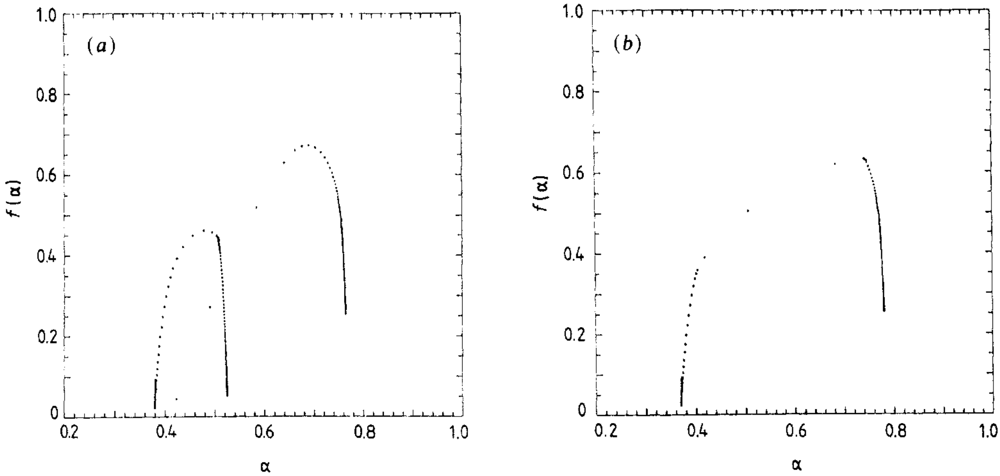

Figure 3. $\varepsilon_0 = 2.5$, $r = 0.5$; (*a*) the $f(\alpha)$ of the up (left) and down (right) clusters (see text); (*b*) the $f(\alpha)$ of the total spectrum.

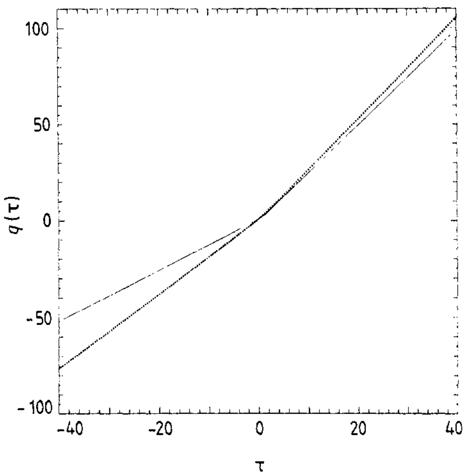

Figure 4. Same parameters as in figure 3; dotted curve: free energy $q(\tau)$ of the up cluster; full curve: $q(\tau)$ of the down cluster.

Hence $q(\tau)$ at the intersection point has a cusp singularity, implying a first-order phase transition (the average scaling exponent μ is discontinuous in τ).

We found this phenomenon for all values of the coupling constants both below and above the Ising critical point. One may ask whether upon partitioning the spectrum into smaller clusters new distinct phases could be isolated.

For example, one can keep the down cluster (with F_{n-1} bands) and split the up cluster in two subclusters, a centre cluster with F_{n-2} bands and an up cluster with F_{n-1} bands. Clearly, the two extremal clusters dominate at $\tau \to -\infty$ and at $\tau \to +\infty$ respectively, but the centre cluster could dominate for finite τ. This possibility can be excluded noticing the following: (*a*) for each cluster (D, C, U) the functions $q(\tau)$ are concave; (*b*) $q_D(0) = q_C(0) = q_U(0) = 1$; (*c*) for $\tau \to \infty$ $q_C(\tau)$ must lie in the strips limited by $q_D(\tau)$ and $q_U(\tau)$.

The form of map (3) depends uniquely on the Fibonacci substitution rule; the specific propagation problem considered enters through the explicit form of the quantity I. Hence we can conclude that the phenomenon discussed above involves any propagation problem on a Fibonacci chain, provided the quantity I preserves a Λ dependences as, e.g., in the discrete Laplacian problem [1, 2].

Chains generated by different substitution rules give rise to different maps [12]: if such maps are conservative, and the conserved quantities keep a Λ dependence, we expect that a similar situation can occur.

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