

Connection between energy spectrum, self-similarity, and specific heat log-periodicity

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As a first step towards the understanding of the thermodynamical properties of quasiperiodic structures, we have performed both analytical and numerical calculations of the specific heats associated with successive hierarchical approximations to multiscale fractal energy spectra. We show that, in a certain range of temperatures, the specific heat displays log-periodic oscillations as a function of the temperature. We exhibit scaling arguments that allow for relating the mean value as well as the amplitude and the period of the oscillations to the characteristic scales of the spectrum. [S1063-651X(98)00408-5]

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I. INTRODUCTION

The discovery of quasicrystals in 1984 [1] aroused a great interest in quasiperiodic structures, as is confirmed by the great number of theoretical [2,3] and experimental [4] works that followed (see also [5]). In particular, the behavior of a variety of particles and quasiparticles (electrons [6], phonons [7], and others [8]) in quasiperiodic structures has been and is currently being studied. A *fractal energy spectrum* is a common feature to such structures (e.g., [9]). As in general these spectra tend to be quite complex, simple models have been studied to enlighten the thermodynamical specificities that such systems may display (a similar approach was used in the 1980s to study the transition from finite- to zero-measure spectra, see, e.g., [3]). Within this vein, we analyzed in [10] one of the simplest fractal spectra (the triadic Cantor set); there it was shown that the specific heat of such a system exhibits a very particular behavior: it oscillates log-periodically around a mean value that equals the fractal dimension of the spectrum.

In this paper we extend the analysis of [10] to the case of multiscale spectra and present a theoretical connection between the structure of the spectrum and the corresponding thermodynamical properties. In particular, we make explicit the relationship between discrete scale-invariance and log-periodic oscillations. We start our discussion with the two-scale (r_1, r_2) fractal set, in its discrete version (Sec. II). Then, in Sec. III, we show that the results of Sec. II can be extended to the continuous two-scale case, as well as to the n -scale problem. Section IV contains the conclusions.

II. TWO-SCALE DISCRETE MODEL

Let us begin by considering a spectrum lying on the (r_1, r_2) two-scale fractal set [11] indicated in Fig. 1(a) (the

restrictions $0 \leq r_1, r_2, r_1 + r_2 \leq 1$ apply). The starting point ($n=0$) for the construction of this spectrum is an arbitrary discrete set of levels lying in an energy interval we take to be $[0,1]$. This is the pattern that will be repeated *ad infinitum* in a self-similar way. The next step consists in compressing the set $n=0$ by factors r_1 and r_2 and putting the two resulting pieces on the bottom and the top of the interval $[0,1]$, respectively [see Fig. 1(a)]. Recursive application of this rule eventually leads to a set of fractal dimension d_f given by $r_1^{d_f} + r_2^{d_f} = 1$ (hence, if $r_1 = r_2 \equiv r$, $d_f = -\ln 2 / \ln r$). This rule can be explicitly written as a recurrence equation for the energy levels $\epsilon_j^{(n)}$ at the n th stage,

$$\{\epsilon_j^{(n+1)}\} = \{r_1 \epsilon_j^{(n)}\} \cup \{1 - r_2 + r_2 \epsilon_j^{(n)}\}. \quad (1)$$

This analytical rule for the construction of the spectrum is the key to obtaining scaling relations for the thermodynamical quantities. The starting point is the partition function for a given hierarchy n :

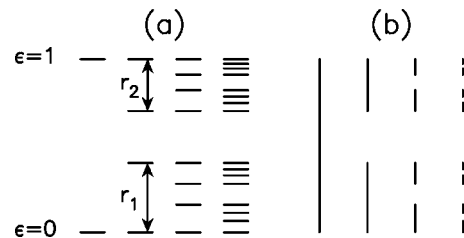


FIG. 1. Energy spectra. The first four steps in the construction of (r_1, r_2) fractal sets. We show a discrete case (a) in which the starting point ($n=0$) is a set of two levels at $\epsilon=0,1$. These levels are then compressed by a factor r_1 (r_2) and put on the bottom (top) of the interval $[0,1]$ ($n=1$), and so on for increasing n . The construction of a continuous example (b) starts from a band of uniform density in $[0,1]$. The iterative rule is the same as in (a), i.e., $n=1$ corresponds to a spectrum whose first and second bands are the intervals $[0, r_1]$ and $[1 - r_2, 1]$, respectively, etc. We take the level density inside each band to be a constant, and the same for all bands in a given hierarchy. In both cases (a) and (b), a fractal emerges at the $n \rightarrow \infty$ limit.

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$$Z^{(n)}(\beta) = \frac{1}{2^n} \sum_{j=1}^{2^n} \exp(-\beta \epsilon_j^{(n)}), \quad (2)$$

where β is the inverse temperature (we are considering a unit Boltzmann constant, i.e., $k_B=1$). A normalization prefactor has been included so that $Z^{(n)}$ is well defined in the limit $n \rightarrow \infty$; in any case, it will not affect the thermodynamics of the system. Now, a recurrence formula for the partition function is readily obtained as a direct consequence of the self-similarity of the energy set (1):

$$Z^{(n+1)}(\beta) = [Z^{(n)}(\beta r_1) + e^{-\beta(1-r_2)} Z^{(n)}(\beta r_2)]/2. \quad (3)$$

Introducing $Z(\beta) \equiv \lim_{n \rightarrow \infty} Z^{(n)}(\beta)$, we have

$$Z(\beta) = [Z(\beta r_1) + e^{-\beta(1-r_2)} Z(\beta r_2)]/2. \quad (4)$$

From now on we will restrict our discussion to the low-temperature regime, as this is the most interesting one. In fact, as the temperature is lowered, the smaller scales of the fractal are progressively revealed, and anomalous effects are expected. Moreover, in the case $T \ll 1$ the analysis gets simplified and some general conclusions can be obtained. In this regime we can safely neglect the exponentially small term in Eq. (4) and derive scaling relations for the partition function, the dimensionless free energy $Q \equiv F/T = -\ln Z$, the total energy E , the entropy S , and the specific heat C :

$$Z(T) = Z(T/r_1)/2, \quad (5)$$

$$Q(T) = Q(T/r_1) + \ln 2, \quad (6)$$

$$E(T) = r_1 E(T/r_1), \quad (7)$$

$$S(T) = S(T/r_1) - \ln 2, \quad (8)$$

$$C(T) = C(T/r_1). \quad (9)$$

Independently of the $n=0$ energy pattern, the relevant scale factor is r_1 (conversely, r_2 governs the scaling laws for *negative* temperatures).

The most interesting of the equalities above is the last one, which expresses the fact that the specific heat is a log-periodic function of the temperature, that is, $C(T) = f(2\pi \ln T / \ln r_1)$, where f is a 2π -periodic function. In other words, if one sets $T = r_1^x$, $C(x)$ results in a periodic function of x (of period one). Consistently, its mean value can be calculated as

$$\begin{aligned} \langle C(T) \rangle &= \int_{x_0}^{x_0+1} C(r_1^x) dx = -\frac{1}{\ln r_1} \int_{r_1^{x_0}}^{r_1^{x_0+1}} C(T) \frac{dT}{T} \\ &= -\frac{S(\tau) - S(r_1 \tau)}{\ln r_1} = -\frac{\ln 2}{\ln r_1}. \end{aligned} \quad (10)$$

In Ref. [1] it was shown that for a one-scale Cantor spectrum (i.e., $r_1=r_2=1/3$), the average value $\langle C(T) \rangle$ coincides with the fractal dimension d_f . The equality above shows that *this is not the case for a two-scale fractal*. We will come back to this point later on to argue that the ‘‘dimension’’ $d = -\ln 2 / \ln r_1$ can be given a simple meaning. We remark

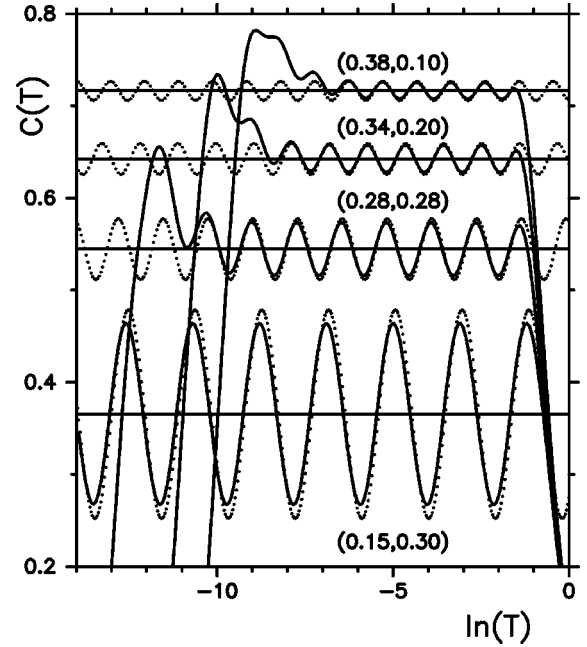


FIG. 2. Specific heat (in units of k_B) vs temperature (in units of the width of the spectrum) for the (r_1, r_2) discrete fractal set of Fig. 1 ($n=8$). Two levels at $\epsilon=0,1$ were taken as the $n=0$ pattern. The curves are parametrized by the scale factors (r_1, r_2) . The horizontal lines indicate the average value $\langle C \rangle = d = -\ln 2 / \ln r_1$. The dotted lines correspond to our prediction $C \approx d + a'' \cos(\omega \ln T) + b'' \sin(\omega \ln T)$, where $\omega = -2\pi / \ln r_1$. The parameters a'' , b'' are related to basic properties of the smoothed spectrum (see text). For high temperatures ($\ln T > 0$), the specific heat decays as T^{-2} , for arbitrary n . The low-temperature breakdown of the oscillatory behavior is pushed towards the left when n increases.

that the result (10) holds as long as $T \ll 1$ (we recall that, as the spectrum is bounded, for high temperatures the specific heat must decay as T^{-2}).

The scaling reasoning has given us information concerning the mean values. In order to discuss the oscillations around the mean value, we resort to a numerical analysis. Starting from Eq. (2) we have computed finite approximations to $C(T)$,

$$C^{(n)}(T) = \frac{\partial}{\partial T} \left[T^2 \frac{\partial \ln Z^{(n)}}{\partial T} \right], \quad (11)$$

and studied its dependences on the hierarchical depth n and the parameters r_1 and r_2 . In Fig. 2, we show some plots of the specific heat vs temperature for different values of (r_1, r_2) and fixed hierarchical depth $n=8$. It is apparent that there is a range of temperatures in which $C(T)$ behaves in the way the above scaling arguments predict. This is a range of intermediate temperatures, $T_{\min} \ll T \ll 1$, where $T_{\min} \sim r_1^n$ is associated to the smallest scale of the ‘‘truncated fractal’’; of course, $T_{\min} \rightarrow 0$ in the limit $n \rightarrow \infty$. Figure 2 clearly displays the following features. $C(T)$ oscillates log-periodically around the mean value $d = -\ln 2 / \ln r_1$ with frequency $\omega = -2\pi / \ln r_1$. Notice that each curve completes about n periods ($n=8$ in the figure, but we have verified this behavior for higher depth n as well). In Fig. 3(a) we show a typical example illustrating the dependence of the amplitudes of the

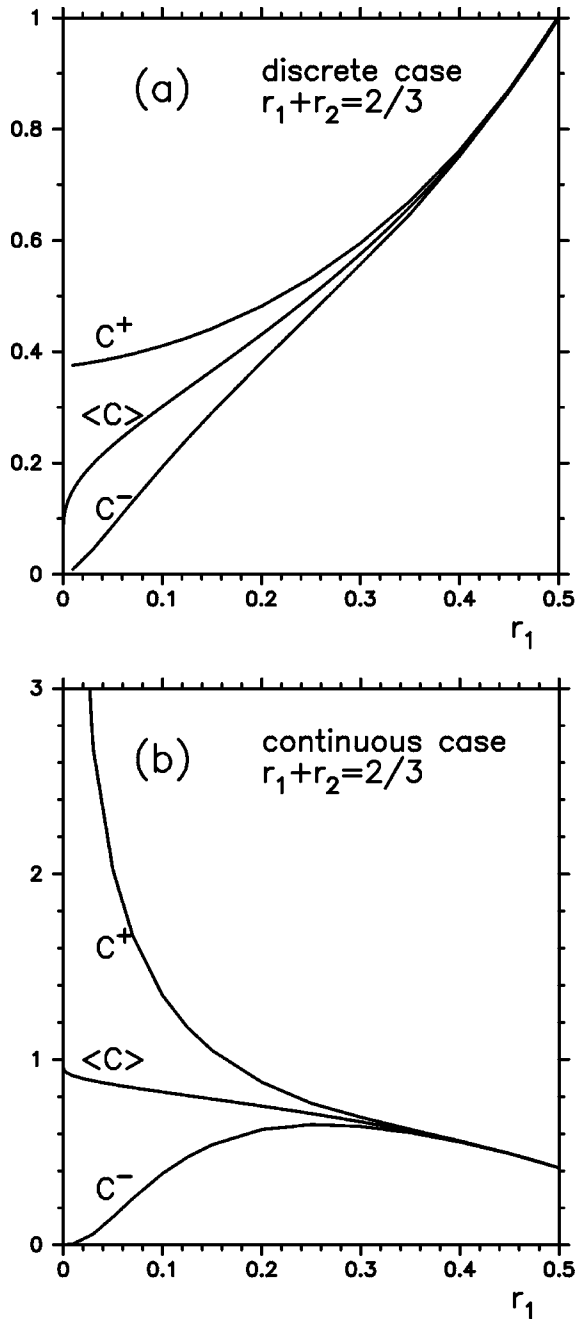


FIG. 3. Amplitudes of the oscillations of the specific heat in the log-periodic regime ($T \ll 1$). Maximum and minimum values of $C(T)$ (respectively C^+ and C^-) for the family of fractal spectra $r_1 + r_2 = 2/3$. Also shown is the average specific heat $\langle C \rangle$. For the discrete case (a), $\langle C \rangle = -\ln 2 / \ln r_1$. In the continuous case (b), $\langle C \rangle = 1 - \ln(r_1 + r_2) / \ln r_1$.

specific heat on the scales (r_1, r_2) . We have plotted the maximum and minimum values of the low-temperature regime of $C(T)$ (denoted, respectively, C^+ and C^-), together with the mean value $\langle C \rangle = -\ln 2 / \ln r_1$ for the family $r_1 + r_2 = 2/3$. The oscillations decrease in amplitude as r_1 decreases, and for r_1 sufficiently small ($r_1 \leq 0.1$) asymmetries become significant.

A point of view that allows for understanding quantitatively the amplitudes of the oscillations consists in relating the thermodynamical properties to those of the spectrum. For instance, a constant value of the specific heat $C = \sigma$ is asso-

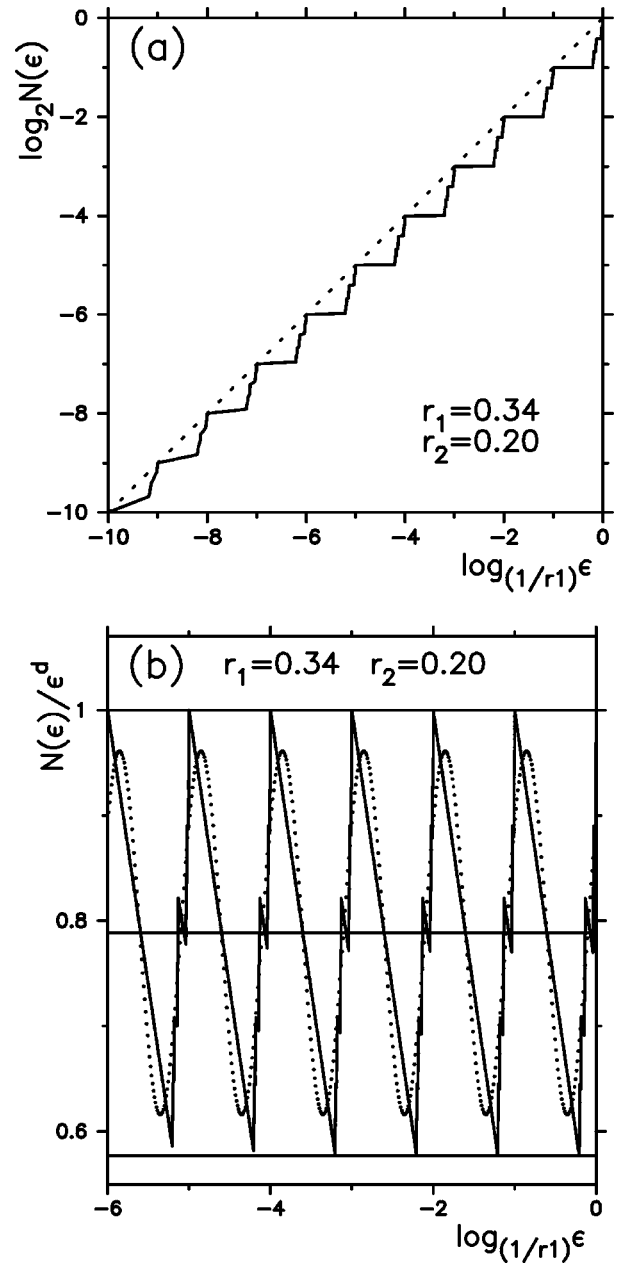


FIG. 4. (a) Integrated density of states N (normalized to unity) vs energy. The full line corresponds to the discrete Cantor spectrum of Fig. 1(a) with $r_1 = 0.34$, $r_2 = 0.20$, and $n = 12$. The dashed line is given by ϵ^d , with $d = -\ln 2 / \ln r_1$, the spectral dimension. (b) Spectral fluctuations. $N(\epsilon)$ after dividing by ϵ^d (full line) and the smooth approximation (dotted line) $\bar{N} / \epsilon^d = a + b \cos(\omega \ln \epsilon - \phi)$, where $\omega = -2\pi / \ln r_1$. a and b are determined by requiring that the exact and the smoothed fluctuations have the same average value and variance. The condition of maximum overlap fixes ϕ .

ciated in general to the fact that the cumulative density of states (or spectral staircase)

$$N(\epsilon) = \int_0^\epsilon \rho(x) dx \quad (12)$$

scales with energy as ϵ^σ (equipartition principle). In our case, it can be verified that the spectral staircase grows approximately as ϵ^d [see Fig. 4(a)], and consequently the aver-

age specific heat is $\langle C \rangle = d$. It is also apparent from Fig. 4(b) that the integrated density of states $N(\epsilon)$ is a log-periodic function of the energy. (Similar results were obtained by Kimball and Frisch for the distribution of normal mode frequencies of fractal-based models [12]; see also [13]). In fact, this feature could have been anticipated by noting that $N(\epsilon)$ also satisfies a simple scaling law:

$$N(r_1 \epsilon) = N(\epsilon)/2, \quad (13)$$

whose general solution can be written as a power law times a log-periodic function [15].

We will now show that an excellent description of the specific heat can be achieved by considering the first non-trivial correction to the bare power-law scaling for $N(\epsilon)$:

$$N(\epsilon) \approx \epsilon^d [a + b \cos(\omega \ln \epsilon - \phi)]. \quad (14)$$

In principle, there is not a unique criterion for choosing the parameters a, b, ϕ . We have determined a and b by requiring that the exact $N(\epsilon)$ and its smooth approximation (14) have the same average value and variance. The condition of maximum overlap between the exact staircase fluctuations N/ϵ^d and the cosine function fixes ϕ . An approximate partition function is now written in terms of the smoothed cumulative level density,

$$\begin{aligned} Z(T) &\approx \beta \int_0^\infty \epsilon^d [a + b \cos(\omega \ln \epsilon - \phi)] \exp(-\beta \epsilon) d\epsilon \\ &= T^d [aa' + bb' \cos(\omega \ln T - \phi) \\ &\quad - bc' \sin(\omega \ln T - \phi)]. \end{aligned} \quad (15)$$

Here the constants a', b', c' are calculated as the integrals:

$$\left. \begin{matrix} a' \\ b' \\ c' \end{matrix} \right\} \equiv \int_0^\infty dx x^d e^{-x} \begin{cases} 1 \\ \cos(\omega \ln x) \\ \sin(\omega \ln x). \end{cases} \quad (16)$$

For not very small values of r_1 one has $a' \gg b', c'$ (e.g., if $r_1 = 0.34$, then $a' \approx 0.9$, $b' \approx 0.002$, and $c' \approx 0.0003$.) After some straightforward manipulations, to first order in the small parameters b'/a' and c'/a' , we obtain the specific heat

$$C(T) \approx d + a'' \cos(\omega \ln T) + b'' \sin(\omega \ln T). \quad (17)$$

This expression can be seen as a log-Fourier expansion of the specific heat up to second-order terms. Instead of presenting (complicated) expressions for the constants a'' and b'' as functions of r_1 and r_2 , we prefer to show the specific heat (17) for a set of selected values of r_1, r_2 (Fig. 2, dotted lines). The agreement of our approximation (17) with the exact (numerical) calculations is excellent for the three upper curves and reasonably good for that corresponding to the smallest r_1 (higher-order terms might be necessary in this case).

III. CONTINUOUS AND MULTISCALE EXTENSIONS

For the sake of completeness, let us also discuss the case of a spectrum constructed by iterative use of the rule (r_1, r_2)

but starting from a *continuous* pattern as shown in Fig. 1(b). For instance, if the zeroth hierarchy is chosen as a continuous spectrum with uniform density in the interval $[0, 1]$, then $n=1$ corresponds to a spectrum whose first and second bands are the intervals $[0, r_1]$ and $[1 - r_2, 1]$, respectively, and so on for increasing n . We have chosen the density to be uniform inside each band. In other words, the number of states in each band is proportional to its length, whereas in the *discrete* case each ‘‘band’’ contains the same number of states; this is the essential difference between what we call *continuous* and *discrete* spectra. Now the partition function is written as

$$Z_{\text{cont}}^{(n)}(\beta) = \frac{1}{(r_1 + r_2)^n} \int_0^1 \rho(\epsilon) \exp(-\beta \epsilon) d\epsilon, \quad (18)$$

where, as in Eq. (2), a normalization prefactor has been included. The analog to Eq. (1) is a recurrence equation for the density of states:

$$\rho^{(n+1)}(\epsilon) = \begin{cases} \rho^{(n)}(\epsilon/r_1) & \text{if } 0 \leq \epsilon \leq r_1 \\ 0 & \text{if } r_1 < \epsilon < 1 - r_2 \\ \rho^{(n)}([\epsilon - 1]/r_2 + 1) & \text{if } 1 - r_2 \leq \epsilon \leq 1, \end{cases} \quad (19)$$

leading to the following result for the partition function:

$$Z_{\text{cont}}(\beta) = \frac{1}{r_1 + r_2} [r_1 Z_{\text{cont}}(\beta r_1) + r_2 e^{-\beta(1-r_2)} Z_{\text{cont}}(\beta r_2)]. \quad (20)$$

In the low-temperature regime ($T \ll 1$), the expression above tends to the scaling relation

$$Z_{\text{cont}}(\beta) = \frac{r_1}{r_1 + r_2} Z_{\text{cont}}(\beta r_1). \quad (21)$$

Note that, as in the discrete case, the scale factor r_1 is responsible for the period of the log-oscillations. Thus the discrete and continuous characteristic frequencies are equal. The essential difference is the presence of r_2 in Eq. (21), which can be traced back to a different distribution of the spectral density (of course, when $r_1 = r_2$ both cases coincide). In consequence, r_2 will also affect the mean value of specific heat, which is easily shown to be

$$\langle C_{\text{cont}} \rangle = 1 - \ln(r_1 + r_2) / \ln r_1 \equiv d'. \quad (22)$$

Equality (22) defines a new dimension d' , which, together with d and d_f , constitute the basic set of characteristic dimensions of our problem. We remark that these dimensions assume different values, except for the particular case $r_1 = r_2$. Even though the mean value (22) differs from its discrete counterpart (10), the continuous and discrete specific heats oscillate in a similar way about their respective averages. However, the small- r_1 asymmetries are more pronounced in the continuous case. These facts can be appreciated by comparing Fig. 3(a) and Fig. 3(b).

The previous analysis for the two-scale spectrum (either discrete or continuous) can also be generalized to the multiscale case. The construction of a multiscale fractal spectrum starts from an arbitrary discrete or continuous set of levels in

the interval $[0,1]$ ($n=0$). Then one makes M rescaled copies of the pattern $n=0$, with different scale factors r_1, \dots, r_M . Each one of these copies is placed in the unit interval at positions a_1, \dots, a_M , so that the copies do not overlap (this requires $a_i + r_i < a_{i+1}$). Iteration of this rule eventually leads to a fractal of dimension $\sum_{i=1}^M r_i^{d_f} = 1$. Analogous considerations to those made for the two-scale case result in the following relationships for the discrete and the continuous multiscale cases, respectively:

$$Z_{\text{disc}}(\beta) = \frac{1}{M} \sum_{i=1}^M e^{-\beta a_i} Z_{\text{disc}}(\beta r_i), \quad (23)$$

$$Z_{\text{cont}}(\beta) = \frac{1}{\sum_{i=1}^M r_i} \sum_{i=1}^M r_i e^{-\beta a_i} Z_{\text{cont}}(\beta r_i). \quad (24)$$

These partition functions lead to the average specific heats ($T \ll 1$)

$$\langle C_{\text{disc}} \rangle = -\ln M / \ln r_1 \equiv d, \quad (25)$$

$$\langle C_{\text{cont}} \rangle = 1 - \ln \left(\sum_{i=1}^M r_i \right) / \ln r_1 \equiv d'. \quad (26)$$

(Naturally, the d and d' we introduced in Sec. II are the $M=2$ particular case of those defined above.) Once more the scaling exponents only depend on r_1 in the discrete case and on the whole set of scaling factors r_j in the continuous (banded) case. As in the two-scale case, these scale factors will be the essential ingredients for a very good approximate description of the thermodynamics of the system.

We point out that the fractals considered in this paper might also be analyzed in their *outbound* and *complete* versions (in the nomenclature of [10]). These variations, which can also be treated within our formalism, will give rise to a thermodynamics analogous to that described above.

IV. CONCLUSIONS

The models we have studied suggest that the hierarchical organization of the energy spectra reflects itself in the specific heat in two ways. Simple scaling arguments show that the average behavior is associated with a noninteger spectral dimension (d and d' in our examples), which in general is different from the fractal dimension (d_f). The corrections to this result are log-periodic oscillations that can be traced back to the log-periodicity of the spectral staircase. The number of oscillations that can be observed is related to the

hierarchical depth of the fractal spectrum, implying that these anomalies may appear in systems displaying a self-similar spectrum up to a *finite* hierarchical depth. These observations, related to multiscale fractal spectra, might also be relevant in the case of the more realistic multifractal ones, because usually a few scales suffice for a good description of a multifractal spectrum.

Moreover, since the effect is a consequence of the scale invariance of the spectrum, it is expected that similar phenomena would generically exist for bosonic and fermionic systems [16]. Let us mention that Petri and Ruocco [13] have observed fractional scaling laws when studying the (Debye) vibrational specific heat of a one-dimensional hierarchical model. However, those authors were mainly concerned with mean values and did not discuss the small amplitude oscillations that can be clearly observed in their results. Furthermore, Luck and Nieuwenhuizen observed that the specific heat of a Fibonacci spin chain oscillates log-periodically with the temperature [14]. They also established a connection between the average specific heat and the integrated density of states. Remarkably, for zero external magnetic field, this spin chain can be mapped onto a system of free fermions (with zero chemical potential) in a fractal spectrum.

Even though it is not surprising that log-periodic corrections (or ‘‘complex exponents’’) are a natural consequence of discrete scale invariance [17], a contribution of the present paper is to have reported and analyzed examples in which the connection between scale invariance (of an energy spectrum) and log-periodicity (of the specific heat as a function of temperature) shows up transparently.

Before concluding, let us comment on a possible connection of the present calculation with the recently introduced nonextensive thermostatistics [18]. Alemany [19] has suggested that this formalism could be connected to systems with fractally structured Boltzmann-Gibbs probability distributions. Although, for our present calculation, we have not succeeded in making a transparent connection along Alemany’s lines, it is worth mentioning one intriguing feature. The generalized specific heat $C_q(T)$ of the quantum one-dimensional harmonic oscillator [20] *does present oscillations* if the entropic index q satisfies $q < 1$. In fact, $C_q(T)/T^{1-q}$ is an oscillatory function of T ; in a similar way $C(T)$ is a periodic function of $\ln T$.

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