



# Specific heat oscillations in quasi-periodic structures

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## Abstract

Most models on quasi-crystals, as well as the related experimental results, exhibit fractal energy spectra. We discuss the relevant thermodynamic implications of this feature by performing both analytical and numerical calculations of the specific heats associated with successive hierarchical approximations to fractal energy spectra. Instructive anomalies are displayed, namely the specific heat exhibits an infinite number of small-amplitude oscillations symmetrically disposed around a characteristic dimension of the spectrum. We also analyse a multifractal spectrum generated dynamically by the logistic map and conjecture a possible connection with Tsallis' generalized thermostats. © 2001 Elsevier Science Ltd. All rights reserved.

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## 1. Introduction

Quasi-crystals are being intensively studied, both theoretically [1–7] and experimentally [8–13] (see [14–19] for a review). The fact that they are in some sense midway between *disorder* (many of their physical properties exhibit an erratic appearance) and *order* (their definition, and construction, follows purely deterministic rules) makes them attractive objects of research. Since their first experimental realization in quasi-periodic GaAs–AlAs heterostructures in 1985 by Merlin and collaborators [20], their interest has only increased. More specifically, the Molecular Beam Epitaxy technique has produced and driven a multiplication of possible such structures (Fibonacci, Thue–Morse, double-period sequences; other possibilities could be Cantor sets, prime numbers, etc.). The behaviour of a variety of particles and quasi-particles (electrons [21,22], photons, plasmon–polaritons, magnons [23]) in quasi-crystals has been and is currently being studied. Now, there is a common feature which can be considered as the basic signature of such structures, and this is a *fractal energy spectrum*. These spectra tend, however, to be quite complex. In order to enlighten the thermodynamic consequences of fractal energy spectra, in Refs. [24,25], one- and multiscale fractal energy spectra were studied within Boltzmann statistics. It was shown that the scale invariance of the spectrum has strong consequences on the thermodynamical quantities. In particular, the specific heat oscillates log-periodically as a function of the temperature. Moreover, general scaling arguments and a detailed analysis of the integrated density of states allowed for a quantitative prediction of the average value (which is related to the average density of states), period and amplitude of the oscillations. Moreover, these results were extended to  $N$ -particle systems described by *quantum* statistics [26]; it was shown that for phonons, and for bosons in general, the Boltzmann scenario survives the inclusion of quantum symmetries. The fermionic case is more delicate, however, in some special cases, log-periodic oscillations can still be observed.

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### 2. Two-scale spectra

Let us begin by analysing a spectrum lying on the  $(r_1, r_2)$  two-scale fractal set [27] indicated in Fig. 1(a). 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  $[0, 1]$ . The next step consists in compressing the set  $n = 0$  by factors  $r_1$  and  $r_2$  and putting the two resulting pieces on bottom and 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

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

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  $n$

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

where  $\beta$  is the inverse temperature (we are considering a unit Boltzmann constant, i.e.,  $k_B = 1$ ). Now, a recurrence formula for the partition function is readily obtained as a direct consequence of the self-similarity of the energy set (1)

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

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

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

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 (4) and derive the following scaling relation for the specific heat  $C$ :

$$C(T) = C(T/r_1). \tag{5}$$

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

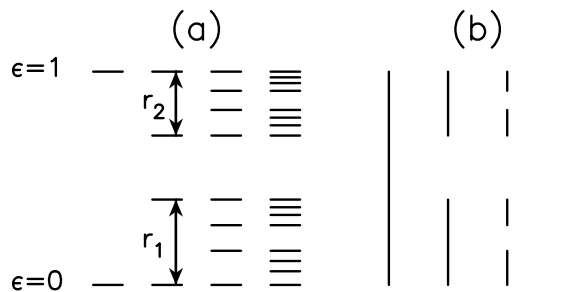


Fig. 1. Energy spectra. The first four steps in the construction of  $(r_1, r_2)$  fractal sets. We show a discrete case (a) in which the starting point ( $n = 0$ ) is a set of two levels at  $\epsilon = 0, 1$ . These levels are then compressed by a factor  $r_1(r_2)$  and put on bottom (top) of the 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.

The equalities above express the fact that the specific heat is a log-periodic function of the temperature. Its mean value is easily seen to be

$$\langle C(T) \rangle = -\frac{\ln 2}{\ln r_1}. \tag{6}$$

The scaling reasoning has given us information concerning the mean values, but, what about the oscillations that can be easily seen in the simulations of Fig. 2? This figure shows some plots of the specific heat versus 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,  $T_{\min} \lll T \lll 1$  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  $n \rightarrow \infty$ . Fig. 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 behaviour for higher depth  $n$  as well).

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

$$N(\epsilon) = \int_0^\epsilon \rho(x) dx \tag{7}$$

scales with energy as  $\epsilon^\sigma$  (equipartition principle). In our case it can be verified that the spectral staircase grows approximately as  $\epsilon^d$  and consequently the average specific heat is  $\langle C \rangle = d$ . It is also clear that the integrated density of states  $N(\epsilon)$  must be 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

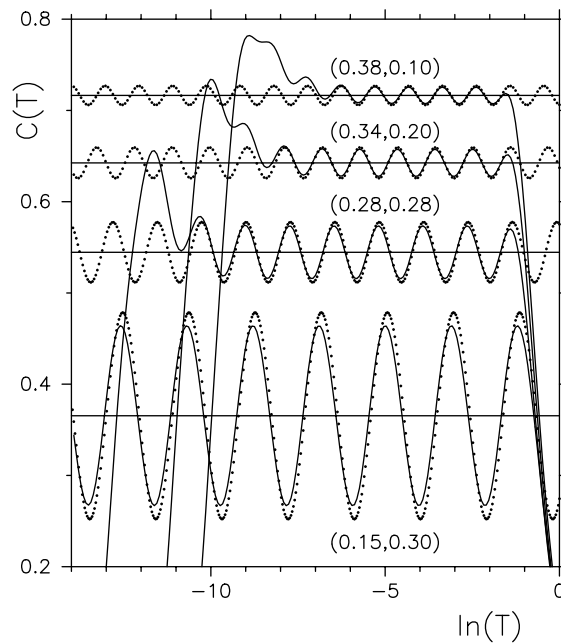


Fig. 2. Specific heat (in units of  $k_B$ ) versus temperature (in units of the width of the spectrum) for the  $(r_1, r_2)$  discrete fractal set of Fig. 1 ( $n = 8$ ). Two levels at  $\epsilon = 0, 1$  were taken as the  $n = 0$  pattern. The curves are parametrized by the scale factors  $(r_1, r_2)$ . 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 behaviour is pushed towards the left when  $n$  increases.

[28]; see also [29]). In fact, these features are a consequence of the fact that  $N(\epsilon)$  also satisfies a simple scaling law

$$N(r_1\epsilon) = N(\epsilon)/2, \quad (8)$$

whose general solution can be written as a power-law times a log-periodic function. An excellent description of the specific heat can be achieved by considering the first non-trivial correction to the bare power-law scaling for  $N(\epsilon)$

$$N(\epsilon) \approx \epsilon^d [a + b \cos(\omega \ln \epsilon - \phi)], \quad (9)$$

the criterion for choosing the parameters  $a$ ,  $b$ ,  $\phi$  being discussed in [25]. After some straightforward manipulations, one obtains the specific heat

$$C(T) \approx d + a'' \cos(\omega \ln T) + b'' \sin(\omega \ln T), \quad (10)$$

where the new constants are expressed in terms of the old ones [25]. This expression can be seen as a log-Fourier expansion of the specific heat up to second-order terms. The comparison of this analytical expression with the numerical results is presented in Fig. 2 (dotted lines). The agreement of approximation (10) 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). Similar results can be obtained for the fractal spectrum of Fig. 1(b), which is the “banded” version of that of Fig. 1(a).

### 3. The logistic spectrum

Now we extend the above considerations to a more sophisticated energy spectrum, namely a *multifractal* one. We introduce it directly through a specific map on the energy levels  $\{\epsilon_n\}$ .

The present calculation is essentially numerical and runs as follows. The energy spectrum is given by the recursive relation

$$\epsilon_{n+1} = g(\epsilon_n), \quad (11)$$

where  $g(x)$  and  $\epsilon_0$  are given. This means that the set of energies we are considering is the *attractor* of the map  $g$ . Notice that, in general,  $\epsilon_0$  will *not* be the ground state, but just the initial condition for the recursive calculation. Once the set of levels are generated, the calculations follows in the usual way, i.e., we calculate the partition function and then the specific heat. In our numerical calculation we stop summing as soon as the desired precision has been obtained for a particular value of  $T$ . The one-dimensional (dissipative) map we have used is the *logistic map* at its chaos threshold ([30–33] and references therein)

$$\epsilon_{n+1} = 1 - a\epsilon_n^2 \quad (12)$$

with  $a = a_c \equiv 1.401155198\dots$  ( $-1 \leq \epsilon_n \leq 1$ ).

This particular map has been chosen because of its frequent relevance in Physics, and because of its dynamic properties (in particular, the multifractality of the attractor at the edge of chaos) are very well known, e.g., the Feigenbaum exponents  $\lambda_F$  and  $\alpha_F$ , the multifractal function  $f(\alpha)$  and entropic index  $q$  [30–33]. In particular, the *fractal* or *Hausdorff* dimensionality of the attractor is  $d_f < 1$ . In Fig. 3 we exhibit the spectrum associated to this map at the chaos thresholds; Fig. 4 shows the associated  $T$ -dependence of the corresponding specific heat. Let us now summarize our main results for the  $T$ -dependence of the specific heat: (i) The spectrum being bounded,  $C(T) \propto 1/T^2$  in the asymptotic  $T \rightarrow \infty$  limit. (ii) Log-periodic oscillations exist decorating the average value. (iii) A remarkable sensitivity exists of  $C$  versus  $T$  with regard to the number of digits used for the critical value  $a_c$ . To be explicit, variations of say  $10^{-4}$  in the value of the chaos threshold produce, in the *low* temperature region, variations of  $C$  which are perfectly detectable within numerical calculations with say double precision.

So we have verified that the behaviour of the specific heat is qualitatively similar to that described for few-scale spectra. However, we still lack an analytical description of the log-periodic oscillations, for example, which are the scales that control the average specific heat, the frequency and amplitudes of the

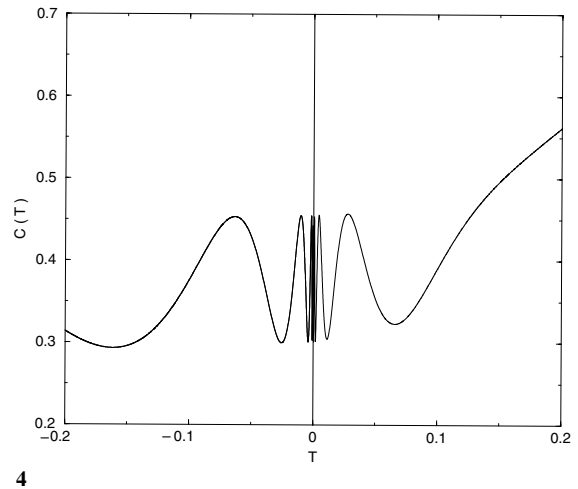
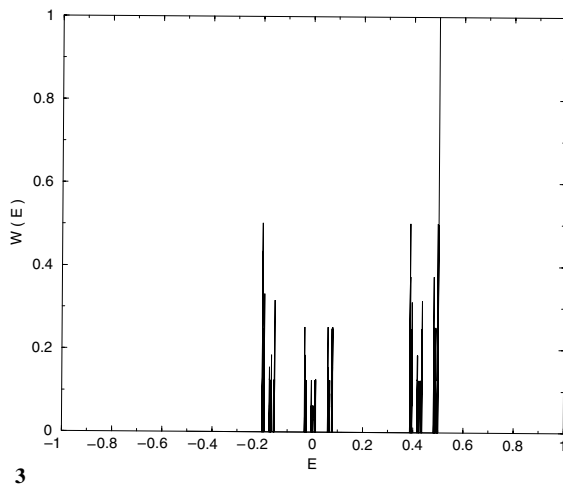


Fig. 3. Density of states for the spectrum generated through the logistic map (see text).

Fig. 4. Specific heat (in units of  $k_B$ ) versus temperature (in units of the width of the spectrum) for the “logistic” spectrum of Fig. 3.

oscillations? A systematic study along these lines of the logistic map and other one-dimensional dissipative maps at their chaos thresholds is in progress and the results will be reported in due time.

#### 4. 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 behaviour is associated to a non-integer spectral dimension, which in general is different from the fractal dimension ( $d_f$ ). The corrections to this result are log-periodic oscillations which can be traced back to the log-periodicity of the integrated density of states. 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, initially related to two-scale fractal spectra, were shown to be also relevant in the case of the more realistic multifractal ones, as that generated by the logistic map.

Before concluding, let us comment on a possible connection of the present results with the non-extensive Tsallis’ thermostatics [34,35]. Alemany [36] has shown that this formalism could be connected to systems with fractally structured Boltzmann–Gibbs probability distributions. Although we have not succeeded yet in making a transparent connection between the log-periodicity of the specific heat and the fractality of the spectrum along Alemany’s lines, it is worth remarking one intriguing feature. The generalized specific heat  $C_q(T)$  of the quantum one-dimensional harmonic oscillator [37] *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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