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Specific heat anomalies associated with Cantor-set energy spectra

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Most physical models on quasicrystals, as well as the related experimental results, exhibit fractal energy spectra. In order to have a deep insight on relevant thermodynamic implications of this feature, we have performed analytical and high precision numerical calculations of the specific heats C_n^{band} and C_n^{disc} associated with successive hierarchical approximations ($n=1,2,3,\ldots$) to bounded Cantor-set energy spectra (constructed with sets of continuous intervals for the *banded* case, and with discrete levels for the *discrete* case). Instructive anomalies are exhibited, namely (i) $C_n^{band}(T)$ and $C_n^{disc}(T)$ differ for all temperatures and finite n (in particular, in units of k_B, $C_n^{disc}(0)=0$ whereas $C_n^{band}(0)=1$), but, through an interesting nonuniform convergence, $C_\infty^{band}(T)=C_\infty^{disc}(T)\equiv C_\infty(T)$ for *all* finite temperatures; (ii) in the $T\to 0$ limit, $C_\infty(T)$ exhibits an *infinite* number of small-amplitude oscillations symmetrically disposed precisely around the fractal dimensionality $d_f=\ln 2/\ln 3$; more precisely, $C_\infty(T)\sim C^*(T)$, where $C^*(T)=C^*(3T)=\Sigma_{k=-\infty}^{\infty}[3^kT\cosh(1/3^kT)]^{-2}$ $=\ln 2/\ln 3+a\sin[2\pi\ln(bT)/\ln 3]+\epsilon(T)$ with $a=1.27\ldots\times 10^{-2}$, $b=1.97\ldots$ and $\epsilon(T)<5\times 10^{-4}$ ($\forall\ T$) (T is measured in units of the outermost width of the Cantor set); (iii) in the $T\to\infty$ limit, $C_\infty(T)\sim 1/8T^2$. In addition to this, we comment on a possible connection of this type of systems with the recently introduced nonextensive thermostatistics. [S1063-651X(97)51511-X]

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Quasicrystals are being intensively studied, both theoretically [1,2] and experimentally [3] (see [4] for a review). The fact that they are in some sense midway between *disorder* (many of their physical properties exhibit an erraticlike appearance) and *order* (their definition, and construction, follows purely deterministic rules) makes them attractive objects of research. Since their first experimental realization (in quasiperiodic GaAs-AlAs heterostructures) in 1985 by Merlin and collaborators [5], 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 behavior of a variety of particles and quasiparticles (electrons [6], photons, plasmon-polaritons, magnons [7]) in quasicrystals 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, we shall herein study the specific heat associated with one of the most simple among them, namely the triadic Cantor set (whose fractal dimension d_f equals ln2/ln3).

Let us consider a scale invariant energy spectrum as indicated in Fig. 1(a); $n=1$ corresponds to a continuous spectrum going from 0 to Δ; $n=2$ corresponds to a spectrum whose first and second branches go from 0 to $\Delta/3$ and $2\Delta/3$ to Δ, respectively; and so on for increasing n. We are interested in the *banded*-spectrum specific heat C_n^{band} as a function of the temperature T (from now on measured in units of Δ; i.e., without loss of generality we shall from now on take $\Delta=1$). We wish to calculate, in particular, $C_\infty^{band}(T)$ $\equiv\lim_{n\to\infty}C_n^{band}(T)$. For instance, in the case $n=1$ we have the partition function [8] (by choosing $k_B=1$; $\beta\equiv 1/T$) $Z_1^{band}(T)=\int_0^1 dE\exp(-\beta E)$, hence the specific heat is given by $C_1^{band}(T)=1-[2T\sinh(1/2T)]^{-2}$; thus obtaining the well known expression of the Langevin paramagnet. Analogously we can obtain $C_n^{band}(T)$ [see Fig. 2(a) for $n=1,2,\ldots,10$]. We verify that, at low temperatures, the successive specific heats oscillate around the fractal dimension $d_f=\ln 2/\ln 3$, and that, at high temperatures, they vanish proportionally to $1/T^2$.

Let us now focus on the *discrete* case. The spectrum we adopt is indicated in Fig. 1(b). For $n=1$, we have two nondegenerate levels at $E=0$ and $E=1$; for $n=2$, we have four levels at $E=0,1/3,2/3,1$; and so on for increasing values of n. The $n=1$ partition function is given by $Z_1^{disc}(T)=1+\exp(-\beta)$ hence, $C_1^{disc}(T)=[2T\cosh(1/2T)]^{-2}$; thus obtaining the well known Schottky anomaly [see Fig. 2(b) for $n=1,2,\ldots,10$].

We address now the general discrete case. The analytical discussion is simplified by considering the following energy spectrum (expressed as a ternary expansion):

$$\overline{E}=c_1/3+c_2/3^2+c_3/3^3+\cdots, \tag{1}$$

where the ternary coefficients $\{c_k\}$ can only take the values 0,2 (if the value 1 were also allowed we would obtain the whole interval [0,1], rather than the Cantor set). The next steps are simple; first we obtain the partition function

$$\overline{Z}_n^{disc}(T)=\sum_{c_1,c_2,\ldots,c_n=0,2}\exp\left[-\beta\left(\frac{c_1}{3}+\frac{c_2}{3^2}+\ldots+\frac{c_n}{3^n}\right)\right]$$
$$=\prod_{k=1}^{n}[1+\exp(-2\beta/3^k)], \tag{2}$$

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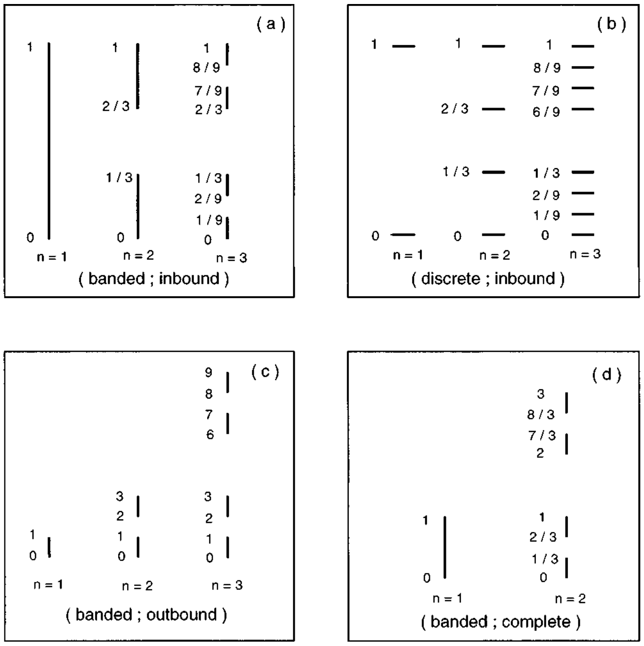

FIG. 1. Energy spectra (in units of $\Delta > 0$): (a) banded, inbound; (b) discrete, inbound; (c) banded, outbound; (d) banded, complete. The triadic Cantor set emerges at the $n \to \infty$ limit.

hence,

$$\overline{C_n^{disc}}(T) = \sum_{k=1}^{n} [3^k T \cosh(1/3^k T)]^{-2}. \tag{3}$$

It is interesting to notice that the specific heat has decoupled into a superposition of n Schottky anomalies each one corresponding to each one of the *scales* of the fractal. As a matter of fact, it can be shown that this model is equivalent to a system of n noninteracting spins$-\frac{1}{2}$ in the presence of a nonuniform external field. Since the spectrum is bounded, in the limit $T \to \infty$, the specific heat must decay as T^{-2}, in fact $\overline{C_\infty^{disc}}(T) \sim 1/T^2[\frac{1}{9} + \frac{1}{81} + \cdots] = 1/8T^2$. Let us now connect the results associated with the discrete spectrum $\{\overline{E}\}$ with those associated with the discrete spectrum $\{E\}$. A straightforward inspection yields $Z_{n+1}^{disc} = [1 + \exp(-\beta/3^n)]\overline{Z_n^{disc}}$. In the large n limit, we obtain $Z_{n+1}^{disc} \sim 2\ \overline{Z_n^{disc}}$, which corresponds to the fact that every band is associated, in the discrete case, with *one* state of the $\overline{E}$ spectrum, instead of *two* states in the E spectrum. Consequently, we have that $C_\infty^{disc} = \overline{C_\infty^{disc}}$.

We can now compare the results for the banded and discrete spectra. Since the energy bands become vanishingly narrow for $n \to \infty$, it is obvious that, although $C_n^{band}(T) \neq C_n^{disc}(T)$ for all *finite* n [e.g., $C_n^{band}(0) = 1$ whereas $C_n^{disc}(0) = 0$], $C_\infty^{band}(T) = C_\infty^{disc}(T) \equiv C_\infty(T)$ for all *finite* temperatures [see in Fig. 2(c) our results for $n = 10$, banded and discrete cases]. More precisely, it can be easily established that $Z_n^{band} = (1/\beta)\tanh[\beta/(2 \times 3^{n-1})]Z_n^{disc}$, hence $C_\infty^{band} = C_\infty^{disc}$.

Let us now address two modified energy spectra for the present problem, say in its banded version. Instead of using the spectrum of Fig. 1(a) (from now on referred to as the *inbound model*), we can use that of Fig. 1(c) (*outbound model*) or that of Fig. 1(d) (*complete model*). It is then clear that, in the $T \to 0$ limit, $C_\infty^{inbound}(T) \sim C_\infty^{complete}(T) \equiv C^*(T)$, and that, in the $T \to \infty$ limit, $C_\infty^{outbound}(T) \sim C_\infty^{complete}(T)$. Moreover, we have that $C^*(T) = \Sigma_{k=-\infty}^{\infty}[3^k T \cosh(1/3^k T)]^{-2}$. We verify an important scale property, namely that $C^*(3T) = C^*(T)$ $(\forall\ T)$. The last step consists of replacing the sum by an integral plus corrections, the corrections being given by the so called Poisson's formula $\Sigma_{k=-\infty}^{\infty} f(k) = \Sigma_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) \exp(2\pi i k x) dx$. Therefore,

$$\begin{aligned} C^*(T) &= \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\exp(2\pi i k x)}{[3^x T \cosh(1/3^x T)]^2} dx \\ &= \frac{\ln 2}{\ln 3} + \frac{2}{\ln 3} \sum_{k=1}^{\infty} \left[A_k \cos\left(\frac{2\pi k \ln T}{\ln 3}\right) \right. \\ &\quad \left. - B_k \sin\left(\frac{2\pi k \ln T}{\ln 3}\right) \right], \end{aligned} \tag{4}$$

where

$$\begin{Bmatrix} A_k \\ B_k \end{Bmatrix} \equiv \int_0^\infty \frac{z}{\cosh^2 z} \times \begin{Bmatrix} \cos \\ \sin \end{Bmatrix} \left(\frac{2\pi k \ln z}{\ln 3} \right) dz. \tag{5}$$

Equation (4) can be rewritten in a more compact way,

$$C^*(T) = \frac{\ln 2}{\ln 3} + \sum_{k=1}^{\infty} a_k \sin\left[\frac{2\pi k \ln(b_k T)}{\ln 3}\right], \tag{6}$$

where $a \equiv a_1 = (2/\ln 3)(A_1^2 + B_1^2)^{1/2} = 1.27 \ldots \times 10^{-2}$ and $b \equiv b_1 = \exp\{(\ln 3/2\pi)[\pi - \arctan(A_1/B_1)]\} = 1.97 \ldots$. The $k = 0$ term has produced the fractal dimension (''average'' value); the coefficients $\{a_k\}$ and $\{b_k\}$ are easily expressed in terms of the above integrals. Then, it is observed that the first two terms ($k = 0$ and $k = 1$) are sufficient to reproduce $C^*(T)$ extraordinarily well; we numerically checked that further corrections are about 2000 times smaller in amplitude (and consist of double frequency and higher harmonic oscillations). $C^*(T)$ is presented in Fig. 2(d).

In order to qualify in what sense d_f is an average, let us notice that $C^*(T)$ is a periodic function of $\ln T$. Consistently, $[\int_T^{3T} C^*(T') dT'/T']/[\int_T^{3T} dT'/T']$ independs from T, and it is easily verified that it equals $\ln 2/\ln 3$. At this point it is interesting to remark that this result can be interpreted as an ''equipartition'' principle. In general, a constant value of the specific heat $C = l$ is associated to the fact that the average density of states scales with energy as E^{l-1}. In our case it can be verified that the density scales as $E^{d_f - 1}$ (see Fig. 3). This implies that the average specific heat is $C_{av} = d_f$. In this sense, the equipartition principle is preserved.

In the context of oscillatory behavior of thermodynamical quantities we point out that similar phenomena have already been observed. For instance, Meurice *et al.* [9], in agreement with a previous discussion [10], have reported oscillations in ''extrapolated slopes'' in Dyson's hierarchical model. Let us also mention that Petri and Ruocco [11] found an expression which is structurally similar to Eq. (3) when studying the vibrational specific heat of a one-dimensional hierarchical model. However, those authors were mainly concerned with

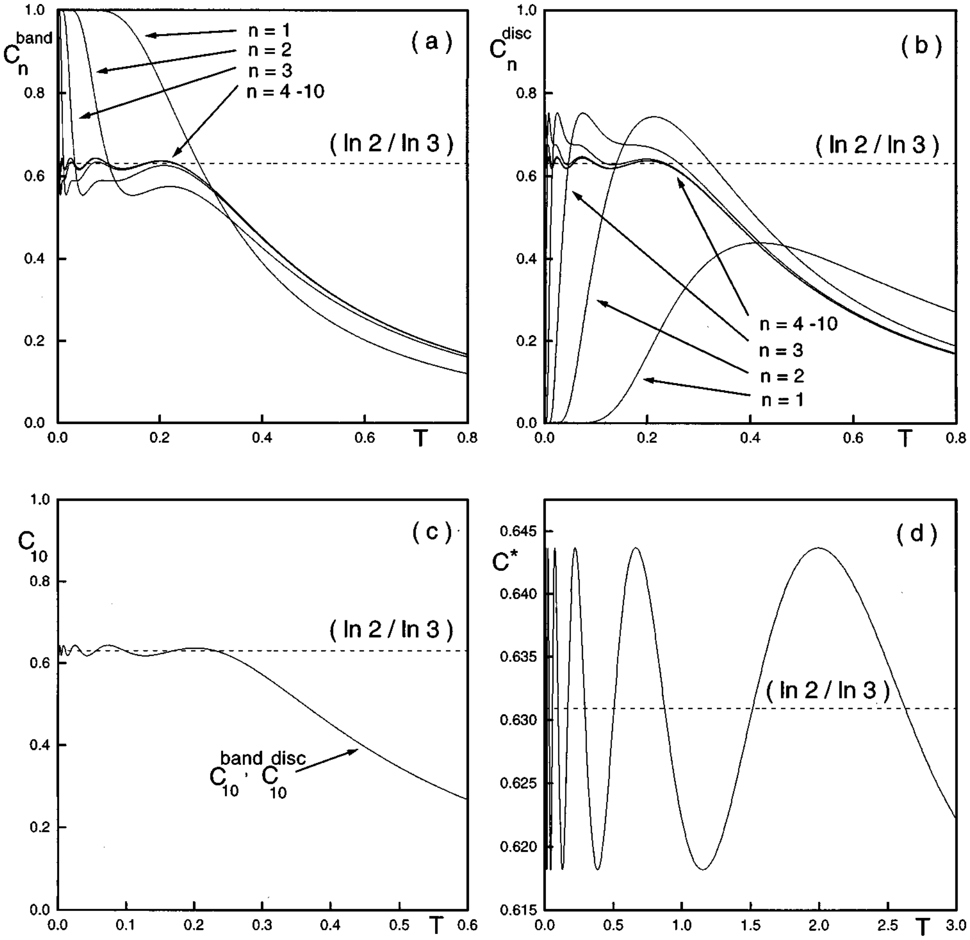

FIG. 2. Specific heat (in units of k_B) vs temperature (in units of $\Delta>0$) of the (a) banded, inbound ($n=1,2,\ldots,10$); (b) discrete, inbound ($n=1,2,\ldots,10$); (c) banded and discrete, inbound ($n=10$); (d) banded and discrete, complete ($n\to\infty$). In all cases the fractal dimension $d_f=\ln2/\ln3=0.630\ldots$ is indicated.

mean values and did not discuss the small amplitude oscillations that can be observed in their results. An interesting contribution of the present paper is to reveal a transparent connection between the scale invariance of the energy spectrum and the oscillations of the specific heat as a function of temperature.

The model we have studied suggests that the fractal structure of a spectrum reflects itself in the specific heat in two ways. The average behavior is associated with a fractal dimension; there are oscillations (around this average value) whose number is related to the hierarchical depth. So, even for a *finite* hierarchy these features could be experimentally observed. In fact, since the effect can appear at arbitrary temperatures, it is quite plausible that similar phenomena would generically exist for bosonic and fermionic systems. In other words, oscillations in thermodynamical functions as a function of temperature would appear as a manifestation of the hierarchical organization of the energy spectrum.

Before concluding, let us comment on a possible connection of the present calculation with the recently introduced nonextensive thermostatistics [12]. This statistics is based on a generalized entropic form, namely $S_q\equiv(1-\Sigma_i p_i^q)/(q-1)$, $q\in\mathbb{R}$ (hence, $S_1=-\Sigma_i p_i \ln p_i$, the standard entropy). The nonextensivity of this form can be seen from the fact that, if A and B are two independent systems (in the sense that the probabilities associated with $A+B$ factorize into those of A and B), then $S_q(A+B)=S_q(A)+S_q(B)+(1-q)S_q(A)S_q(B)$; we imme-

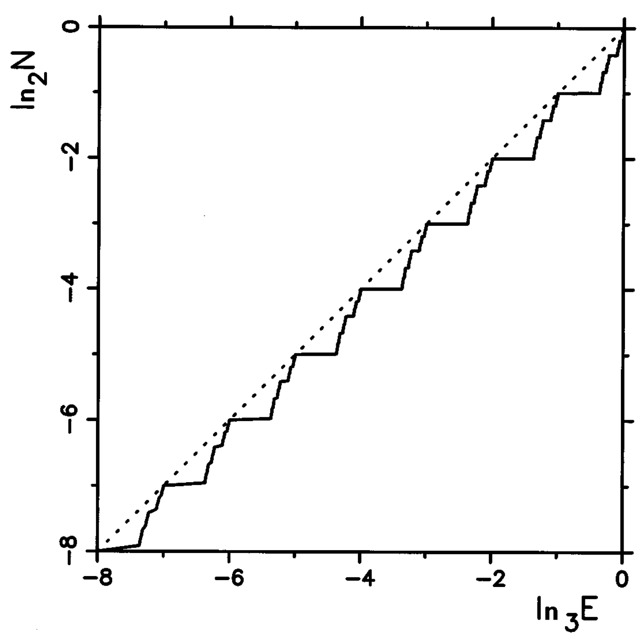

FIG. 3. Integrated density of states N (normalized to unity) vs energy. The full line corresponds to the discrete Cantor spectrum of Eq. (1) with $n=12$. The dashed line is given by E^{d_f}, with $d_f=\ln2/\ln3$, hence the density of states behaves approximately as E^{d_f-1}.

diately verify that, since S_q is non-negative, $q=1$, $q<1$, and $q>1$, respectively, correspond to the extensive, superextensive, and subextensive cases. This formalism has received applications in a variety of situations [13] such as self-gravitating systems, two-dimensional-like turbulence in pure-electron plasma, nonlinear maps, Lévy-like and correlated-like anomalous diffusions, the solar neutrino problem, peculiar velocity distribution of galaxy clusters, cosmology, linear response theory, long-range fluid and magnetic systems, optimization techniques, among others. Alemany [14] has recently suggested that this formalism could be connected to systems with fractally structured Boltzmann-Gibbs probability distributions. Although on the basis of our present calculation does not appear a transparent connection along Alemany's lines, it is worthy mentioning a couple of intriguing features. First, the generalized specific heat $C_q(T)$ of the quantum one-dimensional harmonic oscillator is available in the literature [15], and for $q<1$ it *does present oscillations*; the amplitude of the oscillations decreases when q approaches 1 from below, and they can be as small as the present ones if q is sufficiently close to 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$T$. Second, Bellissard *et al.* [2] have, in some cases, connected quasicrystalline structures with a *zero* Liapunov exponent (this is kind of intuitive since fully ordered and fully disordered structures would naturally fit with negative and positive Liapunov exponents, respectively); a similar connection exists [16] when $q\neq 1$.

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