Thermodynamical fingerprints of fractal spectra

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We investigate the thermodynamics of model systems exhibiting two-scale fractal spectra. In particular, we present both analytical and numerical studies on the temperature dependence of the vibrational and electronic specific heats. For phonons, and for bosons in general, we show that the average specific heat can be associated to the average (power law) density of states. The corrections to this average behavior are log-periodic oscillations, which can be traced back to the self-similarity of the spectral staircase. In the electronic problem, even if the thermodynamical quantities exhibit a strong dependence on the particle number, regularities arise when special cases are considered. Applications to substitutional and hierarchical structures are discussed.

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I. INTRODUCTION

Quasiperiodic structures have been studied intensively in the last 15 years. Aside from their purely theoretical interest, these studies were in part motivated by the discovery of the quasicrystalline state [1] together with the possibility of experimental realization of quasiperiodic superlattices, first achieved in 1985 by Merlin and collaborators [2]. In turn, the rich properties of these structures encouraged the study of systems based on alternative sequences (e.g., Thue-Morse and hierarchical), which, in spite of not being quasiperiodic, still exhibit deterministic (or “controlled”) disorder, i.e., they are neither random nor periodic. One of the most interesting features that many of these problems (either experimental or theoretical) display is a fractal spectrum of excitations. For instance, experiments on Thue-Morse [3] and Fibonacci [2] superlattices have uncovered scale invariant energy spectra. Numerical analysis of linear chains of harmonic oscillators with hierarchical nearest-neighbor couplings and equal masses exhibit spectra related to the triadic Cantor set [4] (the Cantor-like structure is preserved even if masses are also distributed in a hierarchical way [5]). It has also been proved that the energy spectrum of a chain made of identical springs and of masses of two different kinds arranged after the Thue-Morse sequence is a Cantor-like set [6].

Even though controlled disorder typically leads to multifractal spectra, in some cases only a few scales are sufficient for a satisfactory understanding of their thermodynamics. For instance, the phonon spectrum of the chain in [4] is essentially a one-scale Cantor set; the electronic spectra that arise from Fibonacci tight-binding Hamiltonians (either on-site or transfer) are governed by a couple of scale factors [7].

Within this context, few-scale fractal spectra constitute simple prototypes for testing the thermodynamical implications of deterministic disorder. As a first step in this direc-

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The thermodynamical fingerprints of fractal spectra involve the study of spectral properties that remain invariant under scale transformations. This is particularly relevant in the context of disordered systems, where the specific heat and other thermodynamic quantities exhibit a log-periodic behavior. The spectral dimension, which quantifies the effective dimension of the spectrum, is a key concept in this field. For a fractal spectrum, the spectral dimension is given by

\[ D = \frac{\ln 2}{\ln r_1} \]

where \( r_1 \) is the scale factor and \( n \) is the generation number. The spectral staircase is a cumulative distribution function that relates the density of states to the energy, and its smooth form is important for computing thermodynamic quantities.

The specific heat per particle is given by

\[ c(T) = d + a' \cos(\omega \ln T - \phi), \]

where \( a' \) is a function of \( r_1 \) and \( r_2 \). Equation (4) relates the log-periodic nature of the specific heat to that of the spectral staircase.

### III. PHONON STATISTICS

A standard way to study the acoustic properties of a lattice is to consider a nearest-neighbor harmonic chain. This model is represented by the equation of motion

\[ m_j \frac{d^2 u_j}{dt^2} = k_{j-1}u_{j-1} + k_{j+1}u_{j+1} - (k_{j-1} + k_{j+1})u_j, \]

where \( u_j \) is the displacement of the \( j \)-th atom (of mass \( m_j \)) from its equilibrium position and \( k_{j, j+1} \) are the strengths of the couplings between neighboring atoms. Deterministic disorder is introduced by requiring the masses and/or the strengths to follow a statistical distribution (e.g., Thue-Morse, Fibonacci, Fibonacci class [12]) or hierarchical sequences. Assuming that the time dependence in Eq. (5) goes like \( u_j \propto \exp(-\iota \omega t) \), the stationary equation of motion is obtained. Upon diagonalization, one calculates the normal modes and the eigenfrequencies \( \omega \).

### References


[2] V. Balasubramanian, A. S. red and for the sake of notation simplicity, we will take \( n \) fractal that arises in the limit \( n \rightarrow \infty \) and not on the specific pattern for this spectrum to depend only on its hierarchical organization.

The parameters \( a \approx 1, b, \) and \( \phi \) are functions of both \( r_1 \) and \( r_2 \) and result from a detailed analysis of the exact spectral staircase. The smooth cumulative density (2) allows for analytical manipulations while still keeping the principal ingredients of the self-similar spectrum. In fact, in the Boltzmann case, the use of Eq. (2) together with a perturbative approach leads to an accurate expression for the specific heat per particle as a function of the temperature \( T \):

\[ c(T) = d + a' \cos(\omega \ln T - \phi), \]

where \( a' \approx d \) is a function of \( r_1 \) and \( r_2 \) [9]. Equation (4) relates explicitly the log-periodic nature of the specific heat to that of the spectral staircase.
Now we make two approximations in Eq. (5). Our interest is the low-temperature regime, we extend the upper integration limit to infinity and arrive at

\[ c(T) = \frac{1}{2^{n+1}} \int_{0}^{1} \left[ \frac{e^T}{\sinh(e^T)} \right]^2 dN(\epsilon). \]  

(7)

Now we make two approximations in Eq. (7). First, we replace the exact \( N(\epsilon) \) by its smooth version (2). Second, as our interest is the low-\( T \) regime, we extend the upper integration limit to infinity (this is equivalent to considering an unbounded fractal spectrum). After some simple algebra we arrive at

\[ c(T) \approx T^d \left[ a'' + b'' \cos(\omega \ln T - \phi) + c'' \sin(\omega \ln T - \phi) \right]. \]  

(8)

Here \( a'' = a', \quad b'' = b'(1 - c' / \omega d), \quad \) and \( c'' = -b(c' + b' \omega d); \) the parameters \( a', b', c' \) are given by

\[
\begin{pmatrix}
a' \\
b' \\
c'
\end{pmatrix} = \frac{1}{4} \int_{0}^{\infty} dx \frac{x^{d+1}}{\sinh^2(x/2)} \begin{pmatrix} 1 \\ \cos(w \ln x) \\ \sin(w \ln x) \end{pmatrix}.
\]

(9)

Equation (8) is the phonon analog of the Boltzmann result (4). It displays explicitly the average behavior of the specific heat and the log-periodic corrections. In Fig. 2 we plotted the analytical curves (8) for the same set of scaling factors used for the numerically exact calculations. For low temperatures, the agreement between the exact and analytical results is very good [notice that the disagreement in the mean value for the \( (0.30,0.15) \) case actually corresponds to a 3% error]. The scale factor \( r_1 \) is responsible for the period of the oscillations through \( \omega = -2 \pi / \ln r_1 \) [as shown in Fig. 2(b) the period decreases as \( r_1 \) increases]. Moreover, as \( r_1 \) controls the gap scaling with respect to \( T = 0 \), smaller \( r_1 \) values imply comparatively bigger gaps, and, in turn, bigger amplitudes. For fixed \( T \), decreasing \( r_1 \) causes the spectrum to shrink towards \( \epsilon = 0 \), as a consequence the specific heat grows. These are the features observed by Petri and Ruocco in their paper on one-dimensional chains with hierarchical couplings [4]. We can now understand quantitatively their results as being a direct consequence of log-periodic corrections to the pure power-law scaling of the density of states (2).

IV. BOSE AND FERMI STATISTICS

The statistical problem of particles with nonidentically null chemical potential stands at the next level of complexity, both from analytical and numerical points of views. As in this case analytical derivations seem not feasible (except in limiting regimes), so we resort to a numerical procedure. For a fixed average number of particles \( N \) we extracted the chemical potential \( \mu \) as a function of the temperature by solving the equation

\[
N = \sum_{j=1}^{2^{n+1}} \frac{1}{e^{(\epsilon_j - \mu) / T} \pm 1},
\]

(10)

where the sum runs over the levels of the fractal truncated at hierarchical depth \( n \). The sign \(+/-\) corresponds to the Fermi/Bose case. (We are not taking into account spin degeneracies, which will not modify our results.) The numerical solution of Eq. (10) is not a difficult task, however, some care has to be taken with the choice of an appropriate initial value for \( \mu \). Once the chemical potential has been obtained, the specific heat can be calculated as the \( T \) derivative of the average total energy \( E(T) \).

\[
E(T) = \sum_{j=1}^{2^{n+1}} \frac{\epsilon_j}{e^{(\epsilon_j - \mu) / T} \pm 1}.
\]

(11)

A. Bosons

Even though bosonic excitations with non-null chemical potential do not seem to be of main relevance for the thermodynamics of superlattices, we decided to include a discussion on this topic for reasons of completeness, and because bosons in a fractal spectrum display a paradigmatic behavior.
Thus, for very low $N$, one obtains from Eq. 2 that the average particle number in the condensate is given by

\[ N = \frac{\mu}{k_B T} \]

The temperature is illustrated in Fig. 3

![FIG. 3. Bosons in a two-scale fractal spectrum. Fugacity $z$ vs $\ln T$, for different values of particle number $N$ (indicated in the figure). The chosen scales are $(r_1, r_2) = (1/3, 0.2)$ in (a) and $(0.02, 0.2)$ in (b). In both cases $n = 7$.](image)

The dependence of the fugacity $z = \exp(\mu/T)$ with temperature is illustrated in Fig. 3(a). Several curves, parametrized by the average particle number (indicated in the figure) have been drawn. First of all, Fig. 3(a) displays the following limiting features. As $T$ decreases, and the system evolves towards condensation, the chemical potential increases from negative values up to a limiting value close to zero (we recall that our lowest energy is $e = 0$). The number of particles in the condensate is given by $N_0 = z/(1 - z)$. Thus, for very low $T$, together with large $N$, one has $z \approx 1 - 1/N$. In the opposite limit of high temperatures and small $N$, one obtains from Eq. (10) $z \sim N^* = N/2^{n+1}$. In Fig. 3(b) we have chosen a small value of $r_1$ to show that $\mu$ indeed oscillates as the temperature gets through the scales of the spectrum. In this sense, Fig. 3(b) can be thought of as an amplified version of Fig. 3(a).

The dependence of the specific heat per particle on the temperature is illustrated in Fig. 4. Shown are the exact results and the numerical calculation, which uses the smooth expression (2) for the spectral staircase. For low temperatures the agreement is excellent. It is clear that the mean value of the specific heat is indeed associated to the average level density and that it suffices to take into account only the first nontrivial correction to the power-law scaling to explain the oscillations. [It is worth pointing out that this scenario breaks down in the fermionic case (see later)]. We have tested that the curves in Fig. 4 do not change in the thermodynamical limit of increasing both $N$ and the hierarchy $n$ but keeping $N^* = N/2^{n+1}$ fixed, except that the oscillatory behavior extends to lower temperatures of the order of $r_1^n$ (the total number of oscillations of the specific heat is equal to the depth $n$). The relative particle number $N^*$ plays the role of a density, given that the number of levels below a certain energy grows with the volume of the system. When $N^*$ is sufficiently small and the temperature is high enough, the curves tend to those for the Boltzmann statistics [8,9]. This is analogous to the usual statement that the parameter $\lambda \rho$ (where $\lambda$ and $\rho$ are the thermal length and the density, respectively) tells how good is the classical approximation.

Although an analytical description of the problem is lacking, our numerical calculations show that log periodicity is robust enough to resist the inclusion of bosonic symmetries together with the restriction of particle conservation.

### B. Fermions

The results presented in this section are valid for fermions in general, however, we assume that the fractal $(r_1, r_2)$ corresponds to the electronic spectrum of a certain superlattice. From the theoretical point of view, such spectra appear in the simplest model for studying the electronic properties of a lattice, i.e., a stationary tight-binding equation, for instance, in its transfer version:

\[ t_{j+1} \psi_{j+1} + t_j \psi_{j-1} = e \psi_j, \]

where $\psi_j$ denotes the wave function at site $j$ and $\{t_j\}$ are the hopping matrix elements. If these hopping elements are ar-
dependence of prints of the fractal spectrum are clearly seen in the particles \( \sim e^r \) ranged according to the Fibonacci sequence, the spectrum of energies \( \{ \epsilon \} \) is essentially a fractal of the type \( (r_1, r_2) \) (see, e.g., [7]), independently of the boundary conditions. However, the simple scaling is lost if the more general Fibonacci-class [12] sequences are considered.

The numerical scheme used for computing the thermodynamical quantities in the bosonic case can be easily adapted to the electronic problem. Figures 5 and 6 exhibit some relations among chemical potential \( \mu \), average number of particles \( N \), and temperature for the \( r_1 = r_2 = 1/3 \) case. Fingerprints of the fractal spectrum are clearly seen in the dependence of \( \mu \) with temperature (Fig. 5). In the limit of zero temperature, for a given integer particle number \( N \), \( \mu \) takes the value corresponding to the middle of the gap \( (\epsilon_N, \epsilon_{N+1}) \), as happens, e.g., in intrinsic semiconductors. In order to keep \( N \) fixed as temperature grows, the Fermi surface moves in the direction of the lowest density of levels, integrated over an energy interval \( T \). The relative concentration of levels in the neighborhood of the gap is a fluctuating function of the scale \( k_B T \). This gives rise to an oscillatory process that persists until \( T \) overcomes the largest gap \( (\log_3 T = -1) \). From this point on, if \( N^* > 0.5 \) \( (N^* < 0.5) \), \( \mu \) tends in a monotonic way to \( -\infty \) \( (\infty) \). For smaller values of \( r_1 \), oscillations in \( \mu \) are magnified (not shown), analogously to what happens with bosons.

Figure 6 displays the chemical potential as a function of the reduced number of particles \( N^* \) for three values of fixed temperature. This figure gives some insight into the difficulties involved in solving Eq. (10). For low (fixed) temperatures, \( \mu(N) \) tends to the spectral staircase and the numerical problem gets relatively difficult. As temperature grows the staircase gets smoother and numerics simplify. We have taken \( N \) to be continuous, but observe that for integer \( N \) and low temperatures (compared to the gap size) the curves pass through the middle of the gaps, as is clear in Fig. 5.

The specific heat in the fermionic problem depends strongly on the position of the Fermi surface. Thus, we begin by analyzing some simple cases where the number of particles takes special values. For this purpose it is useful to recall the picture of bands and gaps of Fig. 1. Each gap determines a special number of particles \( N^* \), namely, the relative number of particles that would lie below that gap at \( T = 0 \). For instance, the first-generation gap determines \( N^* = 1/2 \). The \( n = 2 \) gaps correspond with \( N^* = 1/4, 3/4 \). Conversely, the denominator and the numerator in \( N^* \) indicate respectively the generation \( n \) of a gap and the number of filled bands of \( n \)th generation, e.g., \( N^* = 1/32 = 1/2^5 \) corresponds to a gap that appeared in the fifth generation and to one filled band of fifth generation.
A first example that illustrates the structure of the specific heat is depicted in Fig. 7. There we consider a spectrum with two different scales $r_1 = 1/3$, $r_2 = 1/9$, and the selected set of numbers $N^* = 1/32, 1/16, 15/16, 31/32$. For the first two cases, $N^* = 1/32, 1/16$, the size of the gap is of the order of the Fermi temperature $T_F$. Once the temperature overcomes the width of that gap, the electrons can fully access the next band above, so that the mean level occupation drops approximately to 1/2. From then on the electrons behave essentially as Boltzmann particles: the specific heat oscillates around a constant average value, as expressed by Eq. (4). The average value and the period are governed by the scaling factor $r_1 = 1/3$ through Eq. (3). The number of oscillations is equal to the generation index $n$: four if $N^* = 1/16$ and five if $N^* = 1/32$. The case of numbers $N^* = 31/32, 15/16$ is equivalent to having respectively $N^* = 1/32, 1/16$ holes and it is then complementary to the previous one. Remarkably, in the case of holes, the dominant scale is $r_2$. The reason for this is that $r_2$ rules the scaling with respect to the upper edge of the spectrum, and, in fact, with respect to the upper (lower) edge of every band (gap); in other words, $r_2$ is the relevant factor for negative temperatures. Equations (3) and (4) are still valid provided that $r_1$ and $r_2$ are interchanged. According to these arguments, the choice $r_2 = r_1^2$ implies that the period of the oscillations for holes is twice that for electrons, which is confirmed by our calculations (see Fig. 7). Horizontal lines correspond to the Boltzmann average result, properly normalized in the case of holes. Increasing the hierarchy $n$ and keeping $N^*$ fixed does not change Fig. 7 because the gap on top of the filled band determines the smallest scale of the fractal that can be resolved.

Other special particle numbers allow for observing a mixed electron-hole behavior. Let us consider, for instance, the cases $N^* = 7/64, 57/64$, corresponding, respectively, to 7 and 57 filled bands of sixth generation (Fig. 8). For $N^* = 7/64$, the Fermi temperature is several scales bigger than the width of the seventh gap, so that the low-$T$ part of the specific heat is associated to hole excitations jumping from the (empty) eighth band down over the sixth-, fifth-, and fourth-generation gaps. These excitations are of Boltzmann nature and govern the specific heat until the temperature becomes of the order of $T_F$. At this point electrons are able to jump up over the third-generation gap between the eighth and ninth bands. The high-$T$ ($T > 3^{-4}$) oscillations are associated to electronic excitations through the third-, second-, and first-generation gaps. Similar considerations apply to the complementary case $N^* = 57/64$. The horizontal lines in Fig. 8 correspond to our predictions for the average specific heat, which take into account the effective number of electrons or holes that contribute to the specific heat in each regime. (The fact that the case $N^* = 7/64$ presents one less oscillation than its complementary is due to an overlap of temperature scales in the transition from hole to electron behavior.)

The general case of an arbitrary number of particles shows a nontrivial mixture of the simple behaviors described before. However, the gross features of the specific heat for arbitrary $N$ can be qualitatively (and sometimes quantitatively) understood as being a reflection of sequences of electronic and hole excitations that alternate themselves in producing the oscillatory patterns shown in Fig. 9. Formulations based on smooth approximations to the density of states, analogous to those made for bosons, are bound to fail in the fermionic case. The intrinsic discontinuity of the Fermi problem, which is critically enhanced by the dual scaling respect to the lower and upper edges of the gaps, is in essence incompatible with smooth approximations (with the exception of too special cases).

V. CONCLUDING REMARKS

We have analyzed the quantum statistics of model systems exhibiting two-scale fractal spectra, with special emphasis on the structure of the specific heat. Our findings extend previous results on classical statistics to show that the thermodynamical manifestations of spectral fractality are robust with respect to the inclusion of quantum symmetries. The general scenario for Boltzmann and bosonic particles can be summarized as follows. In spite of the very fragmented structure of the real density of states, a formulation
that starts from a smooth approximation but takes into account the coarsest log-periodic fluctuations is sufficient for a good description of the specific heat and other averaged quantities. In the case of fermions, even if a treatment that is uniform in the particle number is not possible, many features of the problem can be understood with the help of the simple results for the Boltzmann case.

Our analysis was limited to two-scale fractals. Previous results indicate that provided the scaling towards the inferior limit of the spectrum is uniform, the inclusion of additional scales will not change our conclusions in what concerns the bosonic case. Fermions, however, can feel the scaling with respect to any point of the spectrum. So, the complexity of the fermionic problem would be proportional to the number of relevant scales, in spite of uniform zero-energy scaling.

Let us finish by mentioning that the log periodicities described in this paper may be observable in real physical systems, e.g., in the Fibonacci superlattices [2,18]. In fact, although our discussion was restricted to perfect deterministic systems, both experiments and numerical simulations by Todd et al. [18] indicate that the hierarchical organization of the electronic bands may be preserved even if substantial amounts of (random) disorder are added to the system. From a more general point of view, Saleur and Sornette [19] have demonstrated that the connection between discrete scale invariance and log-periodic oscillations is robust with respect to the presence of disorder.

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