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Non-additive model for specific heat of electrons

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ABSTRACT

By using non-additive Tsallis entropy we demonstrate numerically that one-dimensional quasicrystals, whose energy spectra are multifractal Cantor sets, are characterized by an entropic parameter, and calculate the electronic specific heat, where we consider a non-additive entropy S_q. In our method we consider an energy spectra calculated using the one-dimensional tight binding Schrödinger equation, and their bands (or levels) are scaled onto the $[0, 1]$ interval. The Tsallis' formalism is applied to the energy spectra of Fibonacci and double-period one-dimensional quasiperiodic lattices. We analytically obtain an expression for the specific heat that we consider to be more appropriate to calculate this quantity in those quasiperiodic structures.

1. Introduction

Since the discovery of quasicrystals by Shechtman et al. [1], awarded with the Nobel Prize, and the pioneering work of Merlin et al. [2] on the nonperiodic Fibonacci and Thue–Morse GaAs–AlAs superlattices, quasicrystals have emerged as a new form of matter. Quasicrystals are a particular type of solid that have a discrete point-group symmetry not present in Bravais lattices, like a C_5 symmetry in two dimensions, or icosahedral symmetry in three dimensions [3–6]. In one dimension (1D), the Fibonacci sequence can directly be translated into a layered quasicrystal structure, which is feasible through atomic-precision growth via molecular-beam epitaxy (MBE) [2]. Also, 1D passive photonic (and phononic) quasicrystals have been realized by MBE and other techniques. As a result of these advances, samples can now be prepared consisting of sequences of building blocks of different materials, in that the thickness and composition of individual layers can be controlled with high precision. Several interesting experimental studies have been reported in last two decades, like the transmission of bulk acoustic phonons [7], surface acoustic waves [8], photonic dispersion relation [9] and localization of light waves [10–12], to cite a few. From a theoretical point of view, the behavior of a variety of particles or quasiparticles, such as electrons [13], phonons [14, 15], photons [16,17], polaritons [18] and magnons [19] were investigated. For example, recently, Tanese et al. [20] have reported a fractal energy spectrum of a polariton gas confined in a quasiperiodic one-dimensional cavity described by a Fibonacci sequence. On the theoretical side, very recently, one of us have reported a spin-glass ordering in a two-dimensional square lattice by using the Ising model with ferromagnetic and antiferromagnetic exchange interactions following a quasiperiodic Fibonacci sequence in both directions of a square lattice [21]. A rather fascinating feature of these quasiperiodic structures is that they exhibit collective properties not shared by their constituents. Therefore, the long-range correlations induced by the construction of these systems are expected to be reflected someway in their various spectra (light propagation, electronic transmission, density of states, polaritons, etc.), defining a novel description of disorder or a new class of universality.

On the other hand, the analysis of the thermodynamic properties based on the energy spectrum derived from a fractal structure was pioneered by Tsallis and collaborators [22,23]. Their model was based on the most well-known and simple deterministic fractal geometry, the triadic Cantor set, and they showed 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. Such oscillations also appear in other fractal sets [24,25]. Afterwards, Mauriz and collaborators [27,28] have presented a model based on the polariton's and electron's multifractal energy spectra for artificial structures following the Fibonacci, Thue–Morse and double-period sequences, in order to study their thermodynamic properties. They proved that in the case of Fibonacci quasicrystals, whose incommensurate parameter

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is equal to the golden mean, there are two classes of log-periodic oscillations for the specific heat in the low temperature regime, one for the even and the other for the odd generation number of the sequence, with amplitude of the odd oscillations being bigger than the amplitude of the even one. These results are not observed in others sequences, except for a generalized Fibonacci sequence [29].

In recent years, a trend towards the non-additive statistical physics is rapidly increasing. In this context, the endeavor of the generalization of some of the conventional concepts has been under investigation. A quite interesting generalization of the conventional entropy form has been advanced by Tsallis [30] inspired by fractal and multifractal concepts. The generalized entropy possesses the usual properties of positivity, equiprobability, concavity, irreversibility and generalizes the standard additivity. This new formalism is called the nonextensive statistical mechanical formalism (NSMF) and has been proposed to treat problems with better results than the standard Boltzmann–Gibbs (BG) statistics, for instance, problems involving long-range interactions or long-range memory. The NSMF has been successfully applied to numerous concepts of statistical thermodynamics [34–39] and to many issues in the context of high energy physics [40–43], stellar polytropes [44], thermodynamic of black holes [45], relative information in cosmology [46], quantum entropies [47] and statistics of earthquakes [48].

Based on the fractal properties of these systems and also due to the long-range correlations induced by the construction of these systems, we can infer that the most appropriate statistic to study the thermodynamical properties of these complex systems is the nonextensive statistical mechanical formalism developed by Tsallis [30]. Therefore in this work we investigate the theoretical behavior of some thermodynamical quantities, namely the specific heat, free energy and entropy, calculated by considering the non-additivity effects arising on the system.

2. Energy spectra for quasiperiodic lattices

In this section we briefly describe a transfer matrix treatment[1] for a quasiperiodic chain which follows Fibonacci (FB) and double-period (DP) rules of growth. For this purpose, we will consider a binary sequence of sites in the lattice where the potentials V_n are arranged in a quasiperiodic fashion. By using the transfer matrix treatment, the (discrete) Schrödinger equation in the tight-binding (TB) approximation for this system can be written in the form [13]

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = M(n) \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} \tag{1}$$

where $M(n)$ is the transfer matrix of the system that makes a link from the physical properties of the n-th site to those of the $(n+1)$-th one. After successive applications of the transfer matrices we have $M(n) = M_n M_{n-1} \cdots M_2 M_1$. In this way we can obtain the wave function at arbitrary sites. The numerical evaluation of the products of these transfer matrices is completely equivalent to numerically solve the Schrödinger equation for the quasiperiodic system above.

Here we consider that the potential V_n take only two different values V_A and V_B arranged in accordance with the quasiperiodic Fibonacci and double-period sequences. By shifting the zero energy, we can choose, without loss of generality, these two value of the potentials to be opposite, namely $V_A = V$ and $V_B = -V$, where V is the potential strength.

The Fibonacci structure can be grown experimentally by juxtaposition of layers A and B, such as this superlattice can be constructed recursively as follow: $S_{n+1} = S_n S_{n-1}$ for $n \geq 1$, with $S_0 = B$ and $S_1 = A$. This recursion rule is equivalent to the *inflation* rule $A \to AB$ and $B \to A$. This sequence increases with the Fibonacci number F_n, defined by $F_n = F_{n-1} + F_{n-2}$, with the initial conditions $F_0 = F_1 = 1$. The ratio F_n/F_{n-1} for increasing n converges towards the golden mean $\tau = (1/2)(1+\sqrt{5})$. Analogously, the n-th generation of the double-period sequence can be obtained from the relations $S_n = S_{n-1} S^{\dagger}_{n-1}$, and $S^{\dagger}_n = S_{n-1} S_{n-1}$ (for n $\geq$ 1). The number of letters in this sequence increases as 2^n, and the initial conditions are $S_0 = A$ and $S^{\dagger}_0 = B$. Its inflation rule is given by the transformations $A \to AB$, $B \to AA$.

For the FB quasiperiodic lattice, the transfer matrix is given by the product of F_n matrices M_j $(j = A, B)$, given by

$$M_j = \begin{pmatrix} E - V_j & -1 \\ 1 & 0 \end{pmatrix}. \tag{2}$$

It is easily shown that M_n obeys [13]

$$M_{n+1} = M_{n-1} M_n \tag{3}$$

with $M_0 = M_B$ and $M_1 = M_A$. The double-period (DP) sequence starting matrices are analogous to the Fibonacci sequence, i.e., in our notation, $S_0 = M_1 = M_A$ and $S^{\dagger}_0 = M_0 = M_B$. Note that Eq. (3) depends on energy E. Since the determinant of M_n is the unit, the energy spectrum of the system is determined by E values which satisfy $|Tr(M_n)| \leq 2$, where $Tr()$ means the trace of a matrix. This is equivalent to look for energies where the solutions ψ_n do not grow exponentially. Once obtained, this energy spectra allow us to calculate the specific heat given by the system's allowed bands.

The first connection with physical properties of quasicrystalline superlattices was made by Kohmoto and Banavar [13]. In their work the authors obtain a set of recursion relations and self-consistent maps. These equations define the trace map of the system and are the key for the study of the wavefunction localization and spectral properties. With the aid of those relations and the initial conditions one can determinate the real allowed values of the energy for a given generation number n. Numerical examples for FB and DP quasiperiodic spectra are shown in the references [27,28]. In the next section we will apply these rules to numerically obtain the specific heat.

3. Specific heat

It is our intention in this section to discuss in detail how to obtain an expression for the generalized entropy and specific heat, from the energy spectrum. The starting point for this is the energy spectrum for the continuous fractal set, depicted in Fig. 1, for the FB and DP sequences, where

$$\Delta_i = \epsilon_{2i} - \epsilon_{2i-1} \implies \epsilon_{2i} = \epsilon_{2i-1} + \Delta_i. \tag{4}$$

Thus, when we scale the spectra above onto the $[0, 1]$ interval, we can see that $n = 1$ (where n is the generation number) corresponds to a continuous spectrum going from ϵ_1 to $(\epsilon_1 + \Delta_1)$; $n = 2$ corresponds to a spectrum whose first branch goes from ϵ_1 to $\epsilon_2 = (\epsilon_1 + \Delta_1)$ and the second one goes from ϵ_3 to $\epsilon_4 = (\epsilon_3 + \Delta_2)$ and so on for increasing n. We take the level density (DOS) inside each band to be constant, and the same for all bands in a given hierarchy. In this case, a fractal emerges at the $n \to \infty$ limit. One can, however, make a detailed study considering the influence of a non-uniform DOS [26]. For examples of energy spectra of other quasiperiodic sequences see, e.g., [27–29].

To study such complex systems, we use a non-additive entropy which was introduced by Tsallis in 1988 [30] and was later

[1] See ref. [49] for an example of transfer matrices applied to Cantor sets.