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Analytical investigation of the specific heat for the Cantor energy spectrum

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ABSTRACT

For the energy spectrum obtained for monoscale Cantor set the correct analytical calculations of the specific heat in the frame of the Boltzmann–Maxwell statistics have been performed. These evaluations were realized with the help of Mellin's transform. The accurate analytical expressions for the specific heat in all temperature range were obtained. They demonstrate the log-periodic behavior in low-temperature and non-oscillatory behavior in high-temperature regions, accordingly. The accurate value of the limiting temperature determining the boundary between these two regions was found and evaluated.

1. Introduction

The experimental discovery of quasi-crystals by Shechtman et al. [1] produced a great interest in the understanding of the properties of these systems, as was shown later by the great amount of theoretical and experimental work that followed. 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 [2], 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 quasi-particles (electrons, photons, plasmon-polaritons, magnons) in quasi-periodic sequences has been and is currently being studied [3–11]. 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. [12,13] and [14], 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 [15]; 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.

The aim of this present work is to demonstrate analytical calculations of the specific heat in the frame of the Maxwell–Boltzmann statistics for fractal energy spectrum obtained from monoscale Cantor set in *all* temperature range. The possibility of realization of the correct calculations is based on the general formula for the elements of the Cantor set that has been used in papers [12,14]. In these papers for analytical proof of existence of the log-periodic oscillations that appeared in the specific heat behavior for the simplest case of monoscale energy spectrum of the Cantor set the Poisson summation formula was used. But in the frame of this approach the region of log-periodic behavior was not evaluated properly and expression for the specific heat out of this region was also not shown. But with the help of Mellin's transform it becomes possible to determine the limits of the log-periodic region and find analytical expressions for the specific heat in these two oscillation/non-oscillation regimes. In the given paper with the usage of Mellin's transformation it becomes possible to realize accurate analytical calculations for the specific heat associated with more general monoscale Cantor set in comparison with results considered earlier in paper [14]. It is necessary to note that approach based on Mellin's transform is rather productive and it was applied with success for the solution of the problems related to the anomalous dielectric relaxation [16,17], thermodynamics of spin

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systems with hierarchy-subordinated dynamics [18] and calculation of the moment of inertia of the heated finite Fermi-systems [19] for analytical extraction of the oscillating components of the desired physical values.

2. Monoscale cantor sets thermodynamics

In paper [16] for construction of the fractal energy spectrum the generalized Cantor set model is suggested, which, in turn, can be monoscale or multiscale. The essence of the suggested constructions is reduced to the following scheme. On the initial step $n = 0$ we have the continuous segment $[0, 1]$. On the step $n = 1$ the set $\mathfrak{S}(l, m)$ is generated by division of the initial segment on j (l-accepts the integer values) equal segments of the length l^{-1} numbered from 0 up to $l - 1$. Then $l - m$ segments are excluded and as the result in the Cantor spectrum m segments are remained ($m < l$). In order to keep the spectrum width $\Delta = 1$ the segments with numbers 0 and $l - 1$ cannot be excluded. We should note that at the given l and m, $\binom{m-2}{l-2}$ different combinations of m segments exist (and, hence, $\binom{m-2}{l-2}$ of different sets $\mathfrak{S}(l, m)$). The sets are differentiated from each other with the help of notation $\mathfrak{S}(l, m; b_1, b_2, \dots, b_m)$, where the combination $\{b_1, b_2, \dots, b_m\}$ defines a set containing numbers of non-excluded segments. In accordance with limitations imposed above they should satisfy to condition $0 = b_1 < b_2 < \dots < b_m = l - 1$. After selection of one of possible combinations it should be kept during the whole construction process that is necessary for conservation of the given fractal structure. For the general monoscale $\mathfrak{S}(l, m; b_1, b_2, \dots, b_m)$ the fractal dimension (box-counting dimension) is equaled to $d_{box} = \ln m / \ln l$.

It is necessary also to reproduce an expression for the energy spectrum that is obtained from monoscale Cantor set of the general form $\mathfrak{S}(l, m; b_1, b_2, \dots, b_m)$ in a discrete case

$$\mathfrak{S}_n(l, m; b_1, b_2, \dots, b_m) = E_n^- \cup E_n^+, \tag{1}$$

where

$$E_n^- = \left\{ \sum_{k=1}^{n} \frac{b_k}{l^k} \right\}, \qquad E_n^+ = \left\{ \sum_{k=1}^{n} \frac{b_k}{l^k} + \frac{1}{l^n} \right\}, \tag{2}$$

expressions define the smallest and the highest energies of any interval of the generalized Cantor set, correspondingly. For a monoscale Cantor set, analytical expressions can be derived for the thermodynamic functions. Regarding to the energy spectra given by Eq. (1), the partition function for the monoscale $\mathfrak{S}(l, m; b_1, b_2, \dots, b_m)$ in the nth step of the generation process can be obtained as [14]

$$Z_n(T) = \left[1 + \exp\left(-\frac{\beta}{l^n} \right) \right] \prod_{k=1}^{n} \left[\sum_{b_k} \exp\left(-\frac{\beta b_k}{l^k} \right) \right]. \tag{3}$$

From this expression for the partition function, using the equation $C_n(T) = -\beta^2 \partial^2 \ln Z_n(T)/\partial\beta^2$, the specific heat $C_n(T)$ can be obtained [16]

$$C_n(T) = \left[\frac{2l^n}{\beta} \cosh\left(\frac{\beta}{2l^n} \right) \right]^{-2} + \beta^2 \sum_{k=1}^{n} \frac{\sum_{b_k} \exp(-\frac{\beta b_k}{l^k}) \sum_{b_k} b_k^2 \exp(-\frac{\beta b_k}{l^k}) - [\sum_{b_k} \exp(\frac{\beta b_k}{l^k})]^2}{[l^k \sum_{b_k} \exp(-\frac{\beta b_k}{l^k})]^2}. \tag{4}$$

In the $n \to \infty$ limit, only the second term is survived and then we have

$$C_n(T) = \beta^2 \times \sum_{k=1}^{\infty} \frac{\sum_{b_k} \exp(-\frac{\beta b_k}{l^k}) \sum_{b_k} b_k^2 \exp(-\frac{\beta b_k}{l^k}) - [\sum_{b_k} \exp(\frac{\beta b_k}{l^k})]^2}{[l^k \sum_{b_k} \exp(-\frac{\beta b_k}{l^k})]^2}. \tag{5}$$

This equation looks rather complicated and so it should be evaluated numerically for obtaining the desired temperature dependence of the specific heat. The standard way is in construction of the desired spectra and then the numerical differentiation of the partition function obtained. But an attentive analysis shows that for some specific cases expression (5) can be considerably simplified analytically.

In [14] the simplest case related to consideration of a monoscale Cantor set was considered. This approach is based on division the spectral branch into l subsegments and after that only the first and the last one are selected, i.e. $\mathfrak{S}(l, 2; 0, l - 1)$. But the triadic Cantor set represents itself the simplest case when it becomes possible to perform the summation $\sum_{b_k}$ and thereby simplify Eq. (5). Finally, we have

$$C_\infty(T) = \sum_{k=1}^{\infty} \left[\frac{2l^k T}{l - 1} \cosh\left(\frac{l - 1}{2l^k T} \right) \right]^{-2}. \tag{6}$$

From this expression with the help of the Poisson summation formula it becomes possible to obtain the analytical expression for the specific heat [16], which proves its log-periodic behavior. But we want to stress here that this case is not a unique example which admits the rigorous analytical results.

In the given work we suggest the following monoscale set admitting some simplifications of the general expression (5) for the specific heat. Really, we consider the modified set when after division of the spectral branch on l segments we keep also segments with numbers $c_k = p(k - 1)$, $k = 1, 2, \dots, m$, where p accepts the integer numbers and $l - 1$ must be multiply to the number p except $m = (l - 1)/p + 1$. In the result of these manipulations we obtain monoscale Cantor set of the type $\mathfrak{S}(l, m; 0, p, 2p, .., l - 1)$. In this case the analytical evaluation of summation $\sum_{b_k}$ remains possible and after its realization it allows to simplify expression for the specific heat (5)

$$C_\infty(T) = \sum_{k=1}^{\infty} \left(\frac{p\beta}{2l^k} \right)^2 \left[\frac{1}{\sinh^2(p\beta/2l^k)} - \frac{m^2}{\sinh^2(mp\beta/2l^k)} \right]. \tag{7}$$

In Fig. 1 we demonstrate two finite approximations of the specific heat behavior for monoscale Cantor sets in log-scale. We want to stress three basic points specifying this dependence. Firstly, the behavior of the specific heat at low T represents itself an oscillating function and the number of the oscillations which are controlled by the length of the chosen step participating in the generation process. With increasing of number of periods a new period appears in the low temperature region. The function $C_n(T)$ oscillates around a particular value that is defined by the fractal dimensionality of the set considered. In the cases shown in Fig. 1, we have $d_1 = \ln 6/\ln 11, d_2 = \ln 2/\ln 11$. Thirdly, note that in the oscillating regime, $C_n(T)$ represents itself a log-periodic function. Below, based on exact analytical calculations we are going to prove of the periodicity phenomenon of such type. The log-periodic phenomenon is appeared only in the oscillating regime.

We want to note that the main reason of the log-periodic oscillations in temperature dependence of the specific heat is related to the usage of the fractal model for the energy spectrum. Really, fractals have the property of a discrete scaling invariance, which is a lower symmetry than the scaling invariance [20]. It means that the functional equation for the observed physical value $\Phi(x)$

$$\Phi(\lambda x) = \gamma \Phi(x), \tag{8}$$