Comparison of multifractal and thermodynamical properties of fractal and natural spectra

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Abstract

In this paper, we explain the multifractal and thermodynamical properties of deterministic fractal spectra, and compare the most relevant behaviors with those obtained for some natural spectra with multifractal properties. In particular, we compare the heat capacity, $C(T)$, derived from Cantor-set-type spectra with the ones obtained from several atomic spectra. We find that, although many of the properties of deterministic fractals, previously reported, are also reproduced in natural fractals (oscillations of $C(T)$ in log scale), new features appear in the natural case: the mean value of $C(T)$ is not always related to the multifractal properties, and the oscillations are present in cases for which they disappear in deterministic fractals. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Multifractal analysis has shown to be very useful in several fields of physics, as in the characterization of the wave functions in the Anderson metal–insulator transition [1–3], in the analysis of DNA properties [4,5], or the study of physiological time series [6]. Another field in which the multifractal analysis has shown its applications is the study of the fractal properties of the spectra of chemical elements [7]. In a recent paper [8], we studied the thermodynamic and multifractal properties of deterministic fractal spectra derived from generalized Cantor sets, showing some interesting properties of the heat capacity. The more relevant result is the oscillatory properties of the heat capacity as a function of temperature (in log scale), that make the heat capacity to be a

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log-periodic function in the oscillatory regime. The value around which the oscillations occur results in their dependence on the fractal properties of the spectra.

In this paper, we study the thermodynamics and multifractal properties of some natural spectra, and compare the results to the ones obtained from deterministic fractal spectra. We investigate if the thermodynamical properties of natural fractal spectra can be explained from what we know about the deterministic fractals. This can lead to answer the question of how good are deterministic multifractals (well known and easy to study) to describe the natural ones.

The paper is organized as follows: in Section 2, we describe briefly the procedure to obtain monoscale or multiscale deterministic fractal spectra, and we comment on some of their main thermodynamics and multifractal properties. In Section 3, we present the results obtained from the spectra of several chemical elements, and compare these results with those obtained from deterministic fractals. Finally, in Section 4, we present the conclusions.

2. Thermodynamics of deterministic fractal spectra

One of the most well-known and simple deterministic fractals is the triadic Cantor set. This set is obtained by the repetition of a simple rule: you divide a given segment into three equal parts, and then eliminate the central one. From now on, we will consider all the spectra ranging between 0 and 1, i.e., we will use normalized spectra. The process continues iteratively in all the resulting segments. A plot of the first three iterations can be seen in Fig. 1a. The box-counting dimension \( d_{\text{box}} \) of this set can be easily obtained to give \( d_{\text{box}} = \ln 2 / \ln 3 = 0.63 \ldots \). It is easy to see that, at each step of the generation of the fractal, all the segments present in the set are all equal in size. In this sense we say that the triadic Cantor set is a monoscale fractal. This procedure of fractal generation can be generalized easily (see Ref. [8] for more details) to produce multiscale fractal sets. As an example, in Fig. 1b, we show a set in which, after dividing the unity segment into eight parts, we eliminate the second and fifth subsegment, thus producing three non-equal subsegments. This procedure continues iteratively with all
Fig. 2. Heat capacities as a function of $T$ for the sets shown in Fig. 1a (solid line) and in Fig. 1b (dotted line). We have considered six iterations for the set in Fig. 1a and four iterations for the set in Fig. 1b. The straight solid and dotted lines correspond, respectively, to the average value of the oscillations.

The heat capacity $C$ of a spectrum with the structure of the triadic Cantor set can be obtained analytically (see Refs. [8,9]). For all the results shown in this paper, we have considered for convenience that the Boltzmann’s constant $k_B$ equals unity. The main result is that there exists log-periodic oscillations of $C$ as a function of temperature, being the fractal dimension $d_{box} = \frac{\ln 2}{\ln 3} = 0.63 \ldots$ the average value in the oscillatory regime (see the straight solid line in Fig. 2). The number of oscillations depends on the step in the generation process of the fractal. For a spectrum with infinite number of points, the number of oscillations would also be infinite.

These results are general for all monoscale fractal sets [8] although for more complicated spectra the analytical calculation cannot be carried out. Later on we will describe how to compute $C(T)$ numerically. Nevertheless, when considering multiscale fractal sets, the results are different. The reason is that in this latter case, the fractal dimension $d_{box}$ is not enough to characterize properly the fractal structure due to the presence of multiple scales. In Fig. 2 we show by a dotted line the heat capacity for the set shown in Fig. 1b, for which its $d_{box} = 0.781 \ldots$ Note that in this case, the average value of $C(T)$ (dotted straight line in Fig. 2) is not given by $d_{box}$. The average value in the multiscale case is given by the spectral dimension, $d_E$, which is defined as the fitting
Fig. 3. Log–log plot of the integrated density of states \( g(E) \) as a function of \( E \), for the set in Fig. 1b with six iterations in the generation process. The straight dotted line corresponds to a power-law fit with slope 0.528... 

Exponent of a power-law fit of the integrated density of states \( g(E) \):

\[
g(E) \propto E^{d_E}
\]  

(1)

The reason for this behavior is that for these kinds of fractal sets, \( g(E) \) can be seen as a log-periodic oscillating function around a power law of type (1) (see Fig. 3). It is easy to show using standard statistical mechanics calculations that if \( g(E) \) behaves as \( E^{d_E} \), then the average value of \( C \) is given by \( d_E \), so in the fractal case, where the behavior of type (1) is just approximated, it is natural to obtain oscillations of \( C \) around \( d_E \). In a monoscale fractal set, \( d_E \) coincides with \( d_{\text{box}} \), so this result remains valid. The reason is that in a fit of type (1) the structure of the low part of the spectrum always dominates the trend, and for a monoscale set, this structure is identical to the whole set. In a multiscale set, this is not true, and \( d_E \neq d_{\text{box}} \), and even one can construct multiscale sets with the same \( d_{\text{box}} \) and very different \( d_E \).

Therefore, it seems that one is restricted to a numerical fit of type (1) to predict the average value of \( C \) in multiscale fractals. But in some particular cases, multifractal analysis allows to calculate \( d_E \). In the following, we explain briefly how to obtain the multifractal spectrum of a given set.

2.1. Multifractal spectrum

The most well-known ‘fractal dimension’ is the one we previously called the box-counting dimension \( (d_{\text{box}}) \), that is also known as Haussdorf’s dimension. Given a set (in our case, a one-dimensional discrete set of points), one counts the number of
segments \((n)\) of size \(\varepsilon\) needed to cover the set, and then change the size \(\varepsilon\) and repeat the procedure. The number \(n\) is supposed to scale as a function of \(\varepsilon\) in the form
\[
n(\varepsilon) \propto \varepsilon^{-d_{\text{box}}}.
\]  

(2)

The multifractal spectrum [10] is a generalization of \(d_{\text{box}}\). The starting point is the calculation of the scaling exponent of the different moments of the probability distribution of the set: in our case, we divide the unity segment into \(m\) boxes and we count the number of points of the set inside each box. Let us call \(p_i\) the quotient between the number of points in the \(i\)th box and the total number of points of the set. Then we calculate the partition function \(Z(q,m)\) as
\[
Z(q,m) = \sum_{i=1}^{m} p_i^q.
\]  

(3)

For a fixed value of \(q\), the value of \(m\) is changed (and then, the size \(\varepsilon\) of the boxes used to cover the set, because \(\varepsilon = 1/m\)) in order to obtain a fitting of \(Z\) as a function of \(\varepsilon\) of the type
\[
Z(q,m) \propto \varepsilon^{\tau(q)}.
\]  

(4)

Note that \(\tau(0) = -d_{\text{box}}\). The variable \(q\) can be positive or negative. Because of the definition of \(Z\), the positive values of \(q\) deal with the contribution of the most concentrated regions of the set, that are then characterized by the corresponding \(\tau(q)\), and the opposite can be said for the most rarefied regions of the set and the behavior of \(\tau(q)\) for negative values of \(q\). The function \(D(q)\) (which contains all the ‘dimensions’ of the set) is defined as \(D(q) = \tau(q)/q - 1\). Usually, the multifractal spectrum is represented by the function \(f(x)\), a Legendre transformation of \(D(q)\), where \(\alpha(q) = d\tau(q)/dq\) and \(f(\alpha(q)) = q\alpha - \tau(q)\).

For monoscale fractals, the multifractal spectrum is useless. The reason is that the function \(\tau(q)\) is exactly linear, and has the form
\[
\tau(q) = (q - 1)d_{\text{box}}.
\]  

(5)

As a consequence, the function \(D(q)\) is constant and exactly equal to \(d_{\text{box}}\), and then \(\alpha = d_{\text{box}}\) and \(f = \alpha\). But for multiscale fractals, a true multifractal spectrum appears, because of the inhomogeneous fractal structure of the set. In Fig. 4, we show the multifractal spectrum for the set shown in Fig. 1b, computed as it appears in Ref. [10] (for other multifractal spectra of similar sets, see this reference). The limiting dimensions of the multifractal spectrum characterize the most concentrated and the most rarefied regions of the fractal, and are called \(D_{\infty}\) and \(D_{-\infty}\), respectively. For the multifractal spectrum shown in Fig. 4, we obtain \(D_{\infty} = \ln 3/\ln 8 = 0.528\ldots\) and \(D_{-\infty} = \ln 3/(\ln 8 - \ln 3) = 1.120\ldots\) Note also that the maximum value of \(f(x)\) gives exactly \(d_{\text{box}}\), which in this case is 0.781\ldots\).

The connection between \(d_E\) (and then of \(C\)) and multifractal spectra occurs when the low-energy region (responsible for \(d_E\)) is the most concentrated or the most rarefied one. In these cases, the spectral dimension is then given by \(D_{\infty}\) or \(D_{-\infty}\), respectively.
Fig. 4. Multifractal spectrum of the set shown in Fig. 1b.

Note that the average value of the heat capacity shown in Fig. 2 (dotted line) corresponding to the set in Fig. 1b coincides exactly with $D_\infty$ in Fig. 4. The reason is that the low-energy region is the most dense of the set.

In addition, it is important to note that the oscillations present in $C(T)$ disappear in Cantor fractal spectra for which $d_E > 1$ (see Ref. [8]). This can be better understood with an example: in the set of Fig. 1b, there exist three segments with the same ‘weight’, in the sense that each one of them will lead in the generation process to the same number of points (1/3 of the total), and then all of them have a weight given by 1/3. But their lengths are different: $1/8$, $2/8$ and $3/8$. So their ‘local’ dimensions [10] are $\ln 3/\ln 8$, $\ln 3/(\ln 8 - \ln 2)$ and $\ln 3/(\ln 8 - \ln 3)$, respectively. Note (see Fig. 4) that $\ln 3/\ln 8$ is precisely $D_\infty$ (the most dense region of the set) and $\ln 3/(\ln 8 - \ln 2)$ is $D_{-\infty}$ (because it is the most rarefied region of the set). In sets for which the low-energy region (which controls $d_E$) has a length bigger or equal to its weight, (and then $d_E \geq 1$) the oscillations are never observed. Note that $d_E = 1$ implies that the low-energy region has the same length and weight (as a uniform set) and the fractal structure loses its relevance.

We will apply all these ideas to the spectra of some chemical elements in the following section.

3. Multifractal and thermodynamical properties of natural spectra

In this section, we compare the previous results obtained for deterministic fractals with the results derived from the analysis of the spectra of some chemical elements.\footnote{The experimental data have been retrieved from http://physics.nist.gov.}
all the spectral calculations that follow, we have considered, as before, normalized spectra, in such a way that all the spectral energy levels have been renormalized (preserving the geometrical structure) to the interval [0, 1].

In our study of the relation between the multifractal and the thermodynamical properties of natural spectra, we have found two clear types of behavior: first, a set of natural spectra (as Ce and Mo) for which there is a connection between the multifractal spectrum and the behavior of $C(T)$ (these spectra are then similar to the deterministic multifractals). And second, atomic spectra for which the connection between the multifractal spectrum and $C(T)$ is not so direct (in this group, we can include Co, Fe, Si, Ge, and many others). In the following, we take Ce and Co as our references for each of the two classes, respectively.

We begin by analyzing the spectrum of Ce. In Fig. 5, we show the multifractal spectrum ($f(\alpha)$ as a function of $\alpha$) of the normalized energy spectrum of Ce. As can be seen from the width of $f(\alpha)$, the spectrum of Ce presents great fluctuations in the density of energy levels. The great value of $D_{-\infty}$ indicates the existence of very rarefied regions. On the contrary, the not-so-small value of $D_{\infty}$ allows to conclude that the more dense regions are not very concentrated. It is reasonable to expect the low-energy region (the closer one to the ground state, that in our normalized scale corresponds to zero) to be the most rarefied, because of the quantum structure of the energy levels which, in principle, is more dense far from the ground state. Therefore, if the spectrum presents multifractal properties, the spectral dimension will be given by $D_{-\infty}$. To check this hypothesis, we are going to calculate the heat capacity $C$ of the spectrum as we did before for the deterministic fractal spectra.

Let us call $N$ the total number of energy levels of the spectra, being $e_i$ the $i$th energy level. The heat capacity can be calculated by differentiating the partition function of
the system, or more directly as

\[ C(T) = \frac{\langle E^2(T) \rangle - \langle E(T) \rangle^2}{T^2}, \]  

(6)

where \( T \) is the temperature. In Eq. (6), \( \langle E(T) \rangle \) and \( \langle E^2(T) \rangle \) are, respectively, the averaged energy and the averaged squared energy for a given value of \( T \). These magnitudes can be obtained as

\[ \langle E(T) \rangle = \frac{\sum_{i=1}^{N} e_i \exp(-e_i/T)}{\sum_{i=1}^{N} \exp(-e_i/T)}, \]

\[ \langle E^2(T) \rangle = \frac{\sum_{i=1}^{N} e_i^2 \exp(-e_i/T)}{\sum_{i=1}^{N} \exp(-e_i/T)}. \]

(7)

The heat capacity as a function of \( T \) for the normalized spectrum of Ce is shown in Fig. 6. Several properties of \( C(T) \) deserve to be pointed out. The first, and the most important is that the average value (in the interesting range) of \( C(T) \) is given by \( D_{-\infty} \) as obtained in Fig. 5, the dimension characterizing the most rarefied region of the multifractal spectrum. This indicates, as we expected, that it is the low-energy region (as in the deterministic fractal case) which controls the behavior of \( C(T) \), and that this region is the most rarefied one. The second relevant finding is that a couple of oscillations around \( D_{-\infty} \) are observed in \( C(T) \), as it happened in the deterministic fractal case. And finally, we note that \( C(T) \to 0 \) as \( T \to \infty \). This is natural, because the spectrum is bounded and in this case, for high values of \( T \), \( C(T) \) must tend to zero as \( T^{-2} \).
Although the spectrum of Ce is a non-deterministic fractal set, the properties derived from the geometrical structure of the spectrum present high similarities with the spectra derived from Cantor sets. Nevertheless, there is a point of clear difference between the deterministic and non-deterministic fractal spectra: in the former case, the oscillations of $C(T)$ disappear when the spectral dimension (or $D_{-\infty}$ if the low-energy region is the most rarefied) is bigger than unity, as we referred to in the previous section. However, when only a statistical fractal is considered (as Ce), the oscillations can exist even with a spectral dimension bigger than unity, thus revealing the effect of the non-deterministic behavior.

Finally, the spectrum of Ce presents more similarities with respect to the Cantor-set type, because its integrated density of states $g(E)$ behaves fairly well as a power law, as we show in Fig. 7. Note that the fitting exponent coincides (within numerical error) with $D_{-\infty}$. This characteristic is very important, as we see in the following.

As we commented above, the other general ‘class’ for the behavior of atomic spectra is the one with no connection between the multifractal spectrum and $C(T)$. For all the spectra of this kind we have studied, we always find that the reason for the lack of this connection can be found in the behavior of $g(E)$. Whereas in the case of Ce, the integrated density of states behaves fairly well as a power law (see Fig. 7), for all the elements belonging to this second class we have found that $g(E)$ is not so uniform. In general, what we find is that two spectral regimes in $g(E)$ can be seen. As an example, in Fig. 8 we show the function $g(E)$ for the normalized spectrum of Co (solid line). Note that we can model $g(E)$ by two power laws (two spectral dimensions), one in the low-energy region and the other in the high-energy region. As far as we know, this behavior is never present in deterministic multifractal sets. In spite
Fig. 8. Log–log plot of the integrated density of states \( g(E) \) as a function of \( E \), for the normalized spectrum of Co. The dotted lines correspond to power-law fits with slopes 0.7... and 2.3...

Fig. 9. Heat capacity \( C(T) \) as a function of \( T \) for the normalized spectrum of Co. The horizontal dotted lines correspond to the slopes of \( g(E) \) as shown in Fig. 8. Inset: multifractal spectrum of Co.

of this, we still obtain good fits of \( Z(q,m) \) to single power laws, so the multifractal spectrum is well defined. This lack of uniformity in \( g(E) \) breaks the relation between the multifractal spectrum and \( C(T) \). To illustrate this, in Fig. 9 we show \( C(T) \) as a function of \( T \) (in log scale) obtained from the normalized spectrum of Co. In the inset, we show the multifractal spectrum belonging to the same element. Several features
deserve to be pointed out: first, note that there is not a clear ‘mean value’, and therefore
the value of $D_{-\infty}$ has not any special meaning, as it happened before. Second, note
that the ‘oscillations’ of $C(T)$ are fairly well characterized, not by the multifractal
spectrum but by the two spectral regimes shown in Fig. 8. To show this, in Fig. 9 we
include as horizontal dotted lines the values of the slopes of the two power-law fits of
Fig. 8. Note that each slope characterizes a different region of $C(T)$ giving what we
can consider as a ‘local average value’ of $C(T)$, in contrast to the ‘global average
value’ we found in deterministic fractals and in the other class of natural spectra.

Finally, we would like to make an additional comment, not directly related to the
above discussion. For any spectrum, independent of the connection between $C(T)$ and
the multifractal properties, the behavior of $C(T)$ can also be seen as a kind of ‘spectral
sign’. We have observed that, in general, the properties of $C(T)$ for elements of the
same chemical group are very similar, thus revealing a similar geometric structure, in
spite of the very different values of their corresponding energy levels. To show this,
in Fig. 10, we have plotted the behavior of the heat capacity $C(T)$ obtained for the
spectra of Si (solid line) and Ge (dotted line). Although there exists a displacement
of the ‘oscillations’ (due to the appearance of more high-energy levels for Ge), note
the similarities between both heat capacities. This is a general behavior, that allows to
compare and identify spectra.

4. Conclusions

On the basis of the multifractal and thermodynamical properties of deterministic
fractal spectra, we have studied the behavior of the multifractal spectrum and of the
heat capacity induced by the geometrical structure of natural spectra. Although for the majority of the elements the multifractal spectrum can be obtained, not for all of them there is a connection between the behavior of the heat capacity and the multifractal properties. We have found that only natural spectra for which their integrated density of states is well modeled by a power law present this connection, as it happens with deterministic fractals. In the rest of the cases, the integrated density of states is better described by two power-law fits, and the properties of $C(T)$ are derived from these two regimes without a clear relation to the multifractal spectrum. In addition, the heat capacity of the spectra can be seen as a spectral sign for the elements of the same chemical group.

References