Nonconcave entropies in multifractals and the thermodynamic formalism

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We discuss a subtlety involved in the calculation of multifractal spectra when these are expressed as Legendre-Fenchel transforms of functions analogous to free energy functions. We show that the Legendre-Fenchel transform of a free energy function yields the correct multifractal spectrum only when the latter is wholly concave. If the spectrum has no definite concavity, then the transform yields the concave envelope of the spectrum rather than the spectrum itself. Some mathematical and physical examples are given to illustrate this result which lies at the root of the nonequivalence of the microcanonical and canonical ensembles. On a more positive note, we also show that the impossibility of expressing nonconcave multifractal spectra through Legendre-Fenchel transforms of free energies can be circumvented with the help of a generalized free energy function which relates to a recently introduced generalized canonical ensemble. Analogies with the calculation of rate functions in large deviation theory and dynamical entropies in the thermodynamic formalism of dynamical systems are finally discussed.

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I. INTRODUCTION

Invariant measures generated by nonlinear and complex dynamical systems often show striking scaling and self-similar features that are reminiscent of fractals. However, contrary to ordinary fractals, whose geometric structure is characterized by a single number (the fractal or Hausdorff dimension [1]), the scaling and self-similar properties of measures are usually not captured by a single dimension, say α, but by an infinite set of fractal or singularity dimensions which define the so-called *spectrum of singularities* $f(\alpha)$, also known as the *multifractal spectrum* [2, 3]. The word "multifractal" has been coined [4] in this context precisely to suggest that a measure having multiscaling properties can be pictured abstractly as a superposition of many "pure" fractals, each having a dimension α and a corresponding "weight" $f(\alpha)$ in the superposition.

To be more specific, consider a measure μ defined on a d-dimensional space X. Generalizing the approach followed in fractal geometry, we proceed to partition or "coarse-grain" the space X in small boxes of equal size ε and volume ε^d. The measure contained in each box is

$$p_{\varepsilon,i} = \int_{i^{\text{th}}\ \text{box}} d\mu(x), \tag{1}$$

and from this quantity, a local fractal dimension α_i, also called a crowding index, is defined by using the fact that $p_{\varepsilon,i}$ is expected to scale as $p_{\varepsilon,i} \sim \varepsilon^{\alpha_i}$ in the limit where the boxes' size ε goes to zero. Now, to account for the fact that α_i is not constant over the partition, but varies in general from one box to another, we count the number $n_\varepsilon(\alpha)$ of boxes in the partition whose local dimension is equal to α. From $n_\varepsilon(\alpha)$, the multifractal spectrum $f(\alpha)$ is then simply defined through another scaling relationship, namely $n_\varepsilon(\alpha) \sim \varepsilon^{-f(\alpha)}$ as $\varepsilon \to 0$.

The multifractal spectrum $f(\alpha)$ is not a quantity which is easily calculated analytically or numerically, since it requires the enumeration of all the boxes in the partition of X having a crowding index α lying in some interval $[\alpha, \alpha + \Delta\alpha]$. A more manageable quantity which can be related to $f(\alpha)$ is the so-called *free energy function* $\tau(q)$ defined by the scaling relationship $Z_\varepsilon(q) \sim \varepsilon^{\tau(q)}$, $\varepsilon \to 0$, where

$$Z_\varepsilon(q) = \sum_i p_{\varepsilon,i}^q \sim \sum_i \varepsilon^{-q\alpha_i} \tag{2}$$

is the *partition function* associated with the partition X of μ (the sum above runs over all the boxes of the partition with $p_{\varepsilon,i} \neq 0$ since q can be negative). The calculation of $\tau(q)$ parallels the calculation of free energies in statistical mechanics in that, if $f(\alpha)$ is known, then $\tau(q)$ can be calculated as the *Legendre-Fenchel* (LF) *transform* of $f(\alpha)$ [2]; in symbols,

$$\tau(q) = \inf_{\alpha\in\mathbb{R}} \{q\alpha - f(\alpha)\}. \tag{3}$$

The result that we shall study in this paper is the inverse result, namely that if $\tau(q)$ is known, then $f(\alpha)$ can be calculated from $\tau(q)$ by taking the LF transform of the latter function; in symbols,

$$f(\alpha) = \inf_{q\in\mathbb{R}} \{q\alpha - \tau(q)\}. \tag{4}$$

This result first appeared in [4, 5], and has been used extensively since then to calculate the multifractal spectrum of many phenomena, including turbulence [6, 7, 8, 9, 10, 11], geophysical processes, such as cloud formation and rain precipitations [12, 13, 14], and fluctuations in financial time series [3, 15], among many others [16]. Unfortunately, there is one aspect of Eq.(4) which is often overlooked when deriving it and applying it, namely that *it can only produce concave multifractal spectra*, since LF transforms can only yield concave functions. This basic property of LF transforms does not affect, as such, the calculation of $\tau(q)$ from $f(\alpha)$ because it can be proved

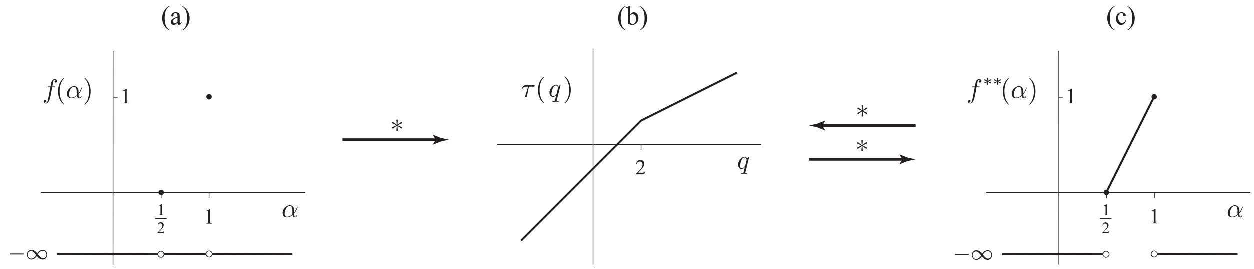

FIG. 1: (a) Multifractal spectrum $f(\alpha)$ for the invariant density of the Ulam map. (b) Corresponding free energy function $\tau(q)$. (c) Legendre-Fenchel transform of $\tau(q)$.

that $\tau(q)$ is an always concave function of q. For calculating the multifractal spectrum, however, there is a problem because $f(\alpha)$ need not be concave, which means that $f(\alpha)$ cannot always be calculated as the LF transform of $\tau(q)$.

Our goal here is to illustrate these observations with a number of basic examples, and to state the precise conditions, based on convex analysis, that ensure that $f(\alpha)$ can be calculated as the LF transform of $\tau(q)$. These conditions will be discussed in the context of two physically-relevant multifractal models: one related to turbulence and another related to diffusion-limited aggregates. In an attempt to offer a workable solution to the problem of calculating nonconcave multifractal spectra, we shall also study a recently generalized canonical ensemble to show that nonconcave spectra can be obtained from a modified version of the LF transform. This part will actually provide an explicit calculation of a nonconcave spectrum $f(\alpha)$ which uses this modified LF transform. We shall briefly comment finally, in the concluding section of the paper, on analogies between nonconcave multifractal spectra and nonconcave entropies in statistical mechanics, large deviation theory, and the thermodynamic formalism of dynamical systems.

II. TWO SIMPLE EXAMPLES

We begin by considering two explicit examples of measures whose multifractal spectra are not given by LF transforms of their free energy functions. The first example was previously discussed in [17] (see also [2]), and will serve here as a starting point to our discussion of the validity of the LF transform of (4). The measure or, rather, the density in this case that we consider is given specifically by

$$\rho(x) = \frac{1}{\pi\sqrt{1-x^2}}, \tag{5}$$

where $x \in [-1,1]$. This density arises as the invariant density of the Ulam map and the Tchebyscheff maps. Applying a partition of size ε on the interval $[-1,1]$, it can be seen that the two boxes of the partition located near the boundary points $x = \pm 1$ have measure $p_{\varepsilon,i} = \varepsilon\rho(x) \sim \varepsilon^{1/2}$, so that $f(\alpha) = 0$ at $\alpha = 1/2$. All the other boxes have measure $p_{\varepsilon,i} \sim \varepsilon$, so that $f(\alpha) = 1$ at $\alpha = 1$, as there are approximately $n_\varepsilon(\alpha) \sim \varepsilon^{-1}$ of these boxes. Combining the two results, and setting $n_\varepsilon(\alpha) = 0$ for $\alpha \notin \{1/2, 1\}$, we obtain

$$f(\alpha) = \begin{cases} 0 & \alpha = 1/2 \\ 1 & \alpha = 1 \\ -\infty & \text{otherwise.} \end{cases} \tag{6}$$

This spectrum is shown in Fig. 1(a). At this point, we go on to prove that $f(\alpha)$ cannot be expressed as the LF transform of $\tau(q)$ by direct calculation. Starting from the asymptotic ($\varepsilon \to 0$) expression of the partition function

$$Z_\varepsilon(q) = \sum_i p_{\varepsilon,i}^q \sim \varepsilon^{q/2} + \varepsilon^{-1}\varepsilon^q, \tag{7}$$

we first find

$$\tau(q) = \min\{q-1, q/2\} = \begin{cases} q/2 & q > 2 \\ q-1 & q \le 2. \end{cases} \tag{8}$$

Then keeping track of the two separate regions $q > 2$ and $q \le 2$, we find

$$\begin{aligned} \inf_{q\in\mathbb{R}}\{q\alpha - \tau(q)\} &= \inf_{q\in\mathbb{R}} \left\{ \begin{array}{ll} q(\alpha - \frac{1}{2}) & q > 2 \\ q(\alpha-1)+1 & q \le 2 \end{array} \right\} \\ &= \begin{cases} 2\alpha - 1 & \alpha \in [1/2, 1] \\ -\infty & \text{otherwise.} \end{cases} \end{aligned} \tag{9}$$

Comparing this result with Eq.(6), we thus see $f(\alpha)$ corresponds to the LF transform of $\tau(q)$ for $\alpha \notin (1/2, 1)$, but differs from it for all other values of α; see Figs. 1(a) and 1(c).

This example can be generalized to illustrate an even more drastic result about $f(\alpha)$ and $\tau(q)$. Consider a dynamical system in d-dimensions whose invariant density is everywhere finite, so that $p_{i,\varepsilon} \sim \varepsilon^d$, except at a finite number k of singular points where $p_{i,\varepsilon} \sim \varepsilon^{\alpha_i} = \varepsilon^{d\xi_i}$ with $\xi_1, \xi_2, \ldots, \xi_k < 1$. The partition function for this density is

$$Z_\varepsilon(q) = \sum_i p_i^q \sim \varepsilon^{-d}\varepsilon^{dq} + \varepsilon^{d\xi_1 q} + \varepsilon^{d\xi_2 q} + \cdots + \varepsilon^{d\xi_k q}, \tag{10}$$

so that

$$\tau(q) = \min\{(q-1)d, d\xi_1 q, d\xi_2 q, \ldots, d\xi_k q\}. \tag{11}$$

The minimum can be calculated explicitly and yields

$$\tau(q) = \begin{cases} d(q-1) & q \leq (1-\xi^*)^{-1} \\ d\xi^* q & q \geq (1-\xi^*)^{-1}, \end{cases} \tag{12}$$

where $\xi^* = \min_i \xi_i$. We see here that the function $\tau(q)$ "overlooks" all the singularities ξ_i, except for the smallest one, and, so, any perturbation of the singularities ξ_i which keeps ξ^* invariant will change $f(\alpha)$ but not $\tau(q)$. In this case, the mapping of $\tau(q)$ to $f(\alpha)$ must be indeterminate, since there is an infinite number of spectra associated with the same free energy.

III. THEORY OF LF TRANSFORMS

The results of the two previous examples are very simple and show at once that $f(\alpha)$ cannot in general be expressed as the LF transform of $\tau(q)$, contrary to what is claimed in most if not all references on the subject. The problem, as was mentioned, is that LF transforms can only yield concave functions, which means that these transforms cannot be used to calculate nonconcave multifractal spectra, including those of the two examples considered before. To make this observation more rigorous, we introduce in this section a few concepts and results of convex analysis [18], beginning with the concept of supporting lines.

A. Supporting lines

We say that a function $f : \mathbb{R} \to \mathbb{R}$ admits a supporting line at α if there exists a constant η such that

$$f(\beta) \leq f(\alpha) + \eta(\beta - \alpha) \tag{13}$$

for all $\beta \in \mathbb{R}$. This requirement means basically that we can draw a line on top of the graph of $f(\alpha)$ which does not go under that graph; see Fig. 2. With this picture in mind, it is easily seen that, if f admits a supporting line at α and is differentiable at α, then the slope η of the supporting line must be such that $f'(\alpha) = \eta$.

The importance of supporting lines comes from their association with LF transforms, and from the fact, more precisely, that they determine whether such transforms are *involutive*, that is, whether they are their own inverse. In the context of $f(\alpha)$ and $\tau(q)$, this means precisely the following. First, we recall that $\tau(q)$ can always be expressed as the LF transform of $f(\alpha)$, so Eq.(3) is always valid independently of the shape of $f(\alpha)$. This follows essentially from the fact that $\tau(q)$ is an always concave function of q [2]. The inverse transform shown in (4), however, is not generally valid, and this is where supporting lines become important. On the one hand, if f admits a supporting line at α, then f at α can expressed as the LF transform of $\tau(q)$ as in Eq.(4). In this case, we say that f is *concave* at α. On the other hand, if f does not admit a supporting line at α, then f at α does not equal the LF transform of $\tau(q)$. In this case, we say that f is *nonconcave* at α. These two complementary results are usually rephrased in convex analysis by defining the function

$$f^{**}(\alpha) = \inf_{q\in\mathbb{R}}\{q\alpha - \tau(q)\}. \tag{14}$$

In terms of $f^{**}(\alpha)$, we then have that $f(\alpha) = f^{**}(\alpha)$ *if and only if f admits a supporting line at α* [18].

For the remaining, it is useful to note that $f^{**}(\alpha)$ corresponds in general to the smallest concave function satisfying $f(\alpha) \leq f^{**}(\alpha)$ for all $\alpha \in \mathbb{R}$. For this reason, $f^{**}(\alpha)$ is called the *concave envelope* or *concave hull* of $f(\alpha)$. This implies, in particular, that if $f(\alpha)$ admits no supporting lines over some open interval, say (α_l, α_h) as in Fig. 2, then $f^{**}(\alpha)$ must be *affine* over that interval, by which we mean that $f^{**}(\alpha)$ has a constant slope over that interval. This last property, which is related to the Maxwell construction [19, 20], is illustrated in Fig. 2.

All of the properties of $f(\alpha)$ and $f^{**}(\alpha)$ in relation to LF transforms can be verified for the two examples considered previously. In the case of the invariant density of the Ulam map, for example, the concave hull of $f(\alpha)$ is the function displayed in (9); it is obviously such that $f(\alpha) \leq f^{**}(\alpha)$ and is concave contrary to $f(\alpha)$. Moreover, it is easily verified from Fig. 1 that the two points $\alpha = 1/2$ and $\alpha = 1$ admit a supporting line, which explains why $f(\alpha) = f^{**}(\alpha)$ there. These two points admit in fact an infinite number of supporting lines. For the point $\alpha = 1/2$, for example, all lines attached to $(1/2, 0)$ with slope in the interval $[2, \infty)$ are supporting in the sense of (13). For $\alpha = 1$, the supporting lines have slopes in the interval $(-\infty, 2]$.

B. Complete relationships

We pursue our analysis of $f(\alpha)$ and $\tau(q)$ by calling attention to the fact that [18]

$$\tau(q) = \inf_{\alpha\in\mathbb{R}}\{q\alpha - f^{**}(\alpha)\}. \tag{15}$$

Therefore, $\tau(q)$ is not only the LF transform of $f(\alpha)$, as stated in Eq.(3), but also the LF transform of $f^{**}(\alpha)$. This result is general: it holds for any function $f(\alpha)$ and its concave envelope $f^{**}(\alpha)$ defined as in Eq.(14) as the double LF transform of $f(\alpha)$ or more compactly:

$$f^{**} = \tau^* = (f^*)^*, \tag{16}$$

where the star stands for the LF transformation. To summarize, we then have $\tau = f^*$, $\tau^* = (f^*)^* = f^{**}$ and $(\tau^*)^* = (f^{**})^* = f^* = \tau$. This chain of equalities can be expressed in a more transparent way using the following

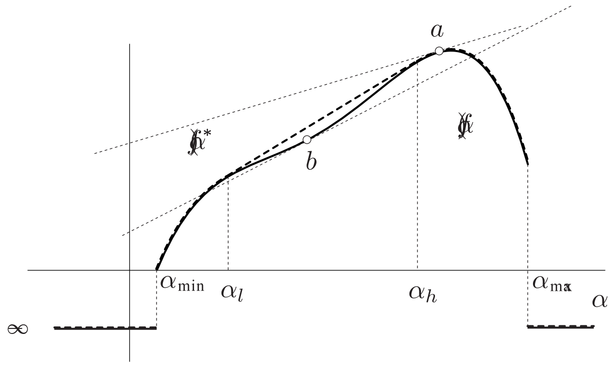

FIG. 2: (a) A generic nonconcave multifractal spectrum $f(\alpha)$ (full line) together with its concave envelope $f^{**}(\alpha)$ (dashed line). The two functions coincide outside the open interval (α_l, α_h). The point a of the multifractal spectrum admits a supporting line (concave point), while the point b does not (nonconcave point).

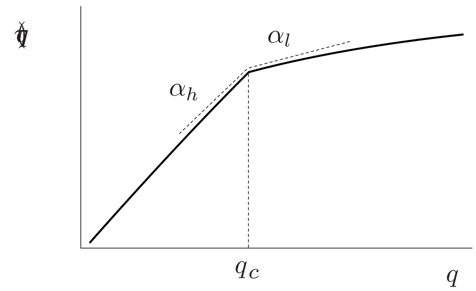

FIG. 3: Free energy function $\tau(q)$ associated with the multifractal spectrum $f(\alpha)$ shown in Figure 2. The LF transform of the concave envelope $f^{**}(\alpha)$ of $f(\alpha)$ yields the same free energy function.

diagram:

$$f(\alpha) \xrightarrow{*} \tau(q) \overset{*}{\rightleftharpoons} f^{**}(\alpha), \tag{17}$$

which makes obvious the fact that there may be more than one spectrum related the same free energy. In fact, all $f(\alpha)$ having the same concave envelope lead to the same $\tau(q)$, as can be verified in the second example considered before. Finally, note that the chain of equalities reduces to $\tau = f^*$ and $\tau^* = f$, or equivalently to

$$\tau(q) \overset{*}{\rightleftharpoons} f(\alpha), \tag{18}$$

when $f(\alpha) = f^{**}(\alpha)$ for all $\alpha \in \mathbb{R}$, that is, when $f(\alpha)$ is everywhere concave.

C. Involutive LF transforms

Having listed all the relationships that exist between $f(\alpha)$, $\tau(q)$ and $f^{**}(\alpha)$, we can now fully address the main issue of this paper, which is to determine when $f(\alpha)$ can safely and completely be calculated as the LF transform of $\tau(q)$. From the chain of equalities and diagrams shown above, this amounts to determine when the LF transform is involutive; that is to say, under which conditions does the diagram (17) reduce to the diagram of (18)?

A first obvious answer to this question is given by recalling what we have just mentioned about the diagram of (18), namely that *if $f(\alpha)$ is everywhere concave, then the multifractal spectra $f(\alpha)$ can completely be calculated as the LF transform of the free energy function $\tau(q)$.* As such, this answer is complete but not very practical because it is based on $f(\alpha)$, and so presupposes that we know $f(\alpha)$. A more useful criterion can be stated from the point of view of $\tau(q)$ alone by using a well-known result of convex analysis which connects nonconcave or affine regions of $f(\alpha)$ with nondifferentiable points of $\tau(q)$. The result goes as follows: suppose that $f(\alpha)$ is nonconcave over some open interval, say (α_l, α_h) as in Fig. 2, or that $f(\alpha)$ is concave but affine over (α_l, α_h). Then $\tau(q)$ is nondifferentiable at some critical value q_c corresponding to the slope of $f^{**}(\alpha)$ over the interval (α_l, α_h). Moreover, the left- and right-derivatives of $\tau(q)$ at q_c equal α_h and α_l, respectively; see Fig. 3.

From this result, we arrive at our criterion by taking the contrapositive: if $\tau(q)$ is everywhere differentiable, then $f(\alpha)$ is concave everywhere with no affine parts. Thus, from the point of view of $\tau(q)$, $f(\alpha)$ *can completely be calculated as the LF transform of $\tau(q)$ if the latter function is everywhere differentiable.* Taking the view that nondifferentiable points of $\tau(q)$ signal the onset of first-order phase transitions for multifractals [21, 22, 23, 24, 25], this is equivalent to saying that $f(\alpha)$ *can completely be calculated as the LF transform of $\tau(q)$ in the absence of first-order phase transitions.* If there is a first-order phase transition, then either $f(\alpha)$ is nonconcave somewhere, in which case $f \neq \tau^*$, or else $f(\alpha)$ is affine somewhere, in which case $f = \tau^*$. Unfortunately, as there is no way to distinguish the two cases from the sole knowledge of $\tau(q)$ (see Figs. 2 and 3), one must resort to calculate $f(\alpha)$ by means which do not rely on $\tau(q)$.

IV. APPLICATION TO PHYSICAL SYSTEMS

Let us now consider examples of multifractals that are of physical relevance.

Our first example is fully developed hydrodynamic turbulence, as described by multifractal turbulence models [4, 7]. The basic idea is that, in the turbulent flow, velocity increments $\delta v(l) = |v(x+l) - v(x)|$ at a given distance l scale with local exponents h, which are distributed on a fractal set with fractal dimension $D(h)$. This notation is taken from Benzi *et al.* [7], and can be translated to our notation using the following identifications:

$$\begin{aligned} h &= \alpha \\ l &= \varepsilon \\ 3 - D(h) &= -f(\alpha) \end{aligned}$$

$$\begin{aligned} p &= q \\ \zeta_p &= \tau(q). \end{aligned} \tag{19}$$

Here ζ_p denote the scaling exponents of moments of velocity increments in the inertial range,

$$\langle(\delta v)^p\rangle \sim l^{\zeta_p}. \tag{20}$$

In multifractal turbulence models, the probability to observe a local exponent h is given by

$$P_l(h) \sim l^{3-D(h)}, \tag{21}$$

which is equivalent to our notation $n_\varepsilon(\alpha) \sim \varepsilon^{-f(\alpha)}$. Moreover, for the scaling exponents p one has

$$\zeta_p = \min_h\{hp + 3 - D(h)\}, \tag{22}$$

which is equivalent to the LF transform of Eq.(3). In practice, one extracts $D(h)$ from the scaling exponents ζ_p, which can be measured in experiments. In our notation, this means that one determines $f(\alpha)$ by the LF transform of the experimentally measured $\tau(q)$. All our arguments of the previous sections apply.

We notice that multifractal turbulence models in their current form can only deal with the convex hull of the spectrum of singularities. The true $f(\alpha)$ spectrum of a turbulent flow is fully determined by the underlying dynamics, the Navier-Stokes equation. There is a priori no reason why this spectrum should be a concave function. Our arguments of the previous section now allow for an experimental check of such anomalous behaviour: a necessary condition for a nonconcave spectrum of singularities generated by the Navier-Stokes equation would be a phase transition point of $\tau(q)$, that is, the scaling exponents ζ_p should be a nondifferentiable function of p at some critical point p_c.

The exponents ζ_p have been measured in many experiments; see, e.g., [8, 9]. Within the experimental uncertainties, they are usually described by a smooth function of p, although one cannot fully exclude the existence of phase transitions (see, e.g., the data in [8] and [9], which show a relatively strong change of slope near $p = 3$). If the existence of such transitions were confirmed, then one would have to check that the underlying spectrum $D(h)$ is either nonconcave or affine somewhere.

Our second example of physical relevance are multifractals as generated by diffusion-limited aggregates (DLA) [26, 27]. Jensen *et al.* [27] provide convincing evidence that the function $\tau(q)$ calculated for the harmonic measure of their DLA cluster exhibits a first-order phase transition at $q = -0.23 \pm 0.05$ (see their Fig. 3). From this result, all that can be said about their $f(\alpha)$ spectrum obtained by LF-transforming $\tau(q)$ (shown in their Fig. 4) is that it is the concave hull $f^{**}(\alpha)$ of the true $f(\alpha)$ spectrum. Note that the spectrum displayed in Fig. 4 of [27] does show an affine part, so it is consistent with the fact that $\tau(q)$ has a nondifferentiable point. However, there is a priori no reason why DLA clusters should possess a concave spectrum of singularities, so that the part where $f(\alpha)$ is seen to be affine could just as well be nonconcave. Therefore, at this point, one may conclude that the true $f(\alpha)$ spectrum of the DLA cluster studied by Jensen *et al.* is as yet unknown.

One last comment may be in order. Although Jensen *et al.* provide evidence to the effect that $\tau(q)$ possesses a nondifferentiable point, the $\tau(q)$ which is calculated in practice is actually always analytic if one deals with finite-size DLA clusters. The spectrum $f^{**}(\alpha)$ which is calculated from $\tau(q)$ is, in this case, necessarily concave and has no affine parts. The nondifferentiable point of $\tau(q)$ and the concomitant affine part of $f^{**}(\alpha)$ appear, formally speaking, only in the "thermodynamic" limit of infinitely large clusters.

V. GENERALIZED FREE ENERGY FUNCTIONS

We now describe and illustrate a method for obtaining nonconcave multifractal spectra from the calculation of a generalized form of the partition function. The method has been proposed recently in [28, 29] in the context of nonconcave microcanonical entropies, and will be illustrated here in the context of the first example considered in Section II. The basic idea of the method is to consider a generalization of the partition function given by

$$Z_\varepsilon(q, g) = \sum_i \varepsilon^{q\alpha_i + g(\alpha_i)}, \tag{23}$$

where α_i represents the local fractal exponent associated with the probability $p_{\varepsilon,i}$, and g is an arbitrary smooth function. This new form generalizes the standard canonical partition function, in the sense that

$$Z_\varepsilon(q, g = 0) = Z_\varepsilon(q) = \sum_i \varepsilon^{q\alpha_i}. \tag{24}$$

For definiteness, we shall adopt the choice $g(\alpha) = \gamma\alpha^2$ with $\gamma \in \mathbb{R}$. Therefore, the generalized partition function that we consider is

$$Z_\varepsilon(q, \gamma) = \sum_i \varepsilon^{q\alpha_i + \gamma\alpha_i^2}. \tag{25}$$

We call this partition function the *Gaussian partition function*; it corresponding free energy function

$$\tau(q, \gamma) = \lim_{\varepsilon\to 0} \frac{\ln Z_\varepsilon(q, \gamma)}{\ln \varepsilon} \tag{26}$$

is called the *Gaussian free energy.* Note that this new free energy is a function of two real parameters, q and γ, and that $\tau(q, \gamma = 0) = \tau(q)$.

The rationale for generalizing the standard free energy function $\tau(q)$ to $\tau(q, \gamma)$ is that it modifies the structure of the LF transform which connects $\tau(q)$ with $f(\alpha)$, and thus modifies the conditions which ensure that $f(\alpha)$ can be written as the LF transform of a free energy function. We spare the reader with the details of this modification which can be found in [28, 29]. For our purpose, we shall only note the generalized versions of the LF transforms that connect $\tau(q,\gamma)$ and $f(\alpha)$; they are given by

$$\tau(q,\gamma) = \inf_{\alpha}\{q\alpha + \gamma\alpha^2 - f(\alpha)\} \tag{27}$$

and

$$f(\alpha) = \inf_{q,\gamma}\{q\alpha + \gamma\alpha^2 - \tau(q,\gamma)\}. \tag{28}$$

The first LF transform holds, like its standard version ($\gamma = 0$), for any spectrum $f(\alpha)$, be it concave or not. The surprising virtue of the second LF transform is that it also holds true for *any* $f(\alpha)$, contrary to the standard version ($\gamma = 0$) which applies only when $f(\alpha)$ is concave. Rather than proving this result, we shall verify that it is valid for the nonconcave multifractal spectrum shown in Fig. 1(a). That is, we shall obtain that nonconcave spectrum by inverting, in the manner of Eq.(28), its associated Gaussian free energy $\tau(q,\gamma)$.

First, we calculate $\tau(q,\gamma)$ starting from $Z_\varepsilon(q,\gamma)$:

$$Z_\varepsilon(q,\gamma) = \sum_i \varepsilon^{q\alpha_i+\gamma\alpha_i^2} \sim \varepsilon^{q/2+\gamma/4} + \varepsilon^{-1}\varepsilon^{q+\gamma}. \tag{29}$$

Taking the limit $\varepsilon \to 0$ yields

$$\tau(q,\gamma) = \min\{q/2+\gamma/4, q+\gamma-1\}. \tag{30}$$

The solution of the minimum can be found explicitly; it has the form

$$\tau(q,\gamma) = \begin{cases} q/2+\gamma/4 & q \geq q_\gamma \\ q+\gamma-1 & q < q_\gamma, \end{cases} \tag{31}$$

where $q_\gamma = -3\gamma/2 + 2$. Next, we apply formula (28) using this solution for $\tau(q,\gamma)$. This leads us to solving the following variational problem:

$$I = \inf_{q,\gamma}\left\{ \begin{array}{ll} q\alpha+\gamma\alpha^2 - q/2 - \gamma/4 & q \geq q_\gamma \\ q\alpha+\gamma\alpha^2 - q - \gamma + 1 & q < q_\gamma \end{array} \right\}. \tag{32}$$

Grouping the variables together, this is equivalent to

$$I = \inf_{q,\gamma}\left\{ \begin{array}{ll} q(\alpha-1/2)+\gamma(\alpha^2-1/4) & q \geq q_\gamma \\ q(\alpha-1)+\gamma(\alpha^2-1)+1 & q < q_\gamma \end{array} \right\}. \tag{33}$$

Let $f_1(\alpha,q,\gamma)$ denote the top expression in the brackets and $f_2(\alpha,q,\gamma)$ the lower one. With this notation, it can be noted that, for $\alpha = 1/2$,

$$f_2(1/2,q,\gamma) > f_1(1/2,q,\gamma) = 0 \tag{34}$$

for all $q < q_\gamma$ and $\gamma \in \mathbb{R}$. Therefore,

$$\inf_{q<q_\gamma,\gamma} f_2(\alpha,q,\gamma) = f_1 = 0, \tag{35}$$

and $I = 0$ at $\alpha = 1/2$. Similarly, for $\alpha = 1$, we have

$$f_1(1,q,\gamma) \geq f_2(1,q,\gamma) = 1 \tag{36}$$

for all $q \geq q_\gamma$ and $\gamma \in \mathbb{R}$, so that $I = f_2 = 1$ at $\alpha = 1$. For all other values of α, it is possible to set q and γ in such a way that $I = -\infty$. Overall, we thus obtain

$$I = \begin{cases} 0 & \alpha = 1/2 \\ 1 & \alpha = 1 \\ -\infty & \text{otherwise}, \end{cases} \tag{37}$$

which is the precise expression of the nonconcave spectrum $f(\alpha)$ of Eq.(6). Accordingly, we have shown that this nonconcave spectrum can be expressed as in Eq.(28) as a modified LF transform of a generalized free energy. We refer the reader again to [28, 29] for more details on this way of calculating nonconcave functions, and on the generality of the method.

VI. CONCLUSION

In summary, we have shown that one must be careful when calculating the singularity spectrum of multifractals as the LF transform of its corresponding free energy, since LF transforms can only yield concave functions. This word of caution has implications for all studies published so far on multifractals, including those on multifractal models of turbulence, as every one of them has taken for granted that the multifractal spectrum is the LF transform of the free energy no matter what the spectrum looks like. This, as we have shown, is only true if the spectrum is concave; if it is nonconcave, then one must resort to calculate it directly from its combinatorial definition. Another possibility is to use a generalization of the canonical ensemble which can be used to extract nonconcave entropies from a generalized version of the free energy function. This way of doing was sketched here in the context of a simple example of nonconcave multifractal spectrum, and is presented in more details in [28, 29].

In closing, we note that all the results mentioned in this paper apply verbatim to other fields of investigation where LF transforms are at play. In statistical mechanics, for example, the LF transform which connects the entropy function of the microcanonical ensemble with the free energy function of the canonical ensemble becomes noninvolutive when the entropy is nonconcave. When this happens, we say that there is nonequivalence of ensembles [30, 31], since one is then unable to obtain the true entropy function of the microcanonical ensemble solely from the knowledge of the free energy of the canonical ensemble. The notion of generalized canonical ensemble has been developed precisely in this context. Similarly, in large deviation theory, it has been known for some time that nonconvex rate functions, which are functions analogous to entropies, cannot be calculated by means of LF transforms of functions analogous to free energy functions [32, 33, 34].

From these analogies, it is but a small step finally to conjecture that nonconcave entropies should also show up in the thermodynamic formalism of dynamical systems

[2, 35]. First-order phase transitions have in fact already been studied in this formalism at the level of an entropy-like quantity referred to as the spectrum of dynamical indices [2]. These typically occur for nonhyperbolic dynamical systems. Therefore, one can only be careful not to assume that the corresponding spectra of dynamical indices can always be expressed as LF transforms of their corresponding free energies or pressure functions, as they are known in this context.

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