Structure factor of Cantor sets

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We write down an infinite-product expression for the structure factor $S(k)$ of a one-parameter family of Cantor sets. From this expression, we find the positions of the zeros and approximate expressions for the positions of the maxima of $S(k)$. Mellin transforms and two averaging methods are used to determine aspects of the asymptotic behavior of $S(k)$ for large k. Two distinct power laws are obtained, depending on the averaging method utilized.

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I. INTRODUCTION

Small-angle scattering is a valuable experimental tool for estimating the dimension of fractal structures (Ref. [1], and references therein), based on the mathematical properties of Fourier transforms, which preserve scale invariance and self-similarity to some degree. In particular, it is shown heuristically in Ref. [1] that a distribution for which the mass within a radius scales as

$$M \sim R^d \; , \tag{1}$$

where d is a dimension, results in a structure factor which scales as

$$S(k) \sim k^{-d} \; . \tag{2}$$

More complicated relations arise when the distribution is bounded by a fractal of a differing dimension [2], or when the distribution is multifractal [3]. An experimental determination of the multifractal distribution requires a more complicated setup, to perform an analog optical-wavelet transform.

For exactly self-similar distributions and distributions with self-similar boundaries it is possible to find analytic expressions for the Fourier transform in terms of products of sums of exponentials or cosines [4–7]. One result of these investigations is that, for various subclasses of the self-similar mass and surface fractals, the structure factor $S(k)$ does not tend to zero in the limit of large k. That is, there are peaks of a fixed nonzero intensity for arbitrarily large k.

This paper addresses the question of how to interpret Eq. (2) in the light of these results, and discusses different approaches to the problem of elucidating the asymptotic structure of $S(k)$, viewed as an analytic function, for a uniform distribution on a Cantor set.

In Sec. II we derive the analytic expression for the Fourier transform, and use it to find the positions and orders of the zeros, and approximate positions and magnitudes of the maxima. In Sec. III we use a geometric mean and a Mellin transform technique to arrive at the estimate

$$S(k) \sim k^{-2d} \; , \tag{3}$$

and use a more direct integral technique which gives the same result as Eq. (2).

II. EXACT RESULTS, ZEROS, AND MAXIMA

A. Evaluation of the Fourier transform

Consider the Cantor sets C_a for $a \geq 2$ defined as the bounded closed nonempty sets of real numbers satisfying

$$C_a = S_a^{(1)}(C_a) \cup S_a^{(2)}(C_a) \; , \tag{4}$$

where

$$S_a^{(1)}(x) = \frac{2x-(a-1)}{2a} \; , \tag{5}$$

$$S_a^{(2)}(x) = \frac{2x+(a-1)}{2a} \tag{6}$$

are similarity transformations. Each of these sets is depicted as a horizontal slice of Fig. 1. C_2 is simply the interval $[-1/2, 1/2]$, while C_∞ consists of two points at $-1/2$ and $1/2$. C_3 is the "middle third" Cantor set, obtained by taking the interval C_2 and successively removing the middle third of any intervals remaining. C_3 is often used as a prototype fractal — it is easy to visualize

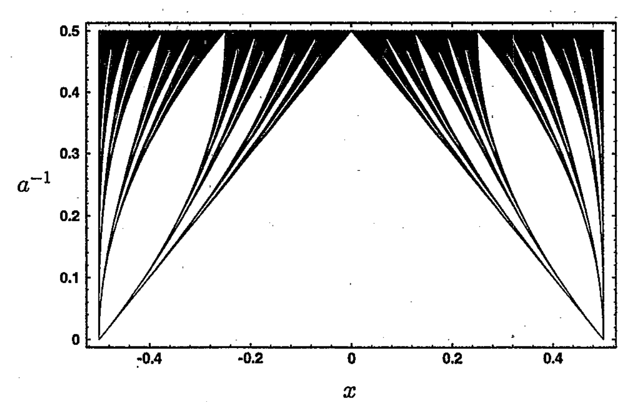

FIG. 1. The Cantor sets C_a given as a function of a^{-1}. See Eqs. (4)–(6).

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and define, and has many of the properties of fractals with more elaborate definitions.

The Hausdorff dimension of C_a is [8]

$$d_H(C_a) = \frac{\ln 2}{\ln a} \ . \tag{7}$$

A uniform mass distribution on C_a, μ_a is defined as d_H- dimensional Hausdorff measure restricted to C_a, and normalized to unity:

$$\int d\mu_a = 1 \ . \tag{8}$$

The self-similarity of C_a leads to the relation

$$\int f(x) d\mu_a(x) = \frac{1}{2}\left[\int f(S_a^{(1)}(x)) d\mu_a(x) + \int f(S_a^{(2)}(x)) d\mu_a(x)\right] \tag{9}$$

for any function f, which, together with Eq. (8), is sufficient to determine all the properties of μ_a that we will need.

The Fourier transform of the distribution is defined as

$$C_a(k) = \int e^{ikx} d\mu_a(x) \ . \tag{10}$$

Substituting this into Eqs. (8) and (9) gives

$$C_a(0) = 1 \ , \tag{11}$$

$$C_a(k) = \cos[k(a-1)/(2a)] C_a(k/a) \ , \tag{12}$$

from which it follows that

$$C_a(k) = \prod_{j=1}^{\infty} \cos[k(a-1)/(2a^j)] \ . \tag{13}$$

The structure factor $S_a(k)$ is given by

$$S_a(k) = C_a(k)^2 \ . \tag{14}$$

The infinite product converges uniformly over any bounded set of complex k, thus $C_a(k)$ and $S_a(k)$ are entire functions. The invariance of the distribution under the transformation $x \to -x$ ensures that $C_a(k)$ is a real function, as shown in Eq. (13). We have evaluated the infinite product numerically, leading to Fig. 2, which illustrates many of the results of this section.

If a is an integer, there is another exact relation involving $C_a(k)$, derivable from Eq. (13), which is particularly useful in describing its behavior for large k:

$$C_a(k + 2a^l m\pi/(a-1)) = (-1)^{m(a^l-1)/(a-1)} C_a(k) \times \frac{C_a(2m\pi/(a-1) + a^{-l}k)}{C_a(a^{-l}k)} \ , \tag{15}$$

where m is any integer, and l is any positive integer. This result often takes a simple form for particular values of the variables, for example, if $a = 3$, $k = 0$, and $m = 1$ it reduces to

$$C_3(3^l\pi) = (-1)^l C_3(\pi) \ . \tag{16}$$

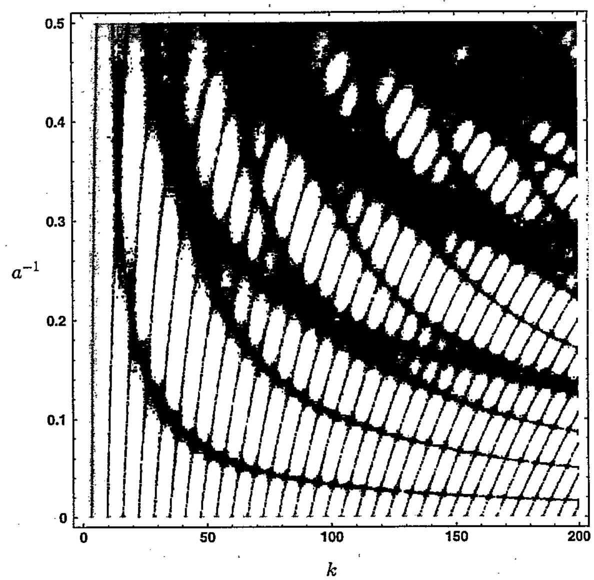

FIG. 2. A plot of $S_a(k)$. White corresponds to a value of 1, while dark corresponds to small values. The intensity is approximately linear in the logarithm of $S_a(k)$. Note the extreme values $a = 2$ and $a = \infty$ for which there are explicit expressions for $S_a(k)$, given in Eqs. (17) and (18). The multiple zeros occurring at odd integral a are clearly visible.

At the extreme values $a = 2$ and $a = \infty$ the Fourier transform of the uniform distribution on C_a is well known to be

$$C_2(k) = \frac{\sin(k/2)}{k/2} \ , \tag{17}$$

$$C_\infty(k) = \cos(k/2) \ . \tag{18}$$

These expressions are also easily obtained from Eq. (13) using Eq. 1.439.1 of Ref. [9].

B. Zeros and connections with number theoretic functions

Substituting the infinite-product expression for the cosine function, found in Eq. 1.431.3 of Ref. [9], into Eq. (13) we obtain

$$C_a(k) = \prod_{j=1}^{\infty} \prod_{m=0}^{\infty} \left[1 - \frac{k^2(a-1)^2}{(2m+1)^2\pi^2 a^{2j}}\right] \ . \tag{19}$$

This representation makes the positions of the zeros explicit. If a is irrational, or is rational with an even numerator, the positions of the zeros corresponding to different j and m never coincide; all the zeros are simple. On the other hand, if a is rational with an odd numerator, there exist zeros of arbitrarily large order. In the particular case of a equal to an odd prime p, the product over j in Eq. (19) may be regrouped to obtain

$$C_p(k) = \prod_{m=0}^{\infty} \left[1 - \frac{k^2(p-1)^2}{(2m+1)^2\pi^2}\right]^{\alpha_p(2m+1)} , \quad (20)$$

where $\alpha_p(n)$ is the exponent of p in the prime decomposition of n. In this case, and also when $a = 2$, the zeros are evenly spaced. $C_a(k)$ is also related to the Riemann ζ function, as demonstrated in the section dealing with Mellin transforms.

C. Maxima

It is quite easy to show by differentiating Eq. (13) that the points at which $S_a'(k) = 0$ are either zeros of $S_a(k)$ or points for which $S_a''(k) < 0$. This implies that there is exactly one maximum of $S_a(k)$ between each of its zeros, because it is bounded and differentiable for all values of k. We assume here that k is real.

Apart from the trivial case at $k = 0$ the first few maxima must be determined numerically. If a is an integer, Eq. (15) may be used to find the position of many maxima in terms of those for small k to a high degree of accuracy. Differentiating Eq. (15) we find the condition under which $S_a(k + a^l 2\pi m/(a-1))$ is a maximum:

$$F_a(k) \equiv f_a(k) + a^{-l}\left[f_a\left(\frac{2\pi m}{a-1} + a^{-l}k\right) - f_a(a^{-l}k)\right] = 0 , \quad (21)$$

where

$$f_a(k) = -\frac{C_a'(k)}{C_a(k)} = \sum_{j=1}^{\infty} \frac{a-1}{2a^j} \tan\left(\frac{k(a-1)}{2a^j}\right) . \quad (22)$$

If l is large and f is well behaved near $2\pi m/(a-1)$, which is true unless one or more of the terms in the sum is close to a singularity of the tan function, a reasonable approximate solution to the equation is $k = k_0$, where k_0 is the position of a maximum, so that

$$f_a(k_0) = 0 . \quad (23)$$

A closer approximation is found using Newton's method, using k_0 as the initial value. f_a and its derivatives are calculated using Taylor series. The result after two iterations is

$$\begin{aligned} k = k_0 &- a^{-l}\frac{f_a(2\pi m/(a-1))}{f_a'(k_0)} \\ &- a^{-2l}\left\{\frac{f_a(2\pi m/(a-1))^2 f_a''(k_0)}{2f_a'(k_0)^3} \right. \\ &\left. + \frac{k_0}{f_a'(k_0)}[f_a'(2\pi m/(a-1)) - f_a'(0)]\right\} \\ &+ O(a^{-3l}) . \end{aligned} \quad (24)$$

If $k_0 = 0$, that is, we are looking for the maximum near $a^l 2\pi m/(a-1)$, the term of order a^{-2l} is exactly zero, and the result is

$$\begin{aligned} k = &-a^{-l}\frac{f_a(2\pi m/(a-1))}{f_a'(0)} \\ &- \frac{a^{-3l}}{f_a'(0)^4}\{f_a(2\pi m/(a-1))^3 f_a'''(0) + f_a'(0)^2 f_a(2\pi m/(a-1))[f_a'(2\pi m/(a-1)) - f_a'(0)]\} + O(a^{-5l}) . \end{aligned} \quad (25)$$

In these expressions the derivatives of $f_a(k)$ evaluated at $k = 0$ may be calculated explicitly using Eq. (22), giving

$$f_a'(0) = \frac{(a-1)^2}{4(a^2-1)} , \quad (26)$$

$$f_a''(0) = 0 , \quad (27)$$

$$f_a'''(0) = \frac{(a-1)^4}{8(a^4-1)} . \quad (28)$$

Thus the positions of the maxima for large k are determined by f_a and its derivatives, evaluated at small values of k, provided that a is an integer.

The values of $S_a(k)$ at these maxima, which give the intensities of diffraction spots, do not follow Eq. (2), except for $a = \infty$. In the other trivial case, $a = 2$, the values of $S_a(k)$ follow Eq. (3), while in all other cases the values of $S_a(k)$ at its maxima vary widely (see Figs. 3–7), with regularities which depend on the number theoretic properties of a. A natural question that arises is how rapidly do the values of $S_a(k)$ at the largest maxima decrease as $k \to \infty$? There are two distinct types of behavior.

If a is an integer, for example, in Fig. 3, it follows from Eq. (15) that

$$S_a(2a^l m\pi/(a-1)) = S_a(2m\pi/(a-1)) , \quad (29)$$

thus the peaks at large k never approach zero, but remain at least as large as the maximum of $S_a(2m\pi/(a-1))$.

This is also the case if a is an irrational Pisot-Vijaraghavan (PV) number, as in Fig. 4. A PV number [10] $x \geq 1$ is a real number which satisfies the equation $\forall n$

$$|x^n - [x^n]| < c^n, \quad (30)$$

for some $c < 1$. $[x^n]$ is the nearest integer to x^n. The PV numbers include all integers, no irreducible rational numbers, and all the remaining algebraic numbers for which all the conjugates are of magnitude less than 1. Each algebraic number has a unique polynomial of minimal degree of which it is a root; its conjugates are the

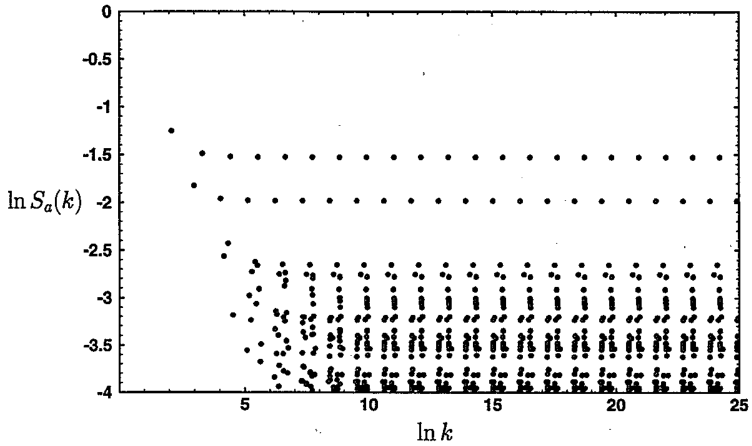

FIG. 3. The maxima of $S_a(k)$ for $a = 3$. The periodicity in $\ln k$ is clear.

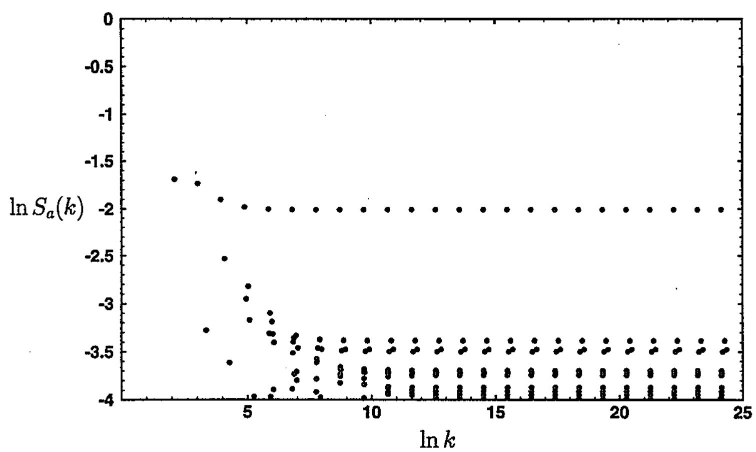

FIG. 4. The maxima of $S_a(k)$ for $a = (\sqrt{5} + 3)/2 = 2.618\ldots$.

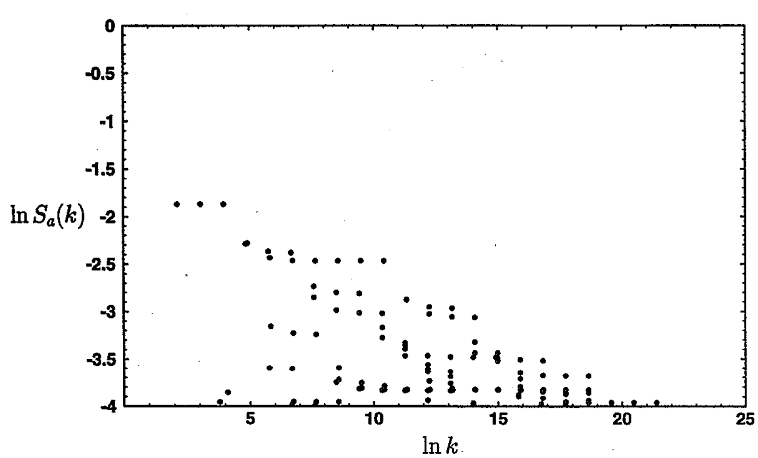

FIG. 5. The maxima of $S_a(k)$ for $a = 5/2$.

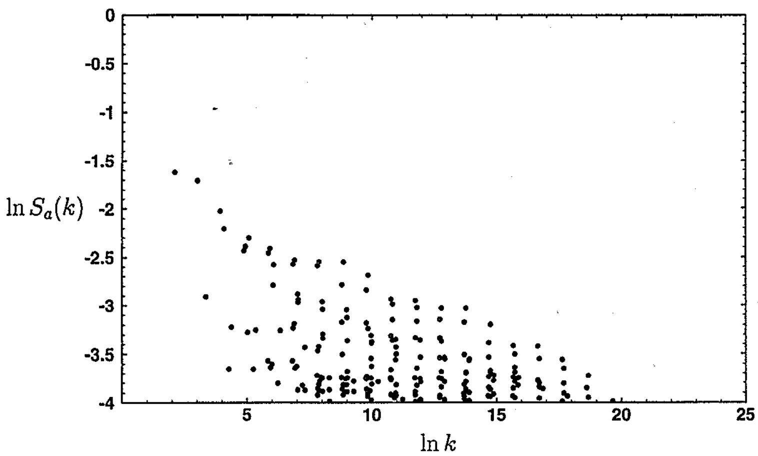

FIG. 6. The maxima of $S_a(k)$ for $a = 8/3$.

remaining roots of that polynomial. PV numbers are discussed in relation to fractals in Refs. [4,7].

Although Eq. (15) does not apply to PV numbers, the large powers of a are sufficiently close to integers that the cosines in Eq. (13) in the evaluation of $S_a(2a^l m\pi/(a-1))$ are almost 1, and this expression approaches a nonzero constant as $l \to \infty$. Hence this case is analogous to that of integral a.

For all other a, for example, rational numbers with even (Fig. 5) or odd (Fig. 6) denominators, or transcendental numbers (Fig. 7), $S_a(k)$ approaches zero for large k. Numerically, it appears that the largest maxima decrease with a power law of the form

$$S_a(k)_{\max} \sim k^{-\alpha(a)} \ , \tag{31}$$

with $\alpha(a) \approx 0.1$ for the values of a chosen. An analytic evaluation of $\alpha(a)$ would require a detailed number theory calculation, which is beyond the scope of this paper. Note that this exponent is much smaller than the exponent in either Eq. (2) or (3). It is interesting to note at this point that a similar situation arises in connection with the Fourier transform of non-PV self-similar quasicrystals [11], for which the spectrum has a complicated structure, but is describable in terms of "mean local exponents."

We now turn to methods of estimating the behavior of $S_a(k)$ as a whole.

III. ASYMPTOTIC POWER LAWS

A. The geometric mean

A simple method of estimating the average decrease of $S(k)$ in the limit of large k is to replace all the terms in the infinite product Eq. (13) for which the argument of the cosine is greater than one by the geometric mean of the $\cos^2$, and all other terms by one.

The geometric mean of the $\cos^2$ function is given by

$$\exp\left[\frac{1}{2\pi}\int_0^{2\pi} \ln\cos^2(x)dx\right] = \frac{1}{4} \ , \tag{32}$$

which leads directly to the estimate

$$S_a(k) \sim k^{-2\ln 2/\ln a} \ . \tag{33}$$

This method is somewhat heuristic, however, it indicates that the exponent $2\ln 2/\ln a$ has some place in the mathematical structure of $S_a(k)$ as $k \to \infty$, a fact which

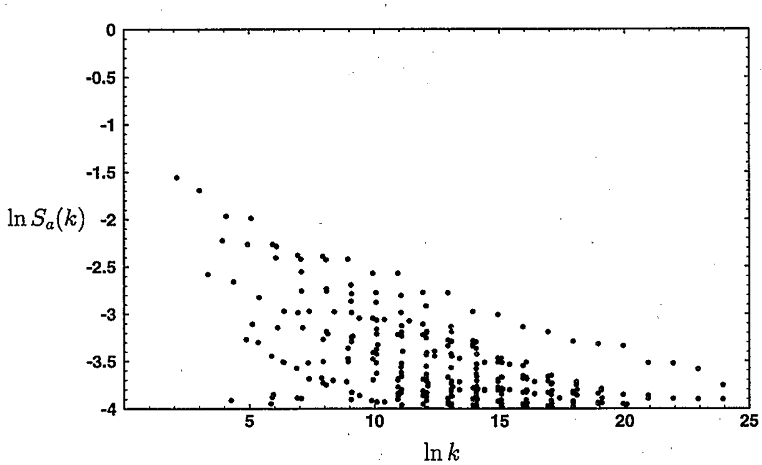

FIG. 7. The maxima of $S_a(k)$ for $a = e = 2.718\ldots$.

is reinforced by its appearance in the Mellin transform of $\ln S_a(k)$, to which we now turn.

B. The Mellin transform

The Mellin representation of a function [12] is a contour integral in the complex plane, which may often be evaluated using Cauchy's theorem to obtain expansions for the function in terms of powers and logarithms. Mellin transform techniques have proved useful in many areas of physics, where only a sum or integral representation of a function is known [13]. The expansions generated using Mellin transforms are not restricted to integer powers, unlike Taylor series and similar constructions, thus they are ideally suited to problems which involve fractals. Mellin transforms have been successfully applied to the electrostatic potential of charge distributions on Julia sets [14].

The Mellin transform of $\ln\cos^2 x$,

$$\int_0^\infty x^{s-1}\ln\cos^2 x dx = -\frac{2^{1-s}}{s}(2^{-s}-1)\cos\frac{\pi s}{2} \times\Gamma(s+1)\zeta(s+1) \;, \quad (34)$$

is not given in Ref. [12] or other common books of integrals and special functions; we obtained this result by integrating by parts, substituting the Mittag-Leffler expansion for $\tan x$ (Eq. 1.421.1 of Ref. [9]), integrating term by term, evaluating the sum to obtain the Riemann zeta function, and using the Riemann relation for $\zeta(z)$ (Eq. 9.535.2 of Ref. [9]).

The expression for $\ln S_a(k)$ [Eqs. (13) and (14)] is a sum over terms of the form $\ln\cos^2 k$. When the Mellin transform is performed this sum becomes a geometric series, giving the Mellin representation of $\ln S_a(k)$ as

$$\ln S_a(k) = \frac{-1}{2\pi i}\int_{c-i\infty}^{c+i\infty} k^{-s}(a-1)^{-s}\frac{2}{s}\frac{2^{-s}-1}{a^{-s}-1}\cos\frac{\pi s}{2} \times\Gamma(s+1)\zeta(s+1)ds\,,\ -2<c<0 \;. \quad (35)$$

The integrand has simple poles at negative even integers, a double pole at $s=0$, and, if $a\neq 2$, simple poles at $s=2\pi ij/\ln a$ for j a nonzero integer.

Closing the contour to the left, we obtain the small-k expansion of $\ln S_a(k)$, noting that the contribution from the semicircular arc vanishes in the large radius limit, if care is taken to avoid the poles on the real axis. It is given by

$$\ln S_a(k) = \sum_{j=1}^{\infty} k^{2j}(a-1)^{2j}\frac{(-1)^j B_{2j}}{2j^2(2j-1)!}\frac{2^{2j}-1}{a^{2j}-1} \;, \quad (36)$$

where B_{2j} is a Bernoulli number, arising from the evaluation of the ζ function at negative odd integers. Exponentiating this series gives the small-k expansion for $S_a(k)$ which is given in Ref. [15] for the case $a=3$. The series has a radius of convergence given by the position of the first zero of $S_a(k)$.

Closing the contour to the right, and ignoring the exponentially large contribution from the arc, which we are unable to evaluate explicitly, we obtain a formal expansion for $\ln S_a(k)$ in the limit $k\to\infty$, given by

$$\ln S_a(k) = -\frac{\ln 2}{\ln a}\ln[2k^2(a-1)^2/a] + \sum_{j\neq 0} k^{-s_j}(a-1)^{-s_j}\frac{2}{s_j}\frac{2^{-s_j}-1}{\ln a}\cos\frac{\pi s_j}{2} \times\Gamma(s_j+1)\zeta(s_j+1) + \int_{\rm arc} \;, \quad (37)$$

$$s_j = \frac{2\pi ij}{\ln a} \;, \quad (38)$$

where the sum is over all positive and negative integers. The sum diverges for almost all values of k. This divergence is canceled by the contribution from the arc, to give $\ln S_a(k)$ for which Eq. (35) is an exact integral representation. We present this result to demonstrate the fractal structure appearing in the first term which implies that, in some sense,

$$S_a(k) \sim k^{-2\ln 2/\ln a} \;. \quad (39)$$

C. Gaussian averaging

Finally we use a method which approximates the behavior of the arithmetic mean of $S_a(k)$ over a large range of k. The integral over $S_a(k)$ which is most amenable to analytic results is

$$P_a(\sigma) = \int_{-\infty}^{\infty} S_a(k)\frac{e^{-(k/\sigma)^2/2}}{\sigma\sqrt{2\pi}}dk \;, \quad (40)$$

which gives the power averaged over a domain of k of order σ, and has a smooth cutoff for $k>\sigma$. A straightforward application of Parseval's formula and the convolution theorem gives

$$P_a(\sigma) = \frac{\sqrt{2\pi}}{\sigma}\int_{-\infty}^{\infty} G_a(\bar{x},(\sigma\sqrt{2})^{-1})^2 d\bar{x} \;, \quad (41)$$

where

$$G_a(\bar{x},\sigma) = \int \frac{e^{-[(x-\bar{x})/\sigma]^2/2}}{\sigma\sqrt{2\pi}}d\mu_a(x) \quad (42)$$

is the convolution of the fractal distribution and a Gaussian distribution.

We now derive some of the properties of $G_a(\bar{x},\sigma)$. Substituting its definition, Eq. (42), into Eq. (9) we obtain the equation

$$G_a(\bar{x},\sigma) = \frac{a}{2}[G_a(a\bar{x}+(a-1)/2,a\sigma) + G_a(a\bar{x}-(a-1)/2,a\sigma)] \;, \quad (43)$$

which relates G_a to itself at two different values of $\bar{x}$.

However, if $\sigma \ll 1$, the limit in which we are most interested, one of these is negligible compared to the other. Replacing the exponential in Eq. (42) by its largest value on the interval $[-1/2, 1/2]$ which contains the fractal, we obtain the bound

$$G_a(\bar{x},\sigma) \leq \frac{\exp[-(2|\bar{x}|-1)^2/(8\sigma^2)]}{\sigma\sqrt{2\pi}} \ , \tag{44}$$

if $|\bar{x}| > 1/2$. This means that Eq. (43) may be written in approximate form as

$$G_a(\bar{x},\sigma) = \begin{cases} \frac{a}{2}G_a(a\bar{x}+(a-1)/2, a\sigma) + O(e^{-(a-2)^2/(8\sigma^2)}) & \text{if} \quad \bar{x} \leq 0 \\ \frac{a}{2}G_a(a\bar{x}-(a-1)/2, a\sigma) + O(e^{-(a-2)^2/(8\sigma^2)}) & \text{if} \quad \bar{x} \geq 0. \end{cases} \tag{45}$$

Thus

$$\begin{aligned} \int_{-\infty}^{\infty} G_a(\bar{x},\sigma)^2 d\bar{x} &= \int_{-\infty}^{0} G_a(\bar{x},\sigma)^2 d\bar{x} + \int_{0}^{\infty} G_a(\bar{x},\sigma)^2 d\bar{x} \\ &= \frac{a^2}{4}\int_{-\infty}^{0} G_a(a\bar{x}+(a-1)/2, a\sigma)^2 d\bar{x} + \frac{a^2}{4}\int_{0}^{\infty} G_a(a\bar{x}-(a-1)/2, a\sigma)^2 d\bar{x} \\ &\quad + O(e^{-(a-2)^2/(8\sigma^2)}) \\ &= \frac{a}{2}\int_{-\infty}^{\infty} G_a(\bar{x}, a\sigma)^2 d\bar{x} + O(e^{-(a-2)^2/(8\sigma^2)}) \ . \end{aligned} \tag{46}$$

In the last step above, a change of variable was made in each integral, and Eq. (44) was used to extend the range of integration. We may ignore the exponentially small corrections in the limit $\sigma \to 0$, and obtain

$$\int_{-\infty}^{\infty} G_a(\bar{x},\sigma)^2 d\bar{x} \sim g_a(\sigma)\sigma^{(\ln 2/\ln a)-1} \ , \tag{47}$$

where g_a is periodic in $\ln\sigma$,

$$g_a(a\sigma) = g_a(\sigma) \ . \tag{48}$$

Now $\sigma G_a(\bar{x},\sigma)$, with $\bar{x}$ fixed, is a monotonically increasing function of σ; this may be seen from Eq. (42). It implies that $g_a(\sigma)$ is bounded by two values whose ratio is at most $2a$.

Finally, from Eqs. (41) and (47) we get

$$P_a(\sigma) \sim h_a(\sigma)\sigma^{\ln 2/\ln a} \ , \tag{49}$$

as $\sigma \to 0$, where

$$h_a(\sigma) = \sqrt{2\pi}2^{(1-\ln 2/\ln a)/2} g_a((\sigma\sqrt{2})^{-1}) \tag{50}$$

is bounded in exactly the same way as $g_a(\sigma)$, above. It is in this sense that Eq. (2) is valid for these Cantor sets.

IV. CONCLUSION

We have seen that the asymptotic scaling law for $S(k)$ depends on the averaging method. By analogy with multifractal theory we might expect a general power law of the form

$$\langle S_a(k)^q \rangle \sim k^{-q\alpha_a(q)} \ , \tag{51}$$

averaging over regions $\Delta k \approx k$. The geometric and arithmetic means of the preceeding section are particular cases of this relation, leading to $\alpha(0) = 2d$, $\alpha(1) = d$, respectively. It may be possible to extend this work to general q for particular values of a. For general a the situation is more complicated, since in the limit $q \to \infty$ only the maxima contribute, requiring the number theoretic properties of a to be included, as discussed in Sec. II.

This work has important ramifications for the experimental determination of fractal dimensions using diffraction techniques. For the distribution considered here, at least, the appropriate estimator of the dimension is the exponent calculated from the arithmetic mean of $S(k)$. This is not, in general, equivalent to a power law fit to $S(k)$ itself. Finally we note again that some studies of this kind have already been presented in the literature [1,7].

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