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STRUCTURE FACTOR OF DETERMINISTIC FRACTALS WITH ROTATIONS

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Abstract

We derive a recursion relation for the Fourier transform of any self-similar multifractal mass distribution. This is then used to find sufficient conditions under which $S(\mathbf{k}) \nrightarrow 0$ as $|\mathbf{k}| \to \infty$. Among two-dimensional distributions for which the similarity transformations contain $2\pi/n$ rotations, it is found that for values of n equal to 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 15, 18 and 30, distributions may be constructed satisfying the above condition. The possible scaling factors in the similarity transformations are strongly constrained by the value of n. In three dimensions, the equivalent condition is that all rotations/reflections are elements of a finite group, together with similar constraints on the scaling factors.

1. INTRODUCTION

It is well known that the scale invariance of fractal mass distributions appears in the diffraction pattern,[1] and this has led to experimental techniques for measuring not only the dimension, but also the whole multifractal spectrum of a distribution.[2]

Investigations into the structure factor $S(\mathbf{k})$ of deterministic mass,[3] surface,[4] and mixed fractals[5] have shown that although the structure factor decreases on the average for large $|\mathbf{k}|$, given by generalisations of the expression in Ref. 1, it need not vanish in the limit $|\mathbf{k}| \to \infty$,

$$S(\mathbf{k}) \nrightarrow 0 \text{ as } |\mathbf{k}| \to \infty . \qquad (1)$$

That is, $S(\mathbf{k})$ contains peaks for arbitrarily large $|\mathbf{k}|$, the intensities of which do not approach zero. None of these investigations considered fractals with rotations in the defining transformations.

In our previous paper,[6] we considered the specific case of the von-Koch snowflake, which contains $\pi/3$ rotations, and found that Eq. (1) holds, due to the existence of the hexagonal lattice and the nature of the transformations used to define the snowflake.

In this paper we consider the more general question of what conditions are sufficient for this property to hold, for self-similar multifractal mass distributions. Similar to the classification of quasiperiodic lattices which also have long range order and (approximate) self-similarity,[7,8] it is found that Eq. (1) holds for fractal distributions defined with rotations inconsistent with periodic lattices. In addition to the octagonal, decagonal, dodecagonal, and icosahedral symmetries of quasicrystals, we find that 14-, 18- and 30-fold rotations are permitted for distributions which satisfy Eq. (1).

2. FUNDAMENTALS

We begin by setting forth the mathematical formalism used in the following sections. It is necessary to use a slightly more general approach than previous authors[3,4] to allow for rotations in the transformations used to define the mass distribution. The mathematical foundation of the theory of fractals, and an introduction to multifractal distributions may be found in Ref. 9.

A self-similar fractal of embedding dimension E is a bounded closed set $\mathbf{F} \subset \mathbf{R}^E$ which may be split into N subsets, each of which being similar to the original,

$$\mathbf{F} = \bigcup_{\alpha=1}^{N} \mathbf{F}_\alpha \tag{2}$$

$$\mathbf{F}_\alpha = S_\alpha \mathbf{F} \,. \tag{3}$$

The similarity transformations S_α each consists of a unitary rotation/reflection matrix U_α, an isotropic dilation factor $0 < c_\alpha < 1$ and a translation vector $\mathbf{t}_\alpha$,

$$S_\alpha \mathbf{x} = c_\alpha U_\alpha \mathbf{x} + \mathbf{t}_\alpha \,. \tag{4}$$

Provided that the sets $\mathbf{F}_\alpha$ are non-overlapping, the Hausdorff dimension of $\mathbf{F}$ satisfies the equation:

$$\sum_{\alpha=1}^{N} c_\alpha^{\dim \mathbf{F}} = 1 \,. \tag{5}$$

We consider a mass distribution on $\mathbf{F}$. The mass density $\rho(\mathbf{x})$ is singular; however, all physical quantities may be found using integrals of the form:

$$I[f(\mathbf{x})] = \int f(\mathbf{x})\rho(\mathbf{x})d^E x \,, \tag{6}$$

which are often finite, and hence easier to handle rigorously than $\rho(\mathbf{x})$. The distribution is normalized to have total mass unity,

$$I[1] = \int \rho(\mathbf{x})d^E x = 1 \,. \tag{7}$$

A self-similar multifractal distribution on $\mathbf{F}$ is one which satisfies the equation:

$$I[f(\mathbf{x})] = \sum_{\alpha=1}^{N} p_\alpha I[f(S_\alpha \mathbf{x})] \,, \tag{8}$$

where f is any function and p_α is the total mass on $\mathbf{F}_\alpha$, thus:

$$\sum_{\alpha=1}^{N} p_\alpha = 1 \,. \tag{9}$$

If the p_α are given by

$$p_\alpha = \frac{c_\alpha}{\sum_{\alpha=1}^{N} c_\alpha} \,, \tag{10}$$

the distribution is monofractal and uniform, with identical regions of the fractal having the same mass. In all other cases the distribution is multifractal, with a range of scaling exponents, depending on the point on the fractal and the quantity referred to.

Equation (8) gives, for the center of mass of the distribution $\langle \mathbf{x} \rangle$,

$$\langle \mathbf{x} \rangle = I[\mathbf{x}] = \sum_{\alpha=1}^{N} p_\alpha (\mathbf{t}_\alpha + c_\alpha U_\alpha \langle \mathbf{x} \rangle) \,. \tag{11}$$

Without loss of generality, we assume that the distribution is centered on the origin, so:

$$\sum_{\alpha=1}^{N} p_\alpha \mathbf{t}_\alpha = 0 \,. \tag{12}$$

Similarly, rescaling or rotating all of the $\mathbf{t}_\alpha$ simply rescales or rotates the distribution; thus, it is possible to fix $\mathbf{t}_1$ to any given non-zero vector in full generality.

The Fourier transform of the distribution, $\tilde{\rho}(\mathbf{k}) = I[\exp(i\mathbf{k}\cdot\mathbf{x})]$, is uniquely determined by Eqs. (7) and (8) which give, using the linearity property of I,

$$\tilde{\rho}(0) = 1 \tag{13}$$

$$\tilde{\rho}(\mathbf{k}) = \sum_{\alpha=1}^{N} p_\alpha e^{i\mathbf{k}\cdot\mathbf{t}_\alpha} \tilde{\rho}(c_\alpha U_\alpha^\dagger \mathbf{k}) \,, \tag{14}$$

where the "†" indicates Hermitian conjugate and is equivalent to U_α^{-1}. This equation permits the numerical evaluation of $\tilde{\rho}(\mathbf{k})$ for any value of $\mathbf{k}$ using a recursive algorithm since the right-hand side of the above equation involves $\tilde{\rho}(\mathbf{k})$ at values of $\mathbf{k}$ which approach zero after a number of iterations. For values of $|\mathbf{k}|$ less than a cutoff ε, $\tilde{\rho}(\mathbf{k})$ is taken to be equal to 1, thus terminating the recursion. Convergence of this procedure as $\varepsilon \to 0$ is guaranteed by the analyticity of $\tilde{\rho}(\mathbf{k})$, together with the fact that the magnitude of the coefficients $(p_\alpha \exp(i\mathbf{k} \cdot \mathbf{t}_\alpha))$ sum to 1, and so do not increase the error in $\tilde{\rho}(\mathbf{k})$ in successive iterations. The analyticity of $\tilde{\rho}(\mathbf{k})$ is shown by expanding the exponential in $I[\exp(i\mathbf{k}\cdot\mathbf{x})]$ in a power series and showing that the resulting series involving terms of the form $I[\prod_{j=1}^{E} x_j^{n_j}]$ is convergent for all $\mathbf{k}$.

The structure factor $S(\mathbf{k})$ may then be simply evaluated as:

$$S(\mathbf{k}) = |\tilde{\rho}(\mathbf{k})|^2 . \tag{15}$$

The alternative definition, as the Fourier transform of the autocorrelation function $g(\mathbf{r})$, is not particularly suitable for deterministic fractals, as $g(\mathbf{r})$ is typically singular.

In order for $\tilde{\rho}(\mathbf{k})$ to be non-vanishing as $|\mathbf{k}| \to \infty$, the phases of the terms in Eq. (14) must add constructively for all but a finite number of iterations. In the following sections, the stringent conditions this imposes on c_α, U_α, $\mathbf{t}_\alpha$ and p_α are investigated for some simple cases following some general discussion.

3. GENERAL REMARKS

The purpose of this paper is to demonstrate the existence of a class of fractals defined using rotations with the property that $\tilde{\rho}(\mathbf{k})$ does not tend to zero in the limit of large, real $\mathbf{k}$. We do not provide an exhaustive classification scheme of such fractals. The fractals we describe all have the following properties:

Condition 1. The exponentials of Eq. (14) required in the evaluation of $\tilde{\rho}(\mathbf{K}_j)$ for some unbounded sequence $\mathbf{K}_j$ are almost all close to 1. Given a set of $\mathbf{t}_\alpha$, the values of $\mathbf{k}$ for which the exponential is exactly 1, lie on a periodic lattice of points, lines or planes, etc., or else $\mathbf{k} = 0$ is the only solution. The phrase "almost all close to 1" can be made rigorous by insisting that, for all j, if the largest difference between the exponentials required to calculate $\tilde{\rho}(\mathbf{k}_j)$ and 1 at each iteration step were sorted into a decreasing sequence, this sequence could be bounded from above by a decreasing geometric sequence which is independent of j. This Condition is automatically satisfied for the terms with $\mathbf{k}$ close to zero, since the recursion relation in Eq. (14) requires values of $\mathbf{k}$ whose absolute value follows a geometric sequence.

Condition 2. The group generated by the U_α is finite. This means, for example, that all rotations are of an angle $2\pi/n$ where n is an integer. It makes the rapid evaluation of $\tilde{\rho}(\mathbf{k})$ possible. It is probably implied by Condition 1, except in the trivial case of the U_α and the $\mathbf{t}_\alpha$ spanning mutually disjoint subspaces, but this is difficult to prove.

It is clear that Condition 1 implies that $\tilde{\rho}(\mathbf{k})$ does not approach zero for large $\mathbf{k}$, except where it is exactly zero for the $\mathbf{K}_j$ due to unspecified behavior at small $\mathbf{k}$. This possibility may be eliminated for any specific distribution by simply evaluating $\tilde{\rho}(\mathbf{k})$ at appropriate points.

Note that we have not assumed that the periodic lattice referred to in Condition 1 exists. It is sufficient that values of $\mathbf{k}$ exist for which $\exp(i\mathbf{k}\cdot\mathbf{t}_\alpha)$ is close to 1 for all α. For a given definition of "close to 1" such points will lie on a quasiperiodic lattice.

4. THE CASE $E = 1$

There are no rotations in one dimension, so this case has been thoroughly dealt with in Ref. 3. It is, however, instructive to review these results, as the two-dimensional case with rotations retains many of the features present in one dimension.

Let c be the smallest number such that all of the c_α may be written as integer powers of c. If c does not exist, the number of values of $\mathbf{k}$ within any interval required in the evaluation of $\tilde{\rho}(\mathbf{K}_j)$ increases without limit as $j \to \infty$. Thus c must exist for Condition 1 to be met.

If c exists, the values of $\mathbf{k}$ required form a geometric sequence with ratio c. Condition 1 is fulfilled if it is possible to align this geometric sequence with the lattice at which the exponentials are close to 1. This is true only if c^{-1} is a Pisot-Vijaraghavan (PV) number. See Ref. 10 for the properties of these numbers.

A PV number $x \geq 1$ is a real number which satisfies the equation $\forall n$

$$|x^n - [x^n]| < a^n , \tag{16}$$

for some $a < 1$. $[x^n]$ 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 remaining roots of that polynomial. The most well known irrational example is the golden ratio $(\sqrt{5}+1)/2$. An important property which may be deduced from Eq. (16) is that, if x is a PV number and y is expressible as a polynomial in x with integer coefficients $\forall n$,

$$|yx^n - [yx^n]| < ba^n \,, \tag{17}$$

for some $0 < a < 1$ and real number b.

Thus the one dimensional self-similar multifractal distributions which satisfy Condition 1 are those for which the $\mathbf{t}_\alpha$ are commensurate (hence the periodic lattice at which the exponentials are equal to 1) and c^{-1} is a PV number, and those for which all the ratios between the $\mathbf{t}_\alpha$ are powers of c^{-1}, which is again a PV number. In the second case, there exists a geometric sequence $\mathbf{K}_j$ at which $\exp(i\mathbf{k}\cdot\mathbf{t}_\alpha)$ is increasingly close to 1 for all α. Both cases rely strongly on the fact that the difference between all the large powers of a PV number and the nearest integer decreases as fast as a geometric sequence.

5. THE CASE $E = 2$

In two dimensions U_α may be described by either a rotation or a reflection. In any case Condition 2 requires that all the U_α leave the vertices of an n-sided regular polygon invariant, for some n. The question arises: for what values of n can Condition 1 be met?

The simplest periodic array occurs when the $\mathbf{t}_\alpha$ are all parallel, with rational ratios (the generalisation to PV ratios is straightforward). In this case, the exponential in Eq. (14) is equal to one on a periodic array of parallel lines in $\mathbf{k}$ space. It is trivial to align the vertices of an n-sided polygon to this array if $n = 1$, 2, 3, 4 or 6. The scale factor c (see last section) may then be the reciprocal of any PV number, and Condition 1 will be met. These values of n are also the symmetries of lattices of points, thus a large range of fractals with these rotations exists for which the Fourier transform does not vanish at large $\mathbf{k}$.

The first non-trivial case is $n = 5$. In Fig. 1, it is seen that it is possible to align only 3 of the

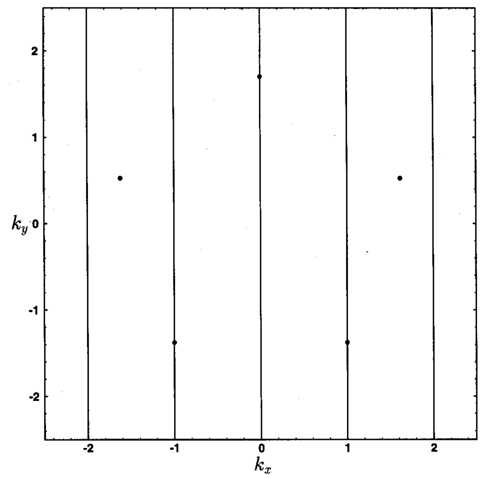

Fig. 1 A pentagon cannot be aligned on an array of parallel lines.

5 vertices of a regular pentagon centered on the origin on an array of parallel lines. However, the two remaining points shown have x-coordinates of $\sin(2\pi/5)/\sin(\pi/5) = (\sqrt{5}+1)/2$. Thus a value of c equal to the reciprocal of $(\sqrt{5}+1)/2$ ensures that the preimages of this pentagon by the transformation in Eq. (14) are increasingly close to the lines as the number of iterations increases, so that Condition 1 is met. The case $n = 10$ follows by simply reflecting Fig. 1 in the x-axis.

For $n = 7$ the same result holds. It is only possible to align 3 of the 7 vertices on an array of parallel lines, but $\sin(3\pi/7)/\sin(\pi/7)$ is PV number, with a minimal polynomial of degree 3. In addition, $\sin(2\pi/7)/\sin(\pi/7)$ may be written as a polynomial in this number with integer coefficients, so by Eq. (17) any distribution with 7-fold rotations with the $\mathbf{t}_\alpha$ parallel and commensurate satisfies Condition 1.

For large values of n, this procedure does not appear to generate fractals which satisfy Condition 1. That is, we have not found any PV number in which all the required ratios of sines may be written as integer polynomials. The exceptions, $n = 5$, 7, 8, 9, 10, 12, 14, 15, 18 and 30, are listed in Table 1, together with the relevant PV number. Note that there is an infinite set of PV numbers of the form $a\sqrt{2}+b$ (and $a\sqrt{3}+b$) with integers a and b, all of

Table 1 Suitable Scaling Factors for Different Values of n

n	c^{-1}	**Minimal Polynomial**
1,2,3,4,6	Any PV number	Polynomial with all but one of it's roots of magnitude less than 1
5,10	$\dfrac{\sin\left(\frac{2\pi}{5}\right)}{\sin\left(\frac{\pi}{5}\right)} = \dfrac{\sqrt{5}+1}{2}$	$x^2 - x - 1$
7,14	$\dfrac{\sin\left(\frac{3\pi}{7}\right)}{\sin\left(\frac{\pi}{7}\right)}$	$x^3 - 2x^2 - x + 1$
8	$\sqrt{2}+1$	$x^2 - 2x - 1$
9,18	$\dfrac{\sin\left(\frac{4\pi}{9}\right)}{\sin\left(\frac{\pi}{9}\right)}$	$x^3 - 3x^2 + 1$
12	$\sqrt{3}+1$	$x^2 - 2x - 2$
30 and its factors	$\dfrac{\sin\left(\frac{7\pi}{15}\right)}{\sin\left(\frac{\pi}{15}\right)}$	$x^4 - 4x^3 - 4x^2 + x + 1$

which satisfy the conditions for $n = 8$ (and $n = 12$ respectively). It is interesting to note at this point that an $n = 12$, $c^{-1} = \sqrt{3} + 2$ (a PV number) set of transformations has been used to define a fractal-like acceptance domain in the construction of a dodecagonal quasicrystal.[11]

Note that the highest degree PV number in Table 1 is of degree 4, and that the ratios of sines and cosines for the first value of n not in Table 1 ($n = 11$) are algebraic numbers of degrees at least 5. Our algorithm for determining if a given number x is PV involves evaluating large powers of x (near x^{200}) to a high degree of precision and should not depend on the degree of x. There may be a deep connection between these properties of PV numbers and the solvability of the minimal polynomial. If this is indeed the case, we expect that a PV number for both $n = 20$ and $n = 24$ should exist, since all the expressions $\sin(2j\pi/20)$ and $\sin(2j\pi/24)$ are algebraic numbers of degree 4 or less.

We conclude this section by giving a few examples of two-dimensional fractal distributions with these properties. All of the distributions here are uniform as defined in Eq. (10). The experimentally measured diffraction pattern of the von Koch snowflake, which has 6-fold symmetry, is given in Ref. 12. See our previous paper[6] for an analytic

Table 2 **Defining Transformations for the Distributions shown in Figs. 2 to 9**

n	s	c_α	θ_α	$\mathbf{t}_\alpha$	p_α
5	5	$\frac{\sqrt{5}-1}{2}$	$\frac{4\pi}{5}$	$\left(\sin\frac{\pi}{5}, \cos\frac{\pi}{5}\right)$	$\frac{1}{2}$
		$\frac{\sqrt{5}-1}{2}$	$\frac{-4\pi}{5}$	$\left(-\sin\frac{\pi}{5}, \cos\frac{\pi}{5}\right)$	$\frac{1}{2}$
7	1	$\frac{\sin\left(\frac{\pi}{7}\right)}{\sin\left(\frac{3\pi}{7}\right)}$	$\frac{2\pi}{7}$	$(1, 0)$	$\frac{1}{3}$
		$\frac{\sin\left(\frac{\pi}{7}\right)}{\sin\left(\frac{3\pi}{7}\right)}$	0	$(0, 0)$	$\frac{1}{3}$
		$\frac{\sin\left(\frac{\pi}{7}\right)}{\sin\left(\frac{3\pi}{7}\right)}$	$\frac{-4\pi}{7}$	$(-1, 0)$	$\frac{1}{3}$
8	1	$\sqrt{2}-1$	$\frac{\pi}{2}$	$(1, 0)$	$\frac{1}{3}$
		$\sqrt{2}-1$	0	$(0, 0)$	$\frac{1}{3}$
		$\sqrt{2}-1$	$\frac{-3\pi}{4}$	$(-1, 0)$	$\frac{1}{3}$
30	30	$\frac{\sin\left(\frac{\pi}{15}\right)}{\sin\left(\frac{7\pi}{15}\right)}$	$\frac{3\pi}{5}$	$(1, 0)$	$\frac{1}{2}$
		$\frac{\sin\left(\frac{\pi}{15}\right)}{\sin\left(\frac{7\pi}{15}\right)}$	$\frac{4\pi}{15}$	$(-1, 0)$	$\frac{1}{2}$

description and figures similar to those given here. There is a 5-fold analog of the von Koch snowflake, shown in Fig. 2, which has the correct value of c. A representation of $|\tilde{\rho}(\mathbf{k})|^2$ is given in Fig. 3. Examples of 7-fold, 8-fold and 30-fold rotations are given in the Figs. 4–9. The transformations used to generate these are given in Table 2. Here θ_α refers to the rotation angle of U_α and s refers to the total number of copies of the distribution. For example, the 5-fold snowflake is generated in two stages; firstly, the transformations given define the upper section of the fractal distribution; second, $s = 5$ rotated copies of the distribution are added together and normalised to give the final result. None of these transformations involve reflections or define distributions which are multifractal.

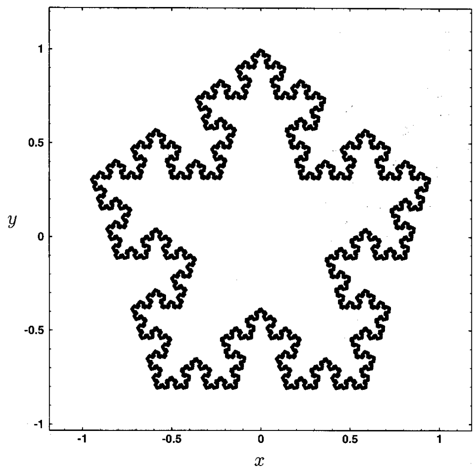

Fig. 2 The 5-fold von-Koch snowflake. The defining transformations for this and succeeding distributions are given in Table 2.

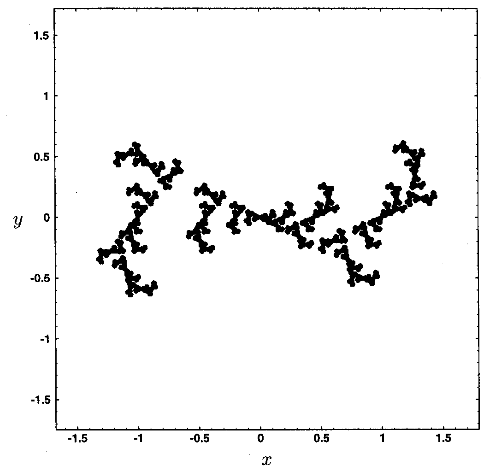

Fig. 4 A fractal with 7-fold rotations.

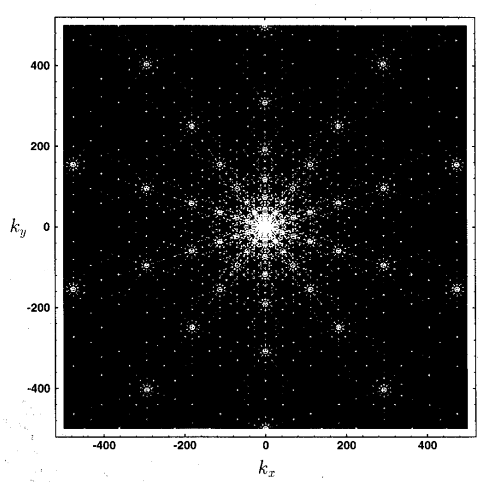

Fig. 3 The structure factor of the 5-fold snowflake $S(\mathbf{k}) = |\tilde{\rho}(\mathbf{k})|^2$. The range of shades black to white corresponds to values of 0 to 0.001.

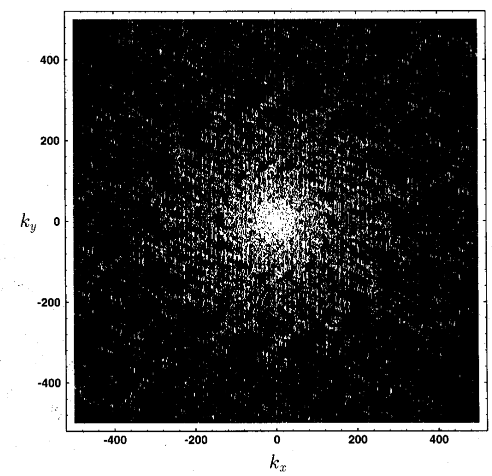

Fig. 5 The structure factor of the $n = 7$ fractal, ranging from 0 to 0.001.

The reason that the 5-fold snowflake with transformations given in Table 2 satisfies the conditions set out at the beginning of this section requires some explanation. The upper section which contains 2/5 of the snowflake is generated by the two transformations given. Thus, if this section is centered on the origin, the translation vectors $\mathbf{t}_1$ and $\mathbf{t}_2$ are equal and opposite by Eq. (12). Shifting the section back

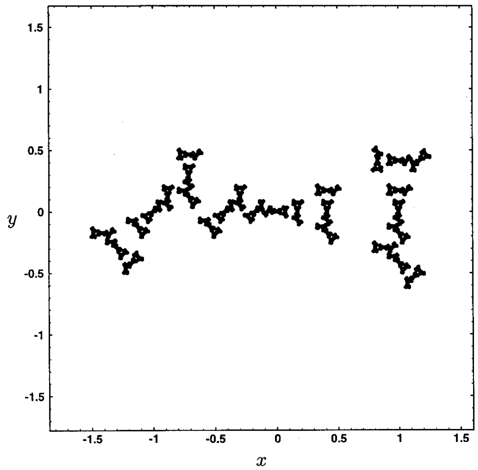

Fig. 6 A fractal with 8-fold rotations.

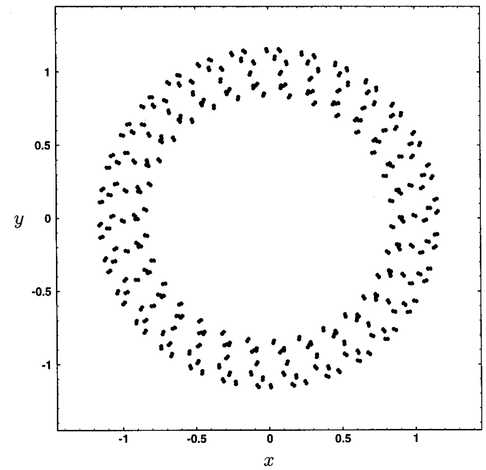

Fig. 8 A fractal with 30-fold rotations.

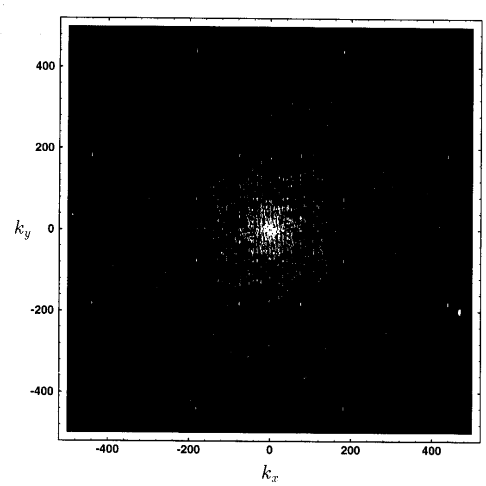

Fig. 7 The structure factor of the $n = 8$ fractal, ranging from 0 to 0.01. The non-zero peaks at large **k** are clearly visible.

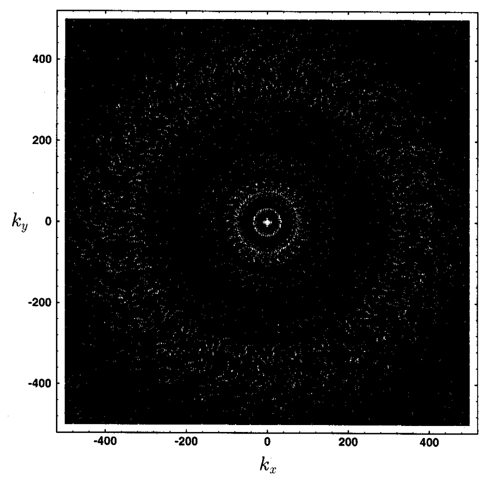

Fig. 9 The structure factor of the $n = 30$ fractal, ranging from 0 to 0.01.

to its original position alters the phases, but not the magnitudes of $|\tilde{\rho}(\mathbf{k})|^2$. Adding the result to 4 rotated copies of the same distribution might possibly cancel the intensities at the required peaks by destructive interference, but this does not happen, as seen in Fig. 3. It is also interesting to note that the "voids", regions of low intensity, in Fig. 3 are shaped like the original snowflake.

6. THE CASE $E = 3$

Rotations in more than 2 dimensions do not commute. This means that classifying the finite groups required for Condition 2 becomes a non-trivial problem. We refer the interested reader to Ref. 13 and the references therein. In three dimensions, the only groups of transformations which map a point out of the plane are the groups of symmetries of the regular polyhedra. Each polyhedron is equivalent to its dual for this purpose, so the group of symmetries of a cube and of an octahedron are isomorphic, and denoted by $\mathcal{W}^*$, and similarly for the dodecahedron and icosahedron ($\mathcal{J}^*$). The group of symmetries of a tetrahedron $\mathcal{T}^*$ is a subgroup of $\mathcal{W}^*$, so there are only 4 cases to consider: $\mathcal{W}^*$, $\mathcal{W}$, $\mathcal{J}^*$ and $\mathcal{J}$, where the unstarred forms are the groups containing only rotations.

$\mathcal{W}^*$, and hence $\mathcal{W}$ are symmetries of the cubic lattice, hence Condition 1 is automatically met if c^{-1} is a PV number; this case is analogous to $n = 4$ of the previous section.

$\mathcal{J}^*$ and $\mathcal{J}$ both contain 5-fold rotations, and so are not the symmetry group of any periodic lattice. Just as for $E = 2$, the problem is now to align the icosahedron with a lattice of points, lines or planes. Writing $\phi = (\sqrt{5}+1)/2$, the 12 vertices of an icosahedron have coordinates $(0, \pm 1, \pm\phi)$, $(\pm\phi, 0, \pm 1)$, $(\pm 1, \pm\phi, 0)$. All of the coordinates are trivially integer polynomials in ϕ, which is a PV number, as noted previously. Thus if $c = \phi^{-1}$ and the $\mathbf{t}_\alpha$ are such that the periodic lattice in Condition 1 is a cubic lattice, Condition 1 is met.

For $E > 3$, the complexity of the problem increases dramatically; however, some general remarks may be made concerning all dimensions. Some groups of rotations have an invariant lattice, thus satisfying Condition 1 if c^{-1} is any PV number. Others are symmetries of polyhedra, but do not have such a lattice, in which case c^{-1} is severely restricted, if values which satisfy Condition 1, and hence Eq. (1) exist at all.

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