Small-angle scattering from 3D Sierpinski tetrahedron generated using chaos game

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Abstract. We approximate a three dimensional version of deterministic Sierpinski gasket (SG), also known as Sierpinski tetrahedron (ST), by using the chaos game representation (CGR). Structural properties of the fractal, generated by both deterministic and CGR algorithms are determined using small-angle scattering (SAS) technique. We calculate the corresponding monodisperse structure factor of ST, using an optimized Debye formula. We show that scattering from CGR of ST recovers basic fractal properties, such as fractal dimension, iteration number, scaling factor, overall size of the system and the number of units composing the fractal.

1. Introduction
A large class of natural objects from nano to macroscales has the property of self-similarity, meaning that they preserve geometrical characteristics under the scale transformations. Such objects are known as fractals and depending on exact or statistical self-similarity they can be classified as deterministic, and respectively stochastic (random) [1]. The presence of fractality in nano and microscale systems has influence on chemical [2, 3], electromagnetic [4], dynamical [5] and other features, therefore the study of relation between structure and shape from one hand, and physical properties from another hand is a topic of significant research interest [6].

One of the common used techniques in investigating nano and microscale fractals is small-angle scattering (SAS; neutron, X-ray, light) which yields the differential elastic cross-section as a function of momentum transfer [7, 8]. The main indicator of the fractal structure is the fractal dimension, and it can be obtained from the power-law behavior of the scattering intensity \( I(q) \) given by [9, 10, 11]

\[
I(q) \sim q^{-\alpha}
\]

where \( q = (4\pi \sin 2\theta)/\lambda, \theta \) is the scattering angle and \( \lambda \) is the wavelength of incident radiation. The exponent \( \alpha \) shows the fractal dimension [12] of the fractal, \( \alpha = D_m \) for mass fractals [9] and \( \alpha = 6 - D_s \) for surface fractals [13, 14, 15], where \( D_m \) is mass fractal dimension and \( D_s \) is surface fractal dimension.

It has been shown recently that besides the fractal dimension, SAS can reveal additional structural parameters, such as: scaling factor, number of units composing the fractal, and the iteration number for both, regular [16, 17] and fat fractals [18, 19, 20, 21], thus making this technique an indispensable tool in studying structural properties of self-similar nano and micro scale objects.
In this paper we calculate numerically, using optimized version of Debye [22] formula developed by Pantos et al. [23], the monodisperse SAS structure factor from three-dimensional ST generated by both deterministic and CGR algorithms, and show that SAS from CGR of ST recovers the main fractal properties, such as fractal dimension, iteration number, scaling factor, overall size of the system and number of fractal units.

2. Small-angle scattering and Debye formula
For monodisperse fractal, the scattering intensity $I(q)$ is defined as [9]

$$I_0(q) = F^2(q)S(q),$$

where $F(q)$ is the form factor and $S(q)$ is the structure factor of the fractal. Since we use a CGR algorithm, defined in Section 3, that generates directly coordinates of positions of scatterers, we can compute intensity spectrum using Debye formula [22]

$$I(q) = NI_s(q) + 2F_s(q)^2\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{\sin qr_{ij}}{qr_{ij}},$$

where $I_s(q)$ is the intensity scattered by each fractal unit, and $r_{ij}$ is the distance between units $i$ and $j$. Computational time of the term $\sin(qr_{ij})/(qr_{ij})$ is increasing proportional to number of units and when it exceeds few hundred this approach become very time consuming. The problem can be resolved by introducing a pair-distance histogram $g(r)$ with a bin-width commensurate with the experimental resolution [23]. Therefore Eq. (3) can be rewritten as

$$I(q) = NI_s(q) + 2F_s^2(q)\sum_{i=1}^{N_{bins}} g(r_i)\frac{\sin qr_i}{qr_i},$$

where $g(r_i)$ is the pair-distance histogram. Since we are interested only in fractal properties of the sample given by structure factor, we can consider $I_s(q) = F_s^2(q) = 1$, and in order to be consistent with previous works [14, 16, 17, 18] we use normalization $I_0(q) = I(q)/N$ and using Eq. 2, we obtain expression for structure factor

$$S(q) = 1 + \frac{2}{N}\sum_{i=1}^{N_{bins}} g(r_i)\frac{\sin qr_i}{qr_i}.$$  (5)

3. Sierpinski tetrahedron and Iterated Function Systems
The Iterated Function System (IFS) of a three-dimensional fractal is given by the set of linear equations $x = a_i x + d_i$, $y = b_i y + e_i$ and $z = c_i z + f_i$ that generates values of $x, y, z$ coordinates. ST centered at the origin, with a side length $a$ can be described by IFS of the affine map, written in a matrix form as

$$w_i \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} a_i & 0 & 0 \\ 0 & b_i & 0 \\ 0 & 0 & c_i \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} d_i \\ e_i \\ f_i \end{bmatrix},$$

where the coefficients $a_i, b_i, c_i, d_i, e_i, f_i$ with $i = 1, 2, 3, 4$ are IFS parameters and given in Tab. 1; $x, y, z$ represent three-dimensional coordinates of generated points.

By definition, chaos game is described by an IFS, and simply the process of CGR is the following:
Table 1. IFS parameters \(a_i, b_i, c_i, d_i, e_i, f_i\) of the affine maps \(w_i\) (first column) for deterministic algorithm and the probabilities \(p_i\) (last column) for random algorithm.

| \(w\) | \(a\) | \(b\) | \(c\) | \(d\) | \(e\) | \(f\) | \(p\) |
|-------|-------|-------|-------|-------|-------|-------|-------|
| 1     | 1/2   | 1/2   | 1/2   | 0     | 0     | \(1/(2\sqrt{3})\) | 1/4   |
| 2     | 1/2   | 1/2   | 1/2   | -1/4  | -1/(4\sqrt{3}) | -1/(4\sqrt{3}) | 1/4   |
| 3     | 1/2   | 1/2   | 1/2   | 1/4   | -1/(4\sqrt{3}) | -1/(4\sqrt{3}) | 1/4   |
| 4     | 1/2   | 1/2   | 1/2   | 0     | \(1/(2\sqrt{3})\) | -1/(4\sqrt{3}) | 1/4   |

(i) Determine a number of subparts into which fractals will be divided at each iteration (four for ST).

(ii) Find coordinates of the vertices of fractal and label them \((1, 2, 3, 4)\).

(iii) Choose a random initial point inside the fractal.

(iv) Randomly (with equal probability) pick one of the labeled vertices and depending on scaling factor \(\beta_s\) put a new point between (on a halfway for ST, since \(\beta_s = 1/2\)) previous point and chosen vertex.

(v) To obtain the fractal continue the same procedure for each generated point.

The set of points that fill ST is generated starting with a random initial point and for every consecutive one, algorithm chooses one of mappings \(w_i\), with a corresponding probability \(p_i\), to act on the previous point.

Figure 1. (Color online) The structure of three-dimensional ST. On the left side are shown points generated by random IFS algorithm where \(n\) is the number of generated points, for \(n = 100, 300, 1000\) and 3000. On the right side are shown tetrahedrons, centered at points generated by deterministic IFS, with side length \(a_m = \beta_s^m a\), where \(\beta_s\) is the scaling factor and \(m\) is the iteration number, for \(m = 0, 1, 2, 3\).

The way of constructing the deterministic ST is following:
(i) Start with the tetrahedron of the side length $a$ (initiator), represented by the iteration number $m = 0$.

(ii) Scale down the initiator by the factor of two (i.e. $\beta_s = 1/2$), and make four copies of it.

(iii) Shift each scaled copy to four different vertices of tetrahedron at $m = 0$ and obtain the ST at $m = 1$.

(iv) Repeat the same procedure for each new tetrahedron in order to obtain the next iteration. For an arbitrary $m$-th iteration, the number of units that compose the ST is given by

$$N_m = 4^m.$$  \(7\)

We calculate the structure factors using the function of the relative positions of the points considered as the centers of the tetrahedrons, neglecting the shape of fractal units. Fig. 1 (left side) clearly shows that with increasing the number of generated points $n$, CGR tends to approximate ST constructed using deterministic approach, when $m \to \infty$ (Fig. 1 (right side)).

4. Results and discussion

For the considered model of ST we calculate numerically the structure factor for deterministic case up to the 5-th iteration. The results are shown in Fig. 2 (left side). The main structural and fractal properties of the sample can be extracted from the intensity spectrum [16]. We clearly see the presence of Guinier region [7], as a plateau at small values of $q$, and the rightmost part of this plateau indicates the overall size of the system as $q = 2\pi/a$, where $a$ is the side length of ST at $m = 0$.

![Figure 2](image-url)

**Figure 2.** (Color online) On the left side is represented the structure factor for the first five iterations of deterministic ST with side length $a$. On the right side is represented the structure factor of the GCR of ST for $n = 20, 80, 320$, and respectively 1280, generated points.

The exponent of scattering vector between the first and the last minima reveals the fractal dimension, which is given by:

$$D = \lim_{m \to \infty} \frac{\log N_m}{\log (a/a_m)} = 2,$$  \(8\)

where $m$ is the iteration number, $a_m = \beta_s^m a$ is the side length of fractal units centered in the points generated by the deterministic IFS of the ST at $m$-th iteration. For the deterministic case, the number of such minima indicates the iteration number of the fractal. The asymptotic behavior of the structure factor at high $q$ region tends to the value $1/N_m$ and gives the information about the number of units composing the fractal at a given iteration [16].
The right side of Fig. 2 represents the intensity spectrum from the CGR of ST, and it shows how the scattering curve is changing with increasing the number of points $n$. The Guinier region depends on the number of points as expected and such dependence becomes negligible as $n \to \infty$ [18]. The fractal region, that reveals the fractal dimension by the slope of the curve, is increasing with $n$, the slope tends to theoretical value given by Eq. 8, and the asymptotes define the number of constituents, by ratio $1/n$.

\[ S(n) \]

\[ qa \]

**Figure 3.** (Color online) The comparison of structure factors of the deterministic ST at iteration number $m = 4$, with the CGR of ST generated for $n = 1024(4xN_m), 1280(5xN_m), 1536(6xN_m)$.

To understand under which condition (i.e. the number of generated points) the CGR algorithm gives a better approximation of the structure of ST, it is necessary to compare directly the structure factor of the deterministic ST at particular iteration with the structure factor using CGR generated for different number of points. Fig. 3 shows the approximation of structure factor of CGR of ST to the deterministic one, for the 4-th iteration. The main characteristic regions (Guinier, fractal) and features (positions of the minima and their number) are in agreement for both algorithms, when the number of points in the CGR is at least 4 or 5 times $N_m$. The asymptotic behavior, as expected tend to the value $1/(\text{number of units})$, that is in agreement with previous theoretical results.

5. Conclusions
We considered the model of the 3D Sierpinski tetrahedron, which is characterized by fractal dimension $D = 2$ and generated using both, deterministic and CGR constructing algorithms. The structure factor of the deterministic ST is calculated using optimized version of Debye
formula [23]. The results give the information about main structural and fractal properties, such as the fractal dimension (from the slope of the curve in the fractal region), the overall size of the fractal (from the Guinier region), the iteration number (from the number of minima), and the number of units composing the fractal (from the asymptotes of spectrum).

The structure factor of the CGR of ST is calculated for different number of generated points, and we show that the fractal properties appear when that number starts to exceed few hundreds. We compared deterministic structure factor with CGR in order to determine the number of generated points that are needed to approximate ST at particular iteration number and we conclude that the number of CGR points should be 4 or 5 times $N_m$, the number of of units of fractal at $m$-th iteration. The results can be used in obtaining the structural properties of fractals with known CGR, using the small-angle scattering technique.

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