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1994 J. Phys.: Condens. Matter 6 4037

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Diffusion-limited aggregation on Penrose lattices

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Received 2 December 1993, in final form 2 February 1994

Abstract. We simulated the diffusion-limited aggregation (DLA) on a pentagonal lattice and on an octagonal lattice; the fractal dimensions of the DLA on these two lattices are found to be 1.53 and 1.57 respectively, exhibiting a weak lattice dependence. We also calculate the vibrational densities of states for the two DLA clusters; the fracton dimensions of the two DLA clusters appear to follow $d_s = 2d_f/(d_f + 1)$.

1. Introduction

Diffusion-limited aggregation (DLA) which describes phenomena such as dielectric breakdown and electrodeposition has been well studied in recent years [1–8]. Either lattice DLA or off-lattice DLA is simulated in two- to six-dimensional spaces [1–8]. Lattice DLA is known to show a slow crossover in the overall shape. While small clusters of only a few thousand particles have a very ramified structure because of strong fluctuations, the shape of large clusters of several million particles is dominated by the structure of the underlying lattice. Large DLA clusters on a square lattice exhibited a ‘+’ overall shape [5].

As is very well known, off-lattice clusters are fractals with an overall fractal dimension $d_f = 1.715 + 0.004$ [6]. Recently, it has been found that large off-lattice DLA clusters have multifractal features [8, 9]. For small x ($x < 1.5$) (x is the ratio of the distance from the cluster origin to the radius r_g of the gyration), the dimension $d_f(x)$ remains constant ($d_f(x) = 1.65 + 0.06$) but for large x , $d_f(x)$ experiences a sharp drop.

Investigations of the dynamical properties of the fractal structure indicate that there is a kind of special vibrational elementary excitation: a fracton [10]. Alexander and Orbach [10] conjectured that the fracton dimension is $d_s = \frac{4}{3}$, but it is learned that this conjecture does not hold for some fractal structures, e.g. loopless fractals [11]. For DLA, Havlin and Ben-Avraham [11] showed that the fracton dimension is given by $d_s = 2d_f/(d_f + 1)$.

Investigations of the physical problems of quasi-periodic lattices has attracted much interest since the discovery of quasi-crystals by Schechtman *et al* [12] in 1984. However, to date, little attention has been paid to the fractal growth problem on quasi-periodic lattices. Owing to the non-periodicity, strictly speaking, the quasi-periodic lattice is not homogeneous; one concludes naturally that the quasi-periodic lattice DLA will differ from lattice DLA or off-lattice DLA. In this paper, we present the first investigation of DLA on quasi-periodic lattices and, for simplicity, we focus on only the isotropic problem.

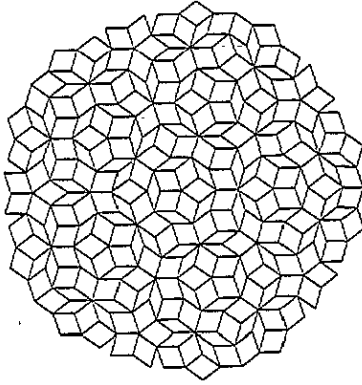


Figure 1. A section of a pentagonal lattice.

2. Quasi-periodic lattice DLA

We consider the diffusion of the particles on quasi-periodic lattices. With $u(x, k)$ labelling the probability that a particle visits site x at its k th step, we have

$$u(x, k+1) = \sum_l \frac{1}{c(x+l)} u(x+l, k) \quad (1)$$

where the sum runs over all the nearest neighbours of site x , $c(x+l)$ representing the coordination number of site $x+l$. For quasi-periodic lattices, $c(x, l)$ is site dependent. Equation (1) is the discrete version of the continuous diffusion equation

$$\frac{\partial u(x, t)}{\partial t} = \nabla[D\nabla u(x, t)] \quad (2)$$

where the diffusion coefficient D is size dependent. In the approximation of $\dot{u}(x, t) = 0$, equation (2) reduces to

$$\nabla[D\nabla u(x, t)] = 0. \quad (3)$$

As is known, the lattice DLA and off-lattice DLA satisfy the Laplace equation $\nabla^2 u(x, t) = 0$ [1]. In fact, a class of fractals is governed by the Laplace equation, namely the Laplace universal class. The quasi-periodic lattice DLA does not satisfy the Laplace equation; therefore, the quasi-periodic lattice DLA will not belong to the Laplace universal class, and it is anticipated that the fractal dimensions of the quasi-periodic lattice DLA will differ from those of lattice DLA or off-lattice DLA.

3. Simulations

3.1. Pentagonal lattice DLA

A pentagonal lattice was first constructed by the use of the generalized dual method [13] before simulation, which is shown in figure 1. The first step in simulation is to put a seed at the centre of the lattice, i.e. at the site with fivefold symmetry. In the simulation, the radius of the launching circle is chosen as $r_{\max} + 5$, and the radius of the killing circle is the larger of $r_{\max} + 10$ and $2r_{\max}$, where r_{\max} represents the maximal radius of the cluster.

The DLA cluster produced on the pentagonal lattice is shown in figure 2; it is composed of 2461 particles. Figure 3 shows the scaling of its mass M with its size. The fractal dimension of the DLA (the slope of the fitting line in figure 3) is evaluated to be $d_f = 1.53 \pm 0.02$.

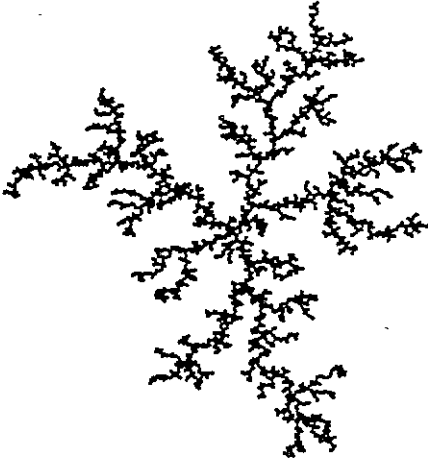


Figure 2. A DLA cluster on a pentagonal lattice.

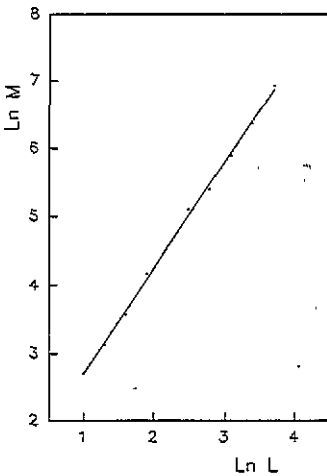


Figure 3. The M - L scaling of the pentagonal lattice DLA, which shows that the fractal dimension is 1.53 ± 0.02 .

3.2. Octagonal lattice DLA

To perform the DLA simulation on an octagonal lattice, similar to the above, we first produced an octagonal lattice by use of the projection method. Figure 4 shows a section of this octagonal lattice. This time, the seed is also placed at the centre of the lattice, but the site has eightfold symmetry. The other constraints in the growth are also similar to the above.

The DLA on the octagonal lattice is shown in figure 5; it is composed of 3286 particles. The scaling of its mass M with its size L gives the fractal dimension $d_f = 1.57 \pm 0.02$, which is shown in figure 6.

On comparison with the usual isotropic models of the periodic lattice DLA and off-lattice DLA, it can be observed that the fractal dimension of the DLA on the quasi-periodic lattices are slightly smaller; they are also different from each other.

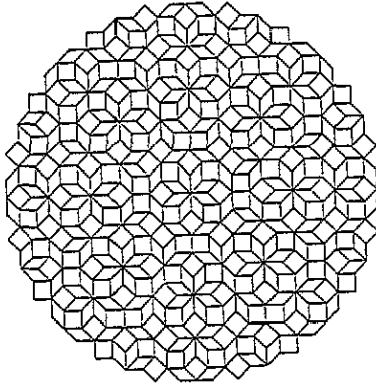


Figure 4. A section of an octagonal lattice.

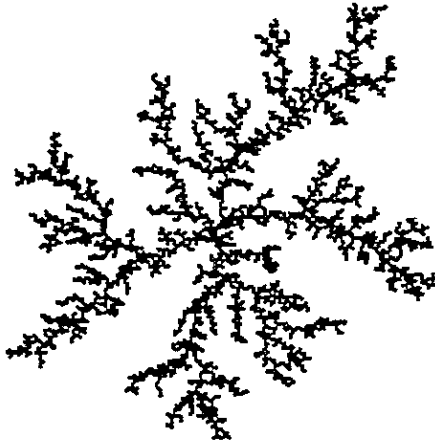


Figure 5. A DLA cluster on an octagonal lattice.

The DLA clusters produced in our simulation, although not large enough, exhaust the computer that we used. As a whole, the construction of quasi-periodic lattice consumes much time. An even larger simulation scale is necessary for this subject. In a crude way, the above results more or less demonstrate the dependence of the fractal dimension of DLA on lattices.

4. Fracton in quasi-periodic lattice DLA

We calculated the vibrational density of states (VDOS) of the pentagonal lattice DLA and the octagonal lattice DLA using the recursion method of Haydock *et al* [14]. The single-parameter Born potential, which is expressed as [15]

$$U = \frac{1}{2}\alpha \sum_{i,j}^{\text{NN}} |u_i - u_j|^2 \quad (4)$$

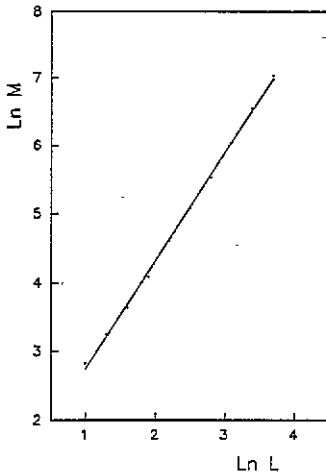


Figure 6. The M - L scaling of the octagonal lattice DLA, which shows that the fractal dimension is 1.57 ± 0.02 .

is adopted, where the sum for i runs over all the sites of the cluster and j over all the nearest neighbours of site i , α represents the force constant and u_i is the displacement of site i . The free-boundary condition is used.

Figure 7 shows the log-log VDOS of the pentagonal lattice DLA cluster (figure 2); the fracton frequency region (the flatter and linear part of the figure) is obviously exhibited. Owing to the fixed size of the cluster, correspondingly there is a lower limit of fracton frequency; beyond the limit, the wavelength will be larger than the cluster size. Similarly, the fixed nearest distance between atoms gives the upper limit of fracton frequency. According to $d_s = 2d_f/(d_f + 1)$ [11], when d_f is 1.53, d_s is about 1.21. We plot a straight line (solid line) with slope $d_s - 1 = 0.21$ in the figure; it is observed that the line fits the fracton DOS quite well.

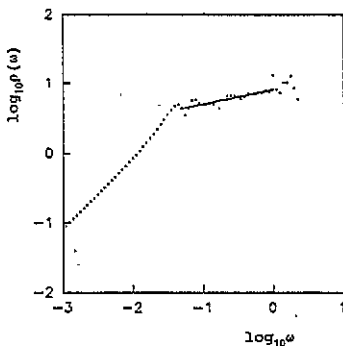


Figure 7. The VDOS of the DLA cluster on the pentagonal lattice.

We show the log-log VDOS of the octagonal lattice DLA cluster in figure 8. Now, $d_s = 2d_f/(d_f + 1)$ ($d_f = 1.57$) gives the fracton dimension to be 1.22. The solid line in the figure has a slope of 0.22; it can be seen this line also fits the fracton DOS roughly.

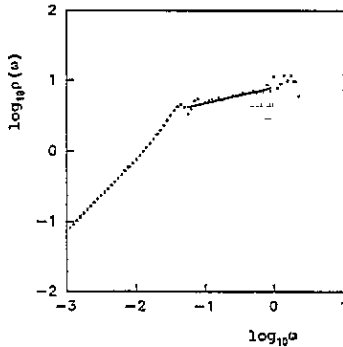


Figure 8. The VDOS of the DLA cluster on the octagonal lattice.

5. Summary

In summary, the simulation of the quasi-periodic lattice DLA shows a weak dependence of the fractal dimensions on the adopted quasi-lattices. For the pentagonal lattice, the fractal dimension of DLA is 1.53 and, for the octagonal lattice, it is 1.57. The computations of the VDOSs of the pentagonal lattice DLA and the octagonal lattice DLA give fracton dimensions which follow $d_s = 2d_f/(d_f + 1)$.

Acknowledgments

Support from The National Natural Science Foundation of China and the Natural Science Foundation of South China University of Technology is acknowledged.

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