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Shelling of Homogeneous Media

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Abstract

A homogeneous medium is characterised by a point set in Euclidean space (for the atomic positions, say), together with some self-averaging property. Crystals and quasicrystals are homogeneous, but also many structures with disorder still are. The corresponding shelling is concerned with the number of points on shells around an arbitrary, but fixed centre. For non-periodic point sets, where the shelling depends on the chosen centre, a more adequate quantity is the *averaged* shelling, obtained by averaging over points of the set as centres. For homogeneous media, such an average is still well defined, at least almost surely (in the probabilistic sense). Here, we present a two-step approach for planar model sets.

1. Introduction

The discovery of quasicrystals and the challenge to describe their structure led to a revived interest in model sets[1, 2, 3, 4]. These sets, also called cut-and-project sets, are pure point diffractive[3, 4] (under some mild assumptions), and can be regarded as generalisations of lattices to an aperiodic setting. Recently, various combinatorial properties of the corresponding point sets in Euclidean space have been investigated[5, 6, 7]. Among those, which are natural generalisations of the lattice case, is the shelling problem, which is considered in this article.

The shelling structure of a point set consists of the number of points on shells around an arbitrary, but fixed centre. For a lattice Γ, the answer does not depend on the centre, as long as it is in Γ. However, the corresponding statement is no longer true for non-periodic point sets. In fact, it might even happen that no two centres give the same result. In such cases, a more adequate quantity is the *averaged* shelling, obtained by taking the average over all points of the set as centres.

This radial distribution function is a characteristic geometric quantity that reflects itself in the corresponding (powder) diffraction spectrum and related objects of physical interest. The underlying combinatorial and algebraic structure is well understood for periodic crystals, but less so for non-periodic arrangements such as mathematical quasicrystals or model sets. Here, we concentrate on the case of planar model sets. In this case, the answer consists of a universal part that encodes properties of the underlying cyclotomic number field, and a non-universal part that depends on the details of the model set construction.

2. Planar Lattices

Before we consider aperiodic model sets, we briefly summarise the result for two periodic planar cases with irreducible point symmetry, the square lattice and the triangular lattice. This is of course well known[8], but we shall follow an approach that generalises to the model set case. We start with the square lattice.

To this end, consider the vertex set of the square lattice as a subset of the complex plane, i.e., as the set of Gaussian integers $\mathbb{Z}[i] = \{a + bi \mid a, b \in \mathbb{Z}\}$, which are the integers in the cyclotomic field $\mathbb{Q}(i)$. The number $c(r^2)$ of lattice points on circles of radius r around the origin is then the number of solutions of the equation $x\overline{x} = r^2$ with $x \in \mathbb{Z}[i]$, where $\overline{x}$ denotes the complex conjugate of x. Note that, if there are solutions at all, the number r^2 must be an integer. Since $r^2 = 0$ is trivial (with $c(0) = 1$), we restrict to $r^2 > 0$ from now on.

To compute the number of solutions, we employ prime factorisation. The cyclotomic field $\mathbb{Q}(i)$ has class number one, so prime factorisation is unique, which means that, up to units, we can uniquely factorise r^2 in terms of primes in $\mathbb{Q}$ or in $\mathbb{Q}(i)$. In the complex field extension from $\mathbb{Q}$ to $\mathbb{Q}(i)$, three situations can occur. If a prime $p \in \mathbb{Z}$ is also a prime in $\mathbb{Z}[i]$, it is called *inert.* If $p \in \mathbb{Z}$ is, up to a unit, the square of a prime in $\mathbb{Z}[i]$, i.e., $p = \varepsilon\pi^2$ with π a prime in $\mathbb{Z}[i]$ and $\varepsilon \in \{\pm i, \pm 1\}$, we say that p *ramifies.* Finally, if $p = \varepsilon\pi\overline{\pi}$ where the primes $\pi, \overline{\pi} \in \mathbb{Z}[i]$ are not related to each other by a unit, the prime p *splits.* The situation for the Gaussian integers is summarised in Table 1. An example for a splitting prime is $5 = (2 + i)(2 - i)$.

Consider the prime factorisation of a positive integer r^2 within $\mathbb{Q}(i)$, up to units. The number of solutions of the equation $x\overline{x} = r^2$ is obtained by counting in how many ways we can distribute the prime factors of r^2 on x and $\overline{x}$, such that they are complex conjugates of each other. If r^2 contains an *inert* prime factor p, we can only do this if it occurs with an even power, say p^{2t}, in which case both x and $\overline{x}$ must contain a factor p^t. If r^2 contains a *ramified* prime factor $p^t \sim \pi^{2t}$, we also have only one choice; both x and $\overline{x}$ contain the factor π^t (up to a unit, to accommodate complex conjugation). Finally, if r^2 is divisible by the power $p^t = \pi^t\overline{\pi}^t$ of a *splitting* prime p, we have (t+1) possibilities: x can contain a factor $\pi^s\overline{\pi}^{t-s}$ for $s = 0, 1, \ldots, t$, with $\overline{x}$ containing the remaining factor $\pi^{t-s}\overline{\pi}^s$. Since we have four units, it is obvious that solutions come in groups of four.

Consequently, for $r^2 > 0$, the shelling number $c(r^2)$ vanishes unless r^2 is an integer such that all inert primes factors of r^2 occur with even powers, whence

$$c(r^2) \;=\; 4 \prod_{\substack{p \mid r^2 \\ p \text{ splits}}} \bigl(t(p) + 1\bigr)\,, \tag{1}$$

Table 1: Splitting of primes in the field extension from $\mathbb{Q}$ to $\mathbb{Q}(i)$.

Primes p in $\mathbb{Z}$	Primes π in $\mathbb{Z}[i]$	
$p = 2$	$2 = -i(1+i)^2 = \varepsilon\pi^2$	ramifies
$p \equiv 1 \bmod 4$	$p = \pi\overline{\pi}$	**splits**
$p \equiv 3 \bmod 4$	$p = \pi$	inert

where the product is over all splitting primes that divide r^2, and $t(p)$ is the maximum power such that $p^{t(p)}$ divides r^2. The actual values can then be derived using the splitting structure as given in Table 1. Noting that $a(r^2) = c(r^2)/4$ is a multiplicative arithmetic function, we can encapsulate the result neatly in terms of a Dirichlet series generating function, which turns out[7] to be the Dedekind zeta function of the cyclotomic field $\mathbb{Q}(i)$.

The situation is very similar for the triangular lattice, which we consider as the set of Eisenstein integers $\mathbb{Z}[\xi_3] = \{a + b\xi_3 \mid a, b \in \mathbb{Z}\}$, where $\xi_3 = \exp(2\pi i/3)$, hence $1 + \xi_3 + \xi_3^2 = 0$. Now, there are six units, ξ_3^k and $\xi_3^k(1 + \xi_3)$, $k \in \{0, 1, 2\}$. The splitting structure is given in Table 2; an example of a splitting prime is $13 = (3 + 2i)(3 - 2i)$. The shelling numbers are again given by equation (1), but with the prefactor 4 replaced by 6.

Table 2: Splitting of primes in the field extension from $\mathbb{Q}$ to $\mathbb{Q}(\xi_3)$.

Primes p in $\mathbb{Z}$	Primes π in $\mathbb{Z}[\xi_3]$	
$p = 3$	$3 = (1 + \xi_3)(1 - \xi_3)^2 = \varepsilon\pi^2$	ramifies
$p \equiv 1 \bmod 3$	$p = \pi\overline{\pi}$	**splits**
$p \equiv 2 \bmod 3$	$p = \pi$	inert

3. Shelling of Planar Modules

In fact, the basic argument generalises[5, 6, 7] to any planar module $\mathbb{Z}[\xi_n]$ with ξ_n a primitive nth root of unity, provided that unique prime factorisation holds, which limits it to the cases where the cyclotomic field $\mathbb{Q}(\xi_n)$ has class number one. This leaves 29 cases of interest, $n \in \{3, 4, 5, 7, 8, 9, 11, 12, 13, 15, 16, 17, 19, 20, 21, 24, 25, 27, 28, 32, 33, 35, 36, 40, 44, 45, 48, 60, 84\}$, which correspond to planar modules with N-fold rotational symmetry, where $N = n$ for even n, and $N = 2n$ for odd n, is the number of units. Apart from the crystallographic cases $n = 3$ and $n = 4$, these modules correspond to dense point sets in the plane. Nevertheless, the shelling numbers for these point sets are again given by equation (1), with the prefactor 4 now replaced by the corresponding value of N. Of course, the appropriate splitting structure of the primes needs to be used. Note that, for the module, there is again

Table 3: Splitting of primes in the field extension from $\mathbb{Q}(\tau)$ to $\mathbb{Q}(\xi)$.

Primes p in $\mathbb{Z}$	Primes P in $\mathbb{Z}[\tau]$	Primes π in $\mathbb{Z}[\xi]$	
$p = 5$	$5 = (\sqrt{5})^2$	$\sqrt{5} \sim (1 - \xi)^2$	ramifies
$p \equiv 1 \bmod 5$	$p = P_1 P_2$	$P_i = \pi_i \overline{\pi}_i$	**splits**
$p \equiv \pm 2 \bmod 5$	$p = P$	$P = \pi$	inert
$p \equiv -1 \bmod 5$	$p = P_1 P_2$	$P_i = \pi_i$	inert

no difference between central and averaged shelling.

As an explicit example, we consider the case $n = 5$, where we may choose $\xi = \xi_5 = \exp(2\pi i/5)$ as the primitive root. We now have three fields that enter; besides $\mathbb{Q}$ and the cyclotomic field $\mathbb{Q}(\xi)$, the third is the maximal real subfield of the latter, $\mathbb{Q}(\tau) = \mathbb{Q}(\sqrt{5})$, where $\tau = \xi + \bar{\xi} = (1+\sqrt{5})/2$ is the golden number. The possible squared radii of the circles are now in $\mathbb{Z}[\tau]$ (i.e., they are integers in the field $\mathbb{Q}(\tau)$), so the splitting that we have to consider in equation (1) is that from $\mathbb{Q}(\tau)$ to $\mathbb{Q}(\xi)$. The splitting structure is given in Table 3.

As mentioned before, this module corresponds to a dense point set in the plane. The model sets of interest [3, 4] are suitable Delone subsets of modules of this type. Therefore, the shelling problem for the module determines the *maximum* number that may occur on shells of a given radius, the actual number depending on how the selection of points takes place.

4. Averaged shelling of model sets

We consider the example of the vertex set of the Tübingen triangle tiling. This set is given by selecting all $x \in \mathbb{Z}[\xi]$ for which $x^\star$, the image under the map $\star: \ \xi \mapsto \xi^2$ which is a Galois automorphism of $\mathbb{Q}(\xi)$, falls into a domain W which is a regular decagon of edge length $\tau/\sqrt{2+\tau}$, i.e., $\varLambda = \{x \in \mathbb{Z}[\xi] \mid x^\star \in W\}$. This choice corresponds to a binary triangle tiling with edge lengths $1/\tau = \tau - 1$ and 1.

To calculate the averaged shelling, we use Weyl's theorem of uniform distribution[9]. The frequency of a difference $x \in \varLambda - \varLambda$ is given by the the relative

Table 4: Averaged shelling for the Tübingen triangle tiling.

r^2	representative	orbit	$t^2 = \sigma(r^2)$	type	av. shelling
$2-\tau$	$\xi+\bar{\xi}$	10	$1+\tau$	1	$6-2\tau$
1	1	10	1	1	$28-14\tau$
$3-\tau$	$\xi^2-\bar{\xi}^2$	10	$2+\tau$	2	$-50+32\tau$
$5-2\tau$	$2+\xi^2$	20	$3+2\tau$	3	$-32+20\tau$
$4-\tau$	$1-\xi-\bar{\xi}^2$	20	$3+\tau$	3	$112-68\tau$
$1+\tau$	$\xi^2+\bar{\xi}^2$	10	$2-\tau$	1	$20-8\tau$
$2+\tau$	$\xi-\bar{\xi}$	10	$3-\tau$	2	$-44+30\tau$
4	2	10	4	1	$-18+12\tau$
$3+\tau$	$1-\xi-\xi^2$	20	$4-\tau$	3	$32-16\tau$
5	$1+2\xi+2\bar{\xi}$	10	5	1	$4-2\tau$
$3+2\tau$	$2+\xi$	20	$5-2\tau$	3	$-264+168\tau$
$2+3\tau$	$1-\xi^2-\bar{\xi}^2$	10	$5-3\tau$	1	$102-58\tau$
$6+\tau$	$1-2\xi-\xi^2$	20	$7-\tau$	3	$260-160\tau$
$5+2\tau$	$2-\xi^2$	20	$7-2\tau$	3	$288-176\tau$
$7+\tau$	$3+\xi+\xi^2$	20	$8-\tau$	3	$-168+104\tau$

overlap area, or covariogram, of the window W and a copy shifted by $x^\star$. Due to the dihedral D_{10} symmetry of the window, the result is the same for the entire D_{10} orbit of $x^\star$, thus it is sufficient to consider one representative, and multiply the covariogram by the length of the orbit. The result for the Tübingen triangle tiling is given in Table 4, which contains all possible radii $r \leq 3$, completing and extending a previously published table[7] where one possible radius was missed. Here, $t^2 = \sigma(r^2) = \sigma(x\overline{x})$ is the squared length of $x^\star$, and σ is algebraic conjugation in the field $\mathbb{Q}(\tau)$, which maps $\sqrt{5} \mapsto -\sqrt{5}$, hence $\sigma(\tau) = -1/\tau = 1 - \tau$.

The averaged shelling numbers are in $\mathbb{Z}[\tau]$ (and probably even in $2\mathbb{Z}[\tau]$), which can be understood from topological properties of the tiling[10, 11] and its symmetry. The frequency module of the tiling, which is the integer span of the frequencies of all finite clusters, is constrained by the existence of topological invariants[10, 11]. Here[11], it is $\frac{1}{10}\mathbb{Z}[\tau]$. As all averaged shelling numbers are finite sums with integer coefficients and weights from the frequency module, the restriction is inherited.

Explicit results for the averaged shelling numbers were also obtained for the eightfold symmetric Ammann-Beenker model set[5] and for the vertex set of the twelvefold symmetric shield tiling[6]. These point sets are obtained from the modules $\mathbb{Z}[\exp(2\pi i/8)]$ and $\mathbb{Z}[\exp(2\pi i/12)]$, with a regular octagon and a regular dodecagon as windows, respectively. In the natural choice of length scales, the Ammann-Beenker tiling contains squares and 45 degree rhombi of egde length one. The shield tiling is made up of equilateral triangles, squares and 'shield'-shaped hexagons, all of the same edge length $\sqrt{2-\sqrt{3}}$.

Table 5: Averaged shelling for planar tilings.

r	square	triangular	Ammann-Beenker	Tübingen	shield
0.518					4.536
0.618				2.764	
0.732					2.000
0.765			1.172		
0.897					0.536
1.000	4.000	6.000	4.000	5.348	8.000
1.176				1.777	
1.239					3.072
1.328				0.361	
1.414	4.000		2.485		6.431
1.506					6.000
1.543				1.974	
1.618				7.056	
1.674					0.210
1.732		6.000	3.029		5.238
1.848			4.887		
1.880					1.525
1.902				4.541	
1.932					9.895
2.000	4.000	6.000	0.828	1.416	4.309

For the Ammann-Beenker tiling and the shield tiling, the averaged shelling numbers lie in index-2 submodules of $\mathbb{Z}[\sqrt{2}]$ and $\frac{1}{2}\mathbb{Z}[1/\sqrt{3}]$, respectively. Details will be given elsewhere[12]. To give a rough impression of the differences between these tilings, their averaged shelling numbers for radii $r \leq 2$ are compared in Table 5. Clearly, an increasing number of radii with small occupation, which are absent in the lattice case, appear as the value of N increases. The growth of the number of possible radii reflects the increasing local complexity of the tiling. Of course, this comparison is somewhat arbitrary, as we might have scaled the tilings differently, for instance such that the shortest distance is the same in all cases. Nevertheless, it becomes evident that nonperiodic systems tend to have a larger number of occupied shells, as expected.

An analogous approach is possible for other combinatorial quantities, such as averaged coordination numbers[12].

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