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Lattice Substitution Systems and Model Sets

by

Jeong-Yup Lee



A thesis submitted to the Faculty of Graduate Studies and Research in partial
fulfillment of the requirements for the degree of Master of Science.

in

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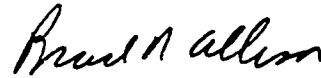
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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled **Lattice Substitution Systems and Model Sets** submitted by **Jeongyup Lee** in partial fulfillment of the requirements for the degree of Master of Science in Mathematics.



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Abstract

The paper studies ways in which the sets of a partition of a lattice in \mathbb{R}^n become regular model sets. The main theorem gives equivalent conditions which assure that a substitution system on a lattice in \mathbb{R}^n gives rise to regular model sets (based on p -adic-like internal spaces), and hence to pure point diffractive sets. The methods developed here are used to show that the n -dimensional chair tiling and the sphinx tiling are pure point diffractive.

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Table of Contents

Chapter 1 - Introduction	1
Chapter 2 - Preliminaries	4
2.1 Definitions and notation	4
2.2 Substitution systems on lattices	5
2.3 Perron-Frobenius theory	7
2.4 Primitive substitution system and boundary measure	8
Chapter 3 - Model Sets	11
3.1 Basic definitions	11
3.2 The main result	12
Chapter 4 - Sphinx Tiling	21
Chapter 5 - The Total Index and Model Sets	25
5.1 Coset part and total index	25
5.2 Total index and model sets	27
Chapter 6 - Chair Tiling	30
References	37
Appendix	39

Chapter 1

Introduction

The world in which we are living is filled with objects, which themselves are actually composed of atoms. Physicists have studied the structure of large assemblages of atoms, which are often very highly ordered objects. A good deal about this structure can be learned through the diffraction patterns, formed when monochromatic radiation (X-rays, electrons, and neutrons) scatters after interacting with the atoms. This is a basic tool of crystallography.

Once aperiodic structures of atoms with pure point diffraction were discovered (for the first time in 1984), many mathematicians and physicists became interested in knowing the structure of arrays of atoms having pure point spectra. Mathematically we consider these atoms as points in \mathbb{R}^n . The pure point diffraction of a point set gives us a glimpse of how nicely the point set is distributed over \mathbb{R}^n . But what is the scientific interpretation of this “*nicely*”? Many researchers have wondered about this and worked on it. Yet at the present it is still a mystery.

There is a general theorem by M. Schlottmann which says that any model set, a term which will be defined later, is pure point diffractive (see Theorem 2). This naturally raises the question of what the model sets are concretely. In this thesis, we find the equivalent and practical conditions for certain discrete point sets of \mathbb{R}^n , created through lattice substitution systems, to be model sets. In this way we get large collections of discrete point sets which have pure point diffraction.

There has been a lot of work on the connection of discrete point sets and pure point diffraction. But so far much of it has stayed in the domain of 1-dimension (or sequences) or in point sets coming from 2-dimensional tilings. In this thesis no such assumptions are necessary, and so it could be considered as a good place to let our viewpoint turn to the space \mathbb{R}^n for general n .

In the subject of long range aperiodic order, there have been two main approaches to building discrete mathematical structures. One is the substitution method and the other is the cut and project or model set method. In the first case the structure is generated by successive substitution of a finite configuration. In the second it is formed by the projection of a lattice from some higher dimensional embedding space.

We get to connect these two methods in this thesis.

We start with a finite number of point sets which are generated by some substitution system (Φ) and are invariant under Φ . The main theorem gives the criteria for these point sets to be model sets.

The connection between substitution systems and cut and project sets is nothing new. The Fibonacci chain is often described in terms of a cut by a strip through \mathbb{Z}^2 . Nonetheless the relationship between them remains very inadequately understood.

The terminology of *model set* in the cut and project theory originated in Meyer's work which actually predates the subject of aperiodic order. In his work he replaced the internal space \mathbb{R}^p in the cut and project scheme by any locally compact abelian group. Since our internal space is p-adic type space, not \mathbb{R}^p , we use Meyer's terminology here in deference to its priority and to emphasize the greater generality of the internal space.

Of relevance to this work is Dekking's criterion which says that the equal length aperiodic tiling in 1-dimension is pure point diffractive if and only if it admits a coincidence. Dekking's approach was through the dynamic systems. Here we are working on n-dimensional objects using purely algebraic and topological tools. Our result implies that if a substitution system Φ admits a coincidence, then it is pure point diffractive. We do not know yet to what extent the condition is *equivalent* to pure point diffractivity.

The setting of the thesis is entirely at the level of point sets, so necessarily the strong conditions implicit in the tiling situation are replaced here by a corresponding algebraic condition on the lattice substitution system: the Perron-Frobenius eigenvalue of the lattice substitution system should equal the determinant of its inflation. This is in fact a compatibility condition which is necessary for the model set connection to exist.

We now present a brief overview of the thesis.

Chapter 2 contains quite a few definitions and most of the basic notation. It makes theorems have a nice shape. One can come back to here to recall the terminology which we use in the next chapters. The major part here consists of some results about Perron-Frobenius(PF) theory and a nice theorem about boundary measure using PF results.

In Chapter 3, we introduce the cut and project scheme, based on projection into \mathbb{R}^n from a lattice in some higher space $\mathbb{R}^n \times G$, where G is some locally compact abelian group, the projection being controlled by a relatively compact set $W \subset G$. If a set in \mathbb{R}^n is controlled by a nonempty compact set $W \subset G$, it is called a model

set. We will learn concrete definitions of model sets and the regular model sets in this chapter. We make use of the boundary measure 0 result, which we will obtain in Chapter 2, in the main theorem. The theorem gives the equivalent conditions for a discrete point set to be a regular model set in the context of lattice substitution systems. One of these conditions is checkable by computation and so provides a practical method of checking for pure point diffractivity.

In Chapter 4, there is an interesting example to which the main theorem can be applied. It is called a sphinx tiling. The sphinx tiling is claimed in [18] as being provable to have pure point diffractivity by a geometric form of “coincidence” established there. We show how to construct the sphinx tiling in \mathbb{R}^2 and how to make the computational matrix to which we can apply our criteria. The result is that the sphinx tiling is pure point diffractive.

In Chapter 5, we introduce the new concepts of coset part and total index. This brings us to regular model sets again and is nicely connected with what we established in Chapter 3. We can learn that the existence of just one coset in our set-up with a substitution system means that the lattice is almost covered by cosets.

In Chapter 6, we show how the theorem in Chapter 5 can be applied to a chair tiling. The chair tiling is a famous example in the subject of aperiodic structures. It has been established for $n = 2$ previously in [18],[4] that the chair tiling in \mathbb{R}^2 is a regular model set. But for the first time we establish this result for the general chair tiling in \mathbb{R}^n . This is helpful to understand the structure of the chair tiling as an aperiodic object. It turns out that the chair tiling is also pure point diffractive.

Although diffraction underlies the motivation of this work, our approach through model sets and Schlottmann’s theorem makes it unnecessary to know anything about it. Still, for the convenience of the reader we have included an Appendix which provides the main definitions and concepts behind diffraction.

Chapter 2

Preliminaries

2.1 Definitions and Notation

We introduce a matrix function system (MFS) on a set X . It looks like a matrix, but its entries are a set of functions and the product of two MFS is formed by the composition of functions at corresponding entries in the matrix. The corresponding substitution matrix $S(\Phi)$ of MFS (Φ) is an ordinary number matrix which is made from Φ .

Let X be a nonempty set. For $m \in \mathbb{Z}_+$, an $m \times m$ *matrix function system* (MFS) on X is an $m \times m$ matrix $\Phi = (\Phi_{ij})$, where each Φ_{ij} is a set (possibly empty) of mappings X to X .

The corresponding matrix $S(\Phi) := (\text{card}(\Phi_{ij}))_{ij}$ is called the *substitution matrix* of Φ . The MFS is *primitive* if $S(\Phi)$ is primitive, i.e. there is an $l > 0$ for which $S(\Phi)^l$ has no zero entries.

In this paper we deal only with MFSs which are *finite* in the sense that $\text{card}(\Phi_{ij}) < \infty$ for all i, j . Of particular importance are the Perron-Frobenius (PF) eigenvalue and the corresponding PF eigenvector (unique up to a scalar factor) of $S(\Phi)$. We will also have use for the *incidence matrix* $I(\Phi)$ of Φ , which is defined by

$$(I(\Phi))_{ij} = \begin{cases} 1 & \text{if } \text{card}(\Phi_{ij}) \neq 0 \\ 0 & \text{else.} \end{cases}$$

Let $P(X)$ be the set of subsets of X . Any MFS induces a mapping on $P(X)^m$ by

$$\Phi \begin{bmatrix} U_1 \\ \vdots \\ U_m \end{bmatrix} = \begin{bmatrix} \bigcup_j \bigcup_{f \in \Phi_{1j}} f(U_j) \\ \vdots \\ \bigcup_j \bigcup_{f \in \Phi_{mj}} f(U_j) \end{bmatrix}, \quad (1)$$

which we call the *substitution* determined by Φ . We sometimes write $\Phi_{ij}(U_j)$ to mean $\bigcup_{f \in \Phi_{ij}} f(U_j)$.

In the sequel, X will be a lattice L in \mathbb{R}^n and the mappings of Φ will always be affine linear mapping of the form $x \mapsto Qx + a$, where $Q \in \text{End}_{\mathbb{Z}}(L)$ is the same for all the maps. Such maps extend to \mathbb{R}^n . For any affine mapping $f : x \mapsto Qx + b$ on L we denote the translational part, b , of f by $t(f)$. We say that $f, g \in \Phi$ are *congruent mod QL* if $t(f) \equiv t(g) \pmod{QL}$. This equivalence relation partitions Φ into congruence classes. For $a \in L$, $\Phi[a] := \{f \in \bigcup_{i,j} \Phi_{ij} \mid t(f) \equiv a \pmod{QL}\}$.

We say that Φ *admits a coincidence* if there is an i , $1 \leq i \leq m$, for which $\bigcap_{j=1}^m \Phi_{ij} \neq \emptyset$, i.e. the same map appears in every set of the i -th row for some i . Furthermore, if $\Phi^M[a]$ is contained entirely in one row of the $\text{MFS}(\Phi^M)$ for some $M > 0, a \in L$, then we say that (\tilde{U}, Φ) admits a *modular coincidence*.

Let Φ, Ψ be $m \times m$ MFSs on X . Then we can compose them :

$$\Psi \circ \Phi = ((\Psi \circ \Phi)_{ij}), \quad (2)$$

where $(\Psi \circ \Phi)_{ij} = \bigcup_{k=1}^m \Psi_{ik} \circ \Phi_{kj}$ and $\Psi_{ik} \circ \Phi_{kj} := \begin{cases} \{g \circ f \mid g \in \Psi_{ik}, f \in \Phi_{kj}\} \\ \emptyset & \text{if } \Psi_{ik} = \emptyset \text{ or } \Phi_{kj} = \emptyset. \end{cases}$

Evidently, $S(\Psi \circ \Phi) \leq S(\Psi) S(\Phi)$ (see (10) for the definition of the partial order).

For an $m \times m$ MFS Φ , we say that $\tilde{U} := [U_1, \dots, U_m]^T \in P(X)^m$ is a *fixed point* of Φ if $\Phi \tilde{U} = \tilde{U}$.

2.2 Substitution Systems on Lattices

Several properties of a profinite group are presented. The reader can just think of the familiar group \mathbb{Z}_p^n (p -adic integer) for the profinite group. We will consider a map from a lattice L in \mathbb{R}^n to its profinite completion \bar{L} . Then a function f with *inflation* Q in L will be a *contraction* in \bar{L} . This gives us a fixed compact set, called an attractor, in \bar{L} .

Let L be a lattice in \mathbb{R}^n . A mapping $Q \in \text{End}_{\mathbb{Z}}(L)$ is an *inflation* for L if $\det Q \neq 0$ and

$$\bigcap_{k=0}^{\infty} Q^k L = \{0\}. \quad (3)$$

Let Q be an inflation. Then $q := |\det Q| = [L : QL] > 1$. We define the Q -adic completion

$$\overline{L} = \overline{L_Q} = \lim_{\leftarrow k} L/Q^k L \quad (4)$$

of L . \overline{L} will be supplied with the usual topology of a profinite group. We have a natural extension of Q on \overline{L} such that $Q\overline{L} = \lim_{\leftarrow k} QL/Q^k L$. In particular, the cosets $a + Q^k \overline{L}$, $a \in L$, $k = 0, 1, 2, \dots$, form a basis of open sets of \overline{L} and each of these cosets is both open and closed. When we use the word *coset* in this paper, we mean either a coset of the form $a + Q^k \overline{L}$ in \overline{L} or $a + Q^k L$ in L , according to the context. An important observation is that any two cosets in \overline{L} are either disjoint or one is contained in the other. The same applies to cosets of L .

We let μ denote Haar measure on \overline{L} , normalized so that $\mu(\overline{L}) = 1$. Thus for cosets,

$$\mu(a + Q^k \overline{L}) = \frac{1}{|\det Q|^k} = \frac{1}{q^k}. \quad (5)$$

We also have need of the metric d on \overline{L} defined via the standard norm:

$$\|x\| := \frac{1}{q^k} \quad \text{if } x \in Q^k \overline{L} \setminus Q^{k+1} \overline{L}, \quad \|0\| = 0. \quad (6)$$

From $\bigcap_{k=0}^{\infty} Q^k L = \{0\}$, we conclude that the mapping $x \mapsto \{x \bmod Q^k L\}_k$ embeds L in \overline{L} . We identify L with its image in \overline{L} . Note that \overline{L} is the closure of L , whence the notation.

An *affine lattice substitution system* on L with inflation Q is a pair (\tilde{U}, Φ) consisting of disjoint subsets $\{U_i\}_{i=1}^m$ of L and an $m \times m$ MFS Φ on L for which $\tilde{U} = [U_1, \dots, U_m]^T$ is a fixed point of Φ , i.e.

$$U_i = \bigcup_{j=1}^m \bigcup_{f \in \Phi_{ij}} f(U_j), \quad i = 1, \dots, m, \quad (7)$$

where the maps of Φ are affine mappings of the form $x \mapsto Qx + a$, $a \in L$, and in which the unions in (7) are *disjoint*. In this paper all our matrix function systems are composed of affine mappings on a lattice and we often drop the words ‘affine lattice’, speaking simply of substitution systems.

We say that the substitution system (\tilde{U}, Φ) is *primitive* if Φ is primitive. A second substitution system (\tilde{U}', Ψ) is called *equivalent* to (\tilde{U}, Φ) if $\tilde{U}' = \tilde{U}$, Ψ and Φ have the same inflation, and $S(\Psi), S(\Phi)$ have the same PF-eigenvalue and right PF-eigenvector (up to scalar factor).

Let (\tilde{U}, Φ) be a substitution system on L . Identifying L as a dense subgroup of \overline{L} , we have a unique extension of Φ to a MFS on \overline{L} in the obvious way. Thus if $f \in \Phi_{ij}$ and $f : x \mapsto Qx + a$, then this formula defines a mapping on \overline{L} , to which we give the same name. Note that f is a *contraction* on \overline{L} , since $\|Qx\| = \frac{1}{q}\|x\|$ for all $x \in \overline{L}$. Thus Φ determines a multi-component iterated function system on \overline{L} . Furthermore defining the compact subsets

$$W_i := \overline{U_i}, \quad i = 1, \dots, m, \quad (8)$$

and using (7) and the continuity of the mapping, we have

$$W_i = \bigcup_{j=1}^m \bigcup_{f \in \Phi_{ij}} f(W_j), \quad i = 1, \dots, m, \quad (9)$$

which shows that $\tilde{W} = [W_1, \dots, W_m]^T$ is the unique *attractor* of Φ (see [3],[8]).

We call (\tilde{W}, Φ) the *associated Q -adic system*. We cannot expect in general that the decomposition in (9) will be disjoint, so we do *not* call (\tilde{W}, Φ) a substitution system.

2.3 Perron-Frobenius Theory

Perron-Frobenius theory has been used in mathematics and physics extensively, since non-negative matrices are so prevalent and the properties of eigenvector and eigenvalue are so powerful when we deal with a matrix. We state a couple of the results from this theory.

For $X, Y \in \mathbb{R}^n$, we write

$$\begin{aligned} X \leq Y & \text{ if } X_i \leq Y_i \text{ for all } 1 \leq i \leq n \\ X < Y & \text{ if } X_i < Y_i \text{ for all } 1 \leq i \leq n. \end{aligned}$$

Similarly, for $A, B \in M_n(\mathbb{R})$

$$\begin{aligned} A \leq B & \text{ if } A_{ij} \leq B_{ij} \text{ for all } 1 \leq i, j \leq n \\ A < B & \text{ if } A_{ij} < B_{ij} \text{ for all } 1 \leq i, j \leq n. \end{aligned} \quad (10)$$

We begin by recalling a couple of results from the Perron-Frobenius theory.

Lemma 1 *Let A be a non-negative primitive matrix with PF-eigenvalue λ . If $0 \leq \lambda X \leq AX$, then $AX = \lambda X$.*

PROOF : We can assume $X \neq 0$. Since $0 \leq \lambda X$ and $\lambda > 0$, $X \geq 0$. Let $X' > 0$ be a PF right-eigenvector of A . Let $\alpha = \max\{\frac{X_i}{X'_i} \mid 1 \leq i \leq m\}$. Then $X \leq \alpha X'$ and X is not strictly less than $\alpha X'$. Claim $X = \alpha X'$. If $X \neq \alpha X'$, then $0 < A^N(\alpha X' - X) = \alpha \lambda^N X' - A^N X$ for some N , since A is primitive. So $\lambda^N X \leq A^N X < \alpha \lambda^N X'$, i.e. $X < \alpha X'$. This is a contradiction. Therefore $AX = \lambda X$. \square

Lemma 2 *Let λ be the PF-eigenvalue of the non-negative primitive matrix A and μ be an eigenvalue of a matrix B where $0 \leq B \leq A$. If $A \neq B$, then $|\mu| < \lambda$.*

PROOF : Let Y be a right eigenvector for eigenvalue μ of B , with $Y = [Y_1, \dots, Y_m]^T$. Let $\bar{Y} = [|Y_1|, \dots, |Y_m|]^T \neq 0$. Then $|\mu| \bar{Y} \leq B \bar{Y} \leq A \bar{Y}$. Let \bar{X}^T be a positive left eigenvector for A with PF-eigenvalue λ . So $|\mu| \bar{X}^T \bar{Y} \leq \bar{X}^T B \bar{Y} \leq \bar{X}^T A \bar{Y} = \lambda \bar{X}^T \bar{Y}$. This shows that $|\mu| \leq \lambda$. If $|\mu| = \lambda$, then $\lambda \bar{Y} \leq A \bar{Y}$. By Lemma 1, $\lambda \bar{Y} = A \bar{Y}$. Since A is a primitive matrix, $\lambda^m \bar{Y} = A^m \bar{Y} > 0$ for some m . So $\bar{Y} > 0$. From $\lambda \bar{Y} \leq B \bar{Y} \leq A \bar{Y} = \lambda \bar{Y}$, we have $A \bar{Y} = B \bar{Y}$. Therefore $A = B$. \square

2.4 Primitive Substitution System and Boundary measure

We will see how the PF-theory is applied to real mathematical problems. One particular condition on the PF-eigenvalue gives us good information about the PF-eigenvector, of which coordinates are boundary measures in our problem. The boundary measure 0 result is crucial information in our work below.

Lemma 3 *Let (\tilde{U}, Φ) be a primitive substitution system. Then for all $l = 1, 2, \dots$, (\tilde{U}, Φ^l) is a primitive substitution system.*

PROOF : Let $i, j, k \in \{1, 2, \dots, m\}$. All the maps $g \in \Phi_{ik}$ have domain U_k and disjoint images in U_i . Moreover all the mappings g are injective. Likewise all the maps f of Φ_{kj} have domain U_j and disjoint images in U_k . Thus all the maps $g \circ f \in \Phi_{ik} \circ \Phi_{kj}$ have domain U_j and disjoint images in U_i . Furthermore $\Phi^2 \tilde{U} = \Phi(\Phi \tilde{U}) = \Phi(\tilde{U}) = \tilde{U}$. So (\tilde{U}, Φ^2) is a substitution system. The argument extends in the same way to (\tilde{U}, Φ^l) . The statement on primitivity is clear. \square

Theorem 1 *Let (\tilde{U}, Φ) be a primitive substitution system with inflation Q on L . Let (\tilde{W}, Φ) be the corresponding associated Q -adic system. Suppose that the PF-eigenvalue of substitution matrix $S(\Phi)$ is $|\det Q|$ and $\bar{L} = \bigcup_{i=1}^m W_i$. Then*

- (\bar{e}) $S(\Phi^r) = (S(\Phi))^r$, $r \geq 1$;
- ($\bar{e}i$) $\mu(W_i) = \frac{1}{q^r} \sum_{j=1}^m (S(\Phi^r))_{ij} \mu(W_j)$, for all $i = 1, \dots, m$, $r \geq 1$;
- ($\bar{e}ii$) $\mu(\partial W_i) = 0$, for all $i = 1, \dots, m$.

PROOF : For every measurable set $E \subset L$ and all $f \in \Phi_{ij}$, $\mu(f(E)) = \mu(Q(E) + a) = \frac{1}{|\det Q|} \mu(E)$, where $f : x \mapsto Qx + a$. In particular, $\mu(f(W_j)) = \frac{1}{q} w_j$, where $w_j := \mu(W_j)$ and $q = |\det Q|$. We obtain

$$w_i \leq \sum_{j=1}^m \frac{1}{q^r} \text{card}((\Phi^r)_{ij}) w_j$$

from (9).

Let $w = [w_1, \dots, w_m]^T$. Since $\bigcup_{i=1}^m W_i = \bar{L}$, the Baire category theorem assures that for at least one i ,

$$\overset{\circ}{W}_i \neq \emptyset \quad (11)$$

and then the primitivity gives this for all i . So $w > 0$ and

$$w \leq \frac{1}{q^r} S(\Phi^r) w \leq \frac{1}{q^r} S(\Phi)^r w, \text{ for any } r \geq 1. \quad (12)$$

Since the PF-eigenvalue of $S(\Phi)^r$ is $q^r = |\det Q|^r$ and $S(\Phi)^r$ is primitive, we have from Lemma 1 that

$$w = \frac{1}{q^r} S(\Phi^r) w = \frac{1}{q^r} S(\Phi)^r w, \text{ for any } r \geq 1. \quad (13)$$

The positivity of w together with $S(\Phi^r) \leq S(\Phi)^r$ shows that $S(\Phi^r) = S(\Phi)^r$. This proves (i) and (ii).

Fix any $i \in \{1, \dots, m\}$, let $\overset{\circ}{W}_i$ contain a basis open set $a + Q^r \bar{L}$ with some $r \in \mathbb{Z}_{\geq 0}$ by (11). Since (\tilde{U}, Φ^r) is a substitution system, $a + Q^r \bar{L} \subset \overset{\circ}{W}_i \subset W_i = \bigcup_{j=1}^m (\Phi^r)_{ij} W_j$. In particular, $(a + Q^r \bar{L}) \cap g(W_k) \neq \emptyset$ for some $k \in \{1, \dots, m\}$ and some $g \in (\Phi^r)_{ik}$. However $g(\bar{L}) = Q^r \bar{L} + b$ for some $b \in L$, so $(a + Q^r \bar{L}) \cap (b + Q^r \bar{L}) \neq \emptyset$. This means $a + Q^r \bar{L} = b + Q^r \bar{L}$. Thus

$$g(W_k) \subset g(\bar{L}) = a + Q^r \bar{L} \subset \overset{\circ}{W}_i. \quad (14)$$

For all $f \in (\Phi^r)_{ij}$, $j \in \{1, 2, \dots, m\}$, f is clearly an open map, so $\bigcup_{j=1}^m (\Phi^r)_{ij}(\overset{\circ}{W}_j) \subset \overset{\circ}{W}_i$. Thus

$$\begin{aligned} \partial W_i = W_i \setminus \overset{\circ}{W}_i &= \left(\bigcup_{j=1}^m (\Phi^r)_{ij}(W_j) \right) \setminus \overset{\circ}{W}_i \\ &\subset \bigcup_{j=1}^m \left((\Phi^r)_{ij}(W_j) \setminus (\Phi^r)_{ij}(\overset{\circ}{W}_j) \right) \\ &\subset \bigcup_{j=1}^m (\Phi^r)_{ij}(\partial W_j). \end{aligned} \tag{15}$$

Note that due to (14) at least one g in $(\Phi^r)_{ij}$ does not contribute to the relation (15).

Let $v_i := \mu(\partial W_i)$, $i = 1, \dots, m$ and $v := [v_1, \dots, v_m]^T$. So $v \leq \frac{1}{q^r} S(\Phi^r)v$. Actually, by what we just said,

$$0 \leq v \leq \frac{1}{q^r} S'v \leq \frac{1}{q^r} S(\Phi^r)v = \frac{1}{q^r} S(\Phi)^r v, \tag{16}$$

where $S' \leq S(\Phi)^r$, $S' \neq S(\Phi)^r$. Now applying the Lemma 1 again we obtain equality throughout (16). But by Lemma 2 the eigenvalues of $\frac{1}{q^r} S'$ are strictly less in absolute value than the PF-eigenvalue of $\frac{1}{q^r} S(\Phi)^r$, which is 1. This forces $v = 0$, and hence $\mu(\partial W_i) = 0$, $i = 1, \dots, m$. \square

Chapter 3

Model Sets

3.1 Basic Definitions

Let us recall the notion of a model set (or cut and project set). A *cut and project scheme* (CPS) consists of a collection of spaces and mappings as follows;

$$\begin{array}{ccccc} \mathbb{R}^n & \xleftarrow{\pi_1} & \mathbb{R}^n \times G & \xrightarrow{\pi_2} & G \\ & & \bigcup_{\tilde{L}} & & \end{array} \quad (17)$$

where \mathbb{R}^n is a real Euclidean space, G is some locally compact Abelian group, and $\tilde{L} \subset \mathbb{R}^n \times G$ is a lattice, i.e. a discrete subgroup for which the quotient group $(\mathbb{R}^n \times G)/\tilde{L}$ is compact. Furthermore, we assume that $\pi_1|_{\tilde{L}}$ is injective and $\pi_2(\tilde{L})$ is dense in G .

A *model set* in \mathbb{R}^n is a subset of \mathbb{R}^n which, up to translation, is of the form $\Lambda(V) = \{ \pi_1(x) \mid x \in \tilde{L}, \pi_2(x) \in V \}$ for some cut and project scheme as above, where $V \subset G$ has non-empty interior and compact closure (relatively compact). When we need to be more precise we explicitly mention the cut and project scheme from which a model set arises. This is quite important in some of the theorems below. Model sets are always Delone subsets of \mathbb{R}^n , that is, they are uniformly discrete and relatively dense. This means that there are radii $r, R > 0$ so that each ball of radius r (resp. R) contains at most (resp. at least) one point of Λ .

We call the model set $\Lambda(V)$ *regular* if the boundary $\partial V = \overline{V} \setminus \overset{\circ}{V}$ of V is of (Haar) measure 0. We will also find it convenient to consider certain degenerate types of model sets. A *weak* model set is a set in \mathbb{R}^n of the form $\Lambda(V)$ where we assume only that V is relatively compact, but not that it has a non-empty interior. When V has no interior, $\Lambda(V)$ is not necessarily relatively dense in \mathbb{R}^n but regularity still means that the boundary of V is of measure 0.

3.2 The Main Result

We start this section by recalling M. Schlottmann's theorem. This makes a natural link with our theorem.

Theorem 2 (Schlottmann [17]) *If $\Lambda = \Lambda(V)$ is a regular model set, then Λ is a pure point diffractive set, i.e. the Fourier transform of its volume averaged autocorrelation measure is a pure point measure.*

□

It is this theorem that is a prime motivation for finding criteria for sets to be model sets.

Now let (\tilde{U}, Φ) be a substitution system with inflation Q on a lattice L of \mathbb{R}^n and let \overline{L} be the Q -adic completion of L . This gives rise to the cut and project scheme.

$$\begin{array}{ccccc}
 \mathbb{R}^n & \xleftarrow{\pi_1} & \mathbb{R}^n \times \overline{L} & \xrightarrow{\pi_2} & \overline{L} \\
 & & \bigcup & & \\
 L & \xleftarrow{\quad} & \tilde{L} & \longrightarrow & L \\
 t & \xleftarrow{\quad} & (t, t) & \longrightarrow & t
 \end{array} \tag{18}$$

where $\tilde{L} := \{ (t, t) \mid t \in L \} \subset \mathbb{R}^n \times \overline{L}$.

We claim that $(\mathbb{R}^n \times \overline{L})/\tilde{L}$ is compact. Since $(\mathbb{R}^n \times \overline{L})/\tilde{L}$ is Hausdorff and satisfies the first axiom of countability, it is enough to show that it is sequentially compact [9]. If $\{(x_i, z_i) + \tilde{L}\}$ is a countable sequence in $(\mathbb{R}^n \times \overline{L})/\tilde{L}$, then there is a subsequence $\{(x_i, z_i) + \tilde{L}\}_S$ with $\{x_i + L\}_S$ convergent sequence, since \mathbb{R}^n/L is compact. We can rewrite $\{(x_i, z_i) + \tilde{L}\}_S$ as $\{(x'_i, z'_i) + \tilde{L}\}_S$, where $\{x'_i\}_{i \in S}$ converges to x in \mathbb{R}^n . Since \overline{L} is compact, there is a convergent subsequence $\{z'_i\}_{i \in S'}$ to some z in \overline{L} . Thus $\{(x'_i, z'_i)\}_{S'}$ converges to (x, z) in $\mathbb{R}^n \times \overline{L}$. Therefore $(\mathbb{R}^n \times \overline{L})/\tilde{L}$ is sequentially compact.

Note also that \tilde{L} is discrete in $\mathbb{R}^n \times \overline{L}$, $\pi_1|_{\tilde{L}}$ is injective and $\pi_2(\tilde{L})$ is dense in \overline{L} .

We have a discrete point set U_i and want to see if it is a model set. Then we project this down to the internal space. Although it satisfies the condition in the internal space to be a model set, it is important to get our original point set back (up to a set of measure 0) when we bring this set over to \mathbb{R}^n which our original point set lies in. Let's call this new point set Λ_i .

In the sequel, the central concern is to relate the sets U_i and the sets $\Lambda_i := W_i \cap L$. Clearly $\Lambda_i \supset U_i$. The next lemma groups a circle of ideas that relate this question to the boundaries and interiors of the W_i .

Lemma 4 *Let $U_i, i = 1, \dots, m$, be point sets of the lattice L in \mathbb{R}^n . Identify L and its image in \bar{L} . Define $W_i := \bar{U_i}$ and $\Lambda_i := W_i \cap L$.*

- (i) *If U_1, \dots, U_m are disjoint and $\mu(\overline{\Lambda_i \setminus U_i}) = 0$ for all $i = 1, \dots, m$, then $\overset{\circ}{W_i} \cap \overset{\circ}{W_j} = \emptyset$ for all $i \neq j$.*
- (ii) *If $L = \bigcup_{i=1}^m U_i$ and $\overset{\circ}{W_i} \cap \overset{\circ}{W_j} = \emptyset$ for all $i \neq j$, where $i, j \in \{1, \dots, m\}$, then $\Lambda_i \setminus U_i \subset \bigcup_{j=1}^m \partial W_j$ for all $i = 1, \dots, m$.*
- (iii) *If $\mu(\partial W_i) = 0$ for all $i = 1, \dots, m$ and $\Lambda_i \setminus U_i \subset \bigcup_{j=1}^m \partial W_j$, then $\mu(\overline{\Lambda_i \setminus U_i}) = 0$.*

PROOF: (i) Suppose there are $i, j \in \{1, \dots, m\}$ with $\overset{\circ}{W_i} \cap \overset{\circ}{W_j} \neq \emptyset$. We can choose $a \in (\overset{\circ}{W_i} \cap \overset{\circ}{W_j}) \cap L$, since L is dense in \bar{L} and $\overset{\circ}{W_i} \cap \overset{\circ}{W_j}$ is open. Choose $k \in \mathbb{Z}_+$ so that $a + q^k \bar{L} \subset \overset{\circ}{W_i} \cap \overset{\circ}{W_j}$. Note that $a + q^k L \subset \Lambda_i \cap \Lambda_j$. Then

$$\begin{aligned} \bigcup_{i=1}^m (\Lambda_i \setminus U_i) &\supseteq ((a + q^k L) \setminus U_i) \cup ((a + q^k L) \setminus U_j) \\ &\supseteq (a + q^k L) \setminus (U_i \cap U_j) \\ &= a + q^k L, \text{ since the } U_i, i = 1, \dots, m, \text{ are disjoint.} \end{aligned}$$

So

$$\begin{aligned} \sum_{i=1}^m \mu(\overline{\Lambda_i \setminus U_i}) &\geq \mu\left(\bigcup_{i=1}^m (\Lambda_i \setminus U_i)\right) \\ &\geq \mu(a + q^k \bar{L}) \\ &> 0, \end{aligned}$$

contrary to assumption.

- (ii) Assume $\overset{\circ}{W_i} \cap \overset{\circ}{W_j} = \emptyset$ for all $i \neq j$. For any $i \in \{1, \dots, m\}$,

$$\begin{aligned} (\Lambda_i \setminus U_i) &\subset \left(\bigcup_{j \neq i} U_j\right) \cap W_i, \text{ since } L = \bigcup_{i=1}^m U_i \\ &\subset \bigcup_{j \neq i} (W_j \cap W_i) \subset \bigcup_{j=1}^m \partial W_j, \text{ since } \overset{\circ}{W_i} \cap \overset{\circ}{W_j} = \emptyset \text{ for all } i \neq j. \end{aligned}$$

- (iii) Obvious. □

Lemma 5 Let $U_i, i = 1, \dots, m$, be disjoint point sets of the lattice L in \mathbb{R}^n . Identify L and its image in \bar{L} . Let $W_i := \bar{U}_i$ in \bar{L} and $\Lambda_i := W_i \cap L$. Suppose that $\mu(\partial W_i) = 0$ for all $i = 1, \dots, m$.

(i) If $\Lambda_i \setminus U_i \subset \bigcup_{j=1}^m \partial W_j$ then, relative to the CPS(18), U_i is a regular weak model set when $\overset{\circ}{W}_i$ is empty, and U_i is a regular model set when $\overset{\circ}{W}_i$ is non-empty. is non-empty.

(ii) If $L = \bigcup_{j=1}^m U_j$ and each U_i is a regular model set, then $\Lambda_i \setminus U_i \subset \bigcup_{j=1}^m \partial W_j$ for all $i = 1, \dots, m$.

PROOF: (i) Assume that $\Lambda_i \setminus U_i \subset \bigcup_{j=1}^m \partial W_j$ for all $i = 1, \dots, m$. Since $\mu(\partial W_i) = 0$ for all $i = 1, \dots, m$,

$$\mu(W_i) = \mu(\overset{\circ}{W}_i) = \mu(\overset{\circ}{W}_i \setminus \bigcup_{j=1}^m \partial W_j) \quad (19)$$

Consider any i with $\overset{\circ}{W}_i \neq \emptyset$. Since $\Lambda_i = W_i \cap L$, $U_i = V_i \cap L$ where $V_i := W_i \setminus (\Lambda_i \setminus U_i)$. Now $V_i \supset \overset{\circ}{W}_i \setminus \bigcup_{j=1}^m \partial W_j$. The latter is open and non-empty. Thus $\overset{\circ}{V}_i \neq \emptyset$ and \bar{V}_i is compact. It follows that $U_i = \Lambda(V_i)$ is a model set. Furthermore from $\overset{\circ}{W}_i \setminus \bigcup_{j=1}^m \partial W_j \subset \overset{\circ}{V}_i \subset V_i \subset \bar{V}_i = W_i$ and (19), $\mu(\bar{V}_i \setminus \overset{\circ}{V}_i) = 0$. So U_i is a regular model set for the CPS (18).

(ii) Suppose that $\overset{\circ}{V}_i \neq \emptyset$, $\mu(\bar{V}_i \setminus \overset{\circ}{V}_i) = 0$, where $U_i = V_i \cap L$, and $L = \bigcup_{j=1}^m U_j$. Then from $\bar{\Lambda}_i \setminus U_i = \bar{\Lambda}(W_i) \setminus \bar{\Lambda}(V_i) \subset \bar{W}_i \setminus \bar{V}_i \subset W_i \setminus \overset{\circ}{V}_i = \bar{V}_i \setminus \overset{\circ}{V}_i$, we have $\mu(\bar{\Lambda}_i \setminus U_i) = 0$ for all $i = 1, \dots, m$. By Lemma 4 (i) and (ii), $\overset{\circ}{W}_i \cap \overset{\circ}{W}_j = \emptyset$ for all $i \neq j$ and $\Lambda_i \setminus U_i \subset \bigcup_{j=1}^m \partial W_j$. \square

Theorem 3 Let (\tilde{U}, Φ) be a primitive substitution system with inflation Q on the lattice L in \mathbb{R}^n . Suppose that the PF-eigenvalue of substitution matrix $S(\Phi)$ is $|\det Q|$ and $L = \bigcup_{i=1}^m U_i$. Then the following are equivalent.

(i) there is a primitive substitution matrix Ψ admitting a coincidence, where (\tilde{U}, Ψ) is equivalent to (\tilde{U}, Φ^M) for some $M \geq 1$.

(ii) The sets U_i , $i = 1, \dots, m$, of \tilde{U} are model sets for the CPS (18).

(iii) For at least one i , U_i contains a coset $a + Q^M L$.

(iv) (\tilde{U}, Φ) admits a modular coincidence.

PROOF :

(i) \rightarrow (ii): Suppose that (\tilde{U}, Ψ) admits a coincidence and is equivalent to (\tilde{U}, Φ^M) . Fix $i \in \{1, \dots, m\}$ with $\cap_{j=1}^m \Psi_{ij} \neq \emptyset$ and let g be in this intersection. Recalling equation (9), and in view of the choice of g , we have

$$\mu(W_i) \leq \left(\sum_{j=1}^m \sum_{f \in \Psi_{ij}} \mu(f(W_j)) \right) - \mu(g(W_k) \cap g(W_l)),$$

for any $k, l \in \{1, \dots, m\}$ with $k \neq l$. On the other hand, from Theorem 1 (ii)

$$\mu(W_i) = \frac{1}{q^M} \sum_{j=1}^m (S(\Psi))_{ij} \mu(W_j) = \sum_{j=1}^m \sum_{f \in \Psi_{ij}} \mu(f(W_j)). \quad (20)$$

Thus, in fact, $\mu(g(W_k) \cap g(W_l)) = 0$ whenever $k \neq l$. It follows at once that $\overset{\circ}{W}_k \cap \overset{\circ}{W}_l = \emptyset$ for all $k \neq l$, since the measure of any open set is larger than 0.

Recall that $\overset{\circ}{W}_i \neq \emptyset$ and $\mu(\partial W_i) = 0$ for all $i = 1, \dots, m$. Then by Lemma 4(ii) and Lemma 5, U_i , $i = 1, \dots, m$, are model sets in CPS(18).

(ii) \rightarrow (iii): Assume that U_i , $i = 1, \dots, m$, are model sets in CPS(18), i.e. $U_i = \Lambda(V_i) = V_i \cap L$ for some V_i with $\overset{\circ}{V}_i \neq \emptyset$. Thus there is a coset $a + Q^M \bar{L} \subset \overset{\circ}{V}_i$ and, since we can always choose the coset representative from the dense lattice L , we can arrange that $a + Q^M L \subset U_i$.

(iii) \rightarrow (iv): Assume that for at least one i , U_i contains a coset $a + Q^M L$. Fix i . Iterate Φ M -times. Then each function f in the substitution system Φ^M has the form $f : x \mapsto Q^M x + b$. For each j , let $G_j := \{ f \in (\Phi^M)_{ij} \mid t(f) \equiv a \pmod{Q^M L} \}$. (Recall that $t(f)$ is the translational part of f). From $U_i = \bigcup_{j=1}^m \bigcup_{f \in (\Phi^M)_{ij}} f(U_j)$, we obtain $a + Q^M L \subset \bigcup_{j=1}^m \bigcup_{f \in G_j} f(U_j)$. In fact

$$a + Q^M L = \bigcup_{j=1}^m \bigcup_{f \in G_j} f(U_j), \quad (21)$$

since the right hand side is clearly inside $a + Q^M L$. From the fact $a + Q^M L \subset U_i$, we get $\Phi^M[a] = \bigcup_{j=1}^m G_j \subset \bigcup_{j=1}^m (\Phi^M)_{ij}$. Therefore Φ^M has a row containing an entire congruence class $\Phi^M[a]$.

(iv) \rightarrow (i): Assume Φ^M has a row, say i -th row, containing an entire congruence class $\Phi^M[a]$. Let $G_j := \Phi^M[a] \cap (\Phi^M)_{ij}$. Then $\bigcup_{j=1}^m \bigcup_{f \in G_j} f(U_j) \subset a + Q^M L$. Recall that $\bigcup_{j=1}^m U_j = L$ and $\tilde{U} = \Phi^M(\tilde{U})$. It follows that the elements of $a + Q^M L$ can

be obtained from the substitution system Φ^M *only* from the mappings of $\Phi^M[a]$, and indeed they must *all* appear as images of the mappings of $\Phi^M[a]$. Thus

$$a + Q^M L = \bigcup_{j=1}^m \bigcup_{f \in G_j} f(U_j) \subset U_i. \quad (22)$$

On the other hand,

$$a + Q^M L = \bigcup_{j=1}^m Q^M(U_j) + a, \quad (23)$$

which is disjoint union.

We now alter our substitution system Φ^M as follows: Define $g : L \rightarrow L$ by $g(x) = Q^M x + a$. We may, by restriction of domain, consider g as a function on U_j , $j = 1, \dots, m$. We define Ψ by

$$\begin{cases} \Psi_{ij} = ((\Phi^M)_{ij} \setminus G_j) \cup \{g\} \\ \Psi_{kj} = (\Phi^M)_{kj} \quad \text{if } k \neq i, \end{cases}$$

for all j . From (22) and (23), the Ψ_{ij} , $j = 1, \dots, m$ consist of maps from U_j to U_i and have the same total effect on U_i as the $(\Phi^M)_{ij}$, $j = 1, \dots, m$. Thus (\tilde{U}, Ψ) is a substitution system admitting a coincidence.

Since $S(\Phi^M)$ is primitive, the incidence matrix $I(\Phi^M)$ is primitive. Then $I(\Psi)$ is also primitive, since $I(\Phi^M) \leq I(\Psi)$. So Ψ is primitive. In addition, Ψ has the inflation Q^M for L which is an inflation in Φ^M .

We claim that $S(\Psi)$, $S(\Phi^{M'})$ have the same PF-eigenvalue and right PF-eigenvector. Then (\tilde{U}, Ψ) is equivalent to (\tilde{U}, Φ^M) .

We verify first that $\tilde{W}_k \cap \tilde{W}_j = \emptyset$ for all $k \neq j$. We can assume that $m > 1$, since there is nothing to prove when $m = 1$. Let $g \in G_l = (\Phi^M)_{il}[a] \neq \emptyset$ for some l . Take any $k \in \{1, \dots, m\}$. There is $M_0 \in \mathbb{Z}_+$ for which $(\Phi^{M_0})_{lk} \neq \emptyset$. Choose $f \in (\Phi^{M_0})_{lk}$. Let $g : x \mapsto Q^M x + a_1$, where $a_1 \equiv a \pmod{Q^M L}$, and $f : x \mapsto Q^{M_0} x + b$ with $b \in L$. Then $g \circ f : x \mapsto Q^{M+M_0} x + Q^M b + a_1$. So $g \circ f \in (\Phi^{M+M_0})_{ik}[a_1 + Q^M b]$. Furthermore $(a_1 + Q^M b) + Q^{M+M_0}(L) \subset a_{\Pi} + Q^M L \subset U_i$.

Let $N := M + M_0$, $c := a_{\Pi} + Q^M b$, and $p := g \circ f$. Note that

$$c + Q^N L = \bigcup_{j=1}^m \bigcup_{h \in H_j} h(U_j), \quad (24)$$

where $H_j = (\Phi^N)_{ij}[c]$.

There are at least two functions in $\bigcup_{j=1}^m H_j$, since $U_j \neq L$ for all j . We can write $c + Q^N L$ in the form

$$c + Q^N L = \bigcup \{ Q^N U_j + Q^N \alpha_h + c \mid j \in \{1, \dots, m\}, h \in H_j, \alpha_h \in L \}, \quad (25)$$

where we have used the explicit form of each of the mappings $h \in H_j$. This union is disjoint, and as a consequence the elements $\alpha_h \in L$ for h in any single H_j are all distinct. In particular we have α_p coming from H_k . From (25) we have

$$L = \bigcup_{j=1}^m \bigcup_{h \in H_j} (U_j + \alpha_h) \quad (26)$$

and separating off U_k ,

$$L = U_k \cup \bigcup_{j=1}^m \bigcup_{h \in H'_j} (U_j + \alpha_h - \alpha_p), \quad (27)$$

where $H'_j := H_j$ if $j \neq k$ and $H'_k := H_k \setminus \{p\}$. Again these decompositions are disjoint. But we also know that U_k and $\bigcup_{j=1, j \neq k}^m U_j$ are disjoint, and it follows that

$$\bigcup_{\substack{j=1 \\ j \neq k}}^m U_j \subset \bigcup_{j=1}^m \bigcup_{h \in H'_j} (U_j + \alpha_h - \alpha_p).$$

Taking closures,

$$\bigcup_{\substack{j=1 \\ j \neq k}}^m W_j \subset \bigcup_{j=1}^m \bigcup_{h \in H'_j} (W_j + \alpha_h - \alpha_p). \quad (28)$$

On the other hand, if we apply Theorem 1(ii) to Φ^N and look at (24) we see that

$$\mu(c + Q^N \bar{L}) = \sum_{j=1}^m \sum_{h \in H_j} \mu(h(W_j)) = \sum_{j=1}^m \sum_{h \in H_j} \mu(Q^N(W_j + \alpha_h) + c),$$

and hence

$$\mu(\bar{L}) = \sum_{j=1}^m \sum_{h \in H_j} \mu(W_j + \alpha_h) = \sum_{j=1}^m \sum_{h \in H_j} \mu(W_j + \alpha_h - \alpha_p).$$

Thus

$$\mu(\bar{L}) = \mu(W_k) + \left(\sum_{j=1}^m \sum_{h \in H'_j} \mu(W_j + \alpha_h - \alpha_p) \right)$$

which, after taking closures in (27), gives

$$\mu \left(W_k \cap \left(\bigcup_{j=1}^m \bigcup_{h \in H_j'} (W_j + \alpha_h - \alpha_p) \right) \right) = 0. \quad (29)$$

Finally from (28) and (29) we obtain

$$\mu(W_k \cap (\bigcup_{\substack{j=1 \\ j \neq k}}^m W_j)) = 0,$$

from which $\overset{\circ}{W}_k \cap \overset{\circ}{W}_j = \emptyset$ for all $k \neq j$. This establishes the claim.

Now

$$\begin{aligned} \mu \left(\bigcup_{j=1}^m g(W_j) \right) &= \frac{1}{|\det Q^M|} \mu \left(\bigcup_{j=1}^m W_j \right) \\ &= \frac{1}{|\det Q^M|} \sum_{j=1}^m \mu(W_j), \\ &\quad \text{from } \mu(\partial W_j) = 0, \quad \overset{\circ}{W}_i \cap \overset{\circ}{W}_j = \emptyset \text{ for all } i \neq j \\ &= \sum_{j=1}^m \mu(g(W_j)). \end{aligned} \quad (30)$$

Again using Theorem 1(ii), this time for Φ^M , we obtain

$$w = \frac{1}{|\det Q^M|} S(\Phi^M) w,$$

where $w = [\mu(W_1), \dots, \mu(W_m)]^T$. The part of this relation in W_i which pertains to the coset $a + Q^M \overline{L}$ is

$$\mu(a + Q^M \overline{L}) = \sum_{j=1}^m \sum_{f \in G_j} \mu(f(W_j)). \quad (31)$$

But from (23)

$$\mu(a + Q^M \overline{L}) = \mu \left(\bigcup_{j=1}^m g(W_j) \right). \quad (32)$$

Together, (30), (31), and (32) show

$$w = \frac{1}{|\det Q^M|} S(\Psi)w.$$

Since $w > 0$ and $S(\Psi)$ is primitive, $S(\Psi)$ has PF-eigenvalue $|\det Q^M|$ and PF-eigenvector w as required. \square

Remark: Let $A = \{a_1, \dots, a_m\}$ be an alphabet of m symbols and let σ be a primitive equal-length alphabetic substitution system on A , that is,

- (i) $\sigma : A \longrightarrow A^q$ for some $q \in \mathbb{Z}_+$;
- (ii) the $m \times m$ matrix $S = (S_{ij})$, whose i, j entry is the number of appearances of a_i in $\sigma(a_j)$, is primitive.

According to Gottschalk [7], for some iteration σ^k of σ , there is a word $w \in A^{\mathbb{Z}}$ which is fixed by σ in the sense that

$$\begin{aligned} \sigma^k(w_0 w_1 \dots) &= w_0 w_1 \dots \\ \sigma^k(\dots w_{-2} w_{-1}) &= \dots w_{-2} w_{-1}. \end{aligned} \tag{33}$$

Replacing σ^k by σ and q^k by q if necessary we can suppose that $k = 1$, and assume then that $\sigma(w) = w$.

We can view w as a tiling of \mathbb{R} by tiles of types a_1, \dots, a_m , all of the same length 1. If we coordinatize each tile by its lefthand end point so that w_l gets coordinate l , then we obtain a partition $U_1 \cup \dots \cup U_m$ of \mathbb{Z} and an $m \times m$ matrix substitution system Φ of q -affine mappings derived directly from σ : namely, $\sigma a_j = a_{i_1} \dots a_{i_q}$ gives rise to the mappings $(x \mapsto qx + l - 1) \in \Phi_{ij}$, $l = 1, \dots, q$.

We take as our cut and project scheme

$$\begin{array}{ccccc} \mathbb{R} & \longleftarrow & \mathbb{R} \times \mathbb{Z}_q & \longrightarrow & \mathbb{Z}_q \\ & & \bigcup & & \\ \mathbb{Z} & \longleftarrow & \tilde{\mathbb{Z}} & \longrightarrow & \mathbb{Z} \\ z & \longleftarrow & (z, z) & \longrightarrow & z \end{array} \tag{34}$$

(see 18), where \mathbb{Z}_q is the q -adic completion of \mathbb{Z} .

According to Theorem 3, the U_i are model sets for (34) if and only if for some iteration σ^M of σ , there is a $k \in \mathbb{Z}$ for which all the mappings $f_l : x \mapsto q^M x + l$ with $l \equiv k \pmod{q^M}$ lie in one row of Φ^M .

Since $\sigma^M a_j$ has q^M letters in it, there are q^M mappings in the j th column of Φ^M . Furthermore, since the letters of $\sigma^M a_j$ are represented by contiguous tiles, their coordinates fall in a range of consecutive integers, and so the mappings of the j th column of Φ^M are the maps f_l , where $0 \leq l < q^M$, in some order. In particular, all of the mappings in Φ^M are of this restricted form. It follows that modular coincidence is equivalent to the existence of a row of Φ^M , say the i th row, and a k , $0 \leq k < q^M$, so that f_k belongs to *each* of $\Phi_{i1}^M, \dots, \Phi_{im}^M$.

This condition precisely says that there is a k so that the k th position of $\sigma^M(a_j)$ contains the same letter a_i for all j . This is the well-known coincidence condition of Dekking [6], and he has proved that for non-periodic primitive equal-length substitutions, this condition is equivalent to pure point diffractivity. It is straightforward to show that $S(\Phi)$ has its PF-eigenvalue equal to $|\det Q|$. Thus we have

Corollary 1 *Let σ be a primitive equal-length ($= q$) alphabetic substitution with a fixed bi-infinite word w , and assume that w is not periodic. Let Φ be the corresponding matrix substitution system and let $\mathbb{Z} = U_1 \cup \dots \cup U_m$ be the corresponding partition of \mathbb{Z} . Then the following are equivalent:*

- (i) *there is an M so that σ^M has a coincidence in the sense of Dekking;*
- (ii) *Φ has a modular coincidence;*
- (iii) *the U_i 's are model sets for (34);*
- (iv) *the U_i 's are pure point diffractive.*

We note that this interesting *equivalence* of model sets and pure point diffractivity is more than we can yet prove in the higher dimensional substitution systems.

Chapter 4

Sphinx tiling

In this section we take up the sphinx tiling. This is a substitution tiling whose subdivision rule is shown in Figure 1 and Figure 2.

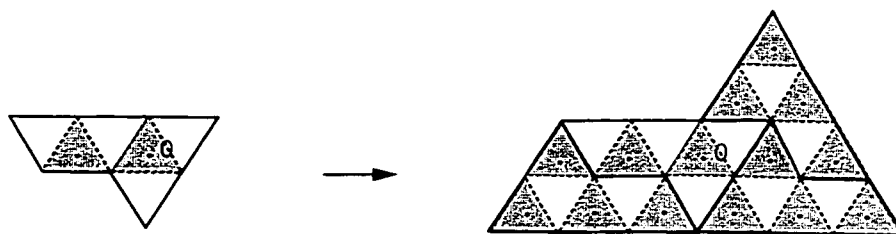


Figure 1: Sphinx Inflation [Type 1]

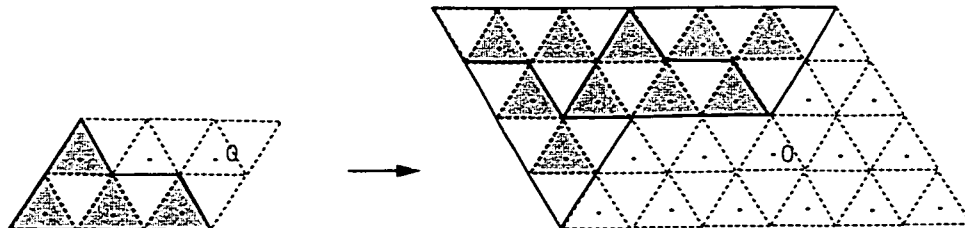


Figure 2: Sphinx Inflation [Type 2]

It has 12 sphinx-like tiles (up to translation). If we choose a single point in the same way in each sphinx then we arrive at 12 sets of points. We wish to show that each of these sets is a regular model set. Actually we make a slight alteration to this, choosing several points from each tile, but this is equivalent to our original problem.

Each sphinx can be viewed as consisting of 6 equilateral triangles of two orientations. In this way, any sphinx tiling determines a tessellation of the plane by equilateral triangles. We consider the centre points of the triangles of one orientation. These clearly form a lattice L , once we have chosen one of them as the origin. Note that some sphinxes have two points and others have four points in L . We give

names at each tile and the points in it as shown in Figure 3. Then the 12 types of sphinx partition L into 36 subsets forming a matrix substitution system. We show that these are model sets for a 2-adic-like cut and project scheme of the form of (18).

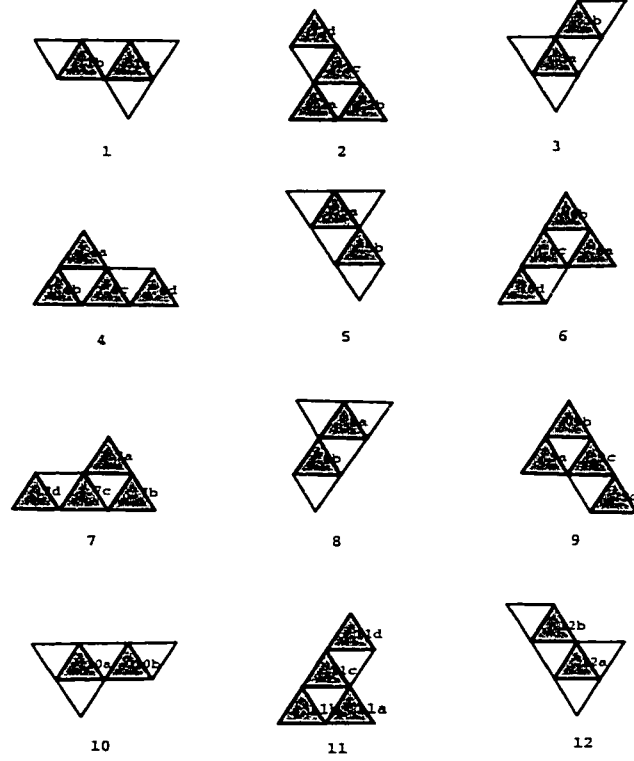


Figure 3: 12 Sphinx Tiles

With the origin as shown, the coordinates are chosen so that in the standard rectangular system $(1,0)$ is the lattice point directly to the right of $(0,0)$. It is more convenient to replace this by an oblique coordinate system: $L = \{ ae + bw \mid a, b \in \mathbb{Z} \}$, where $e = (1,0)$, $w = (\frac{1}{2}, \frac{\sqrt{3}}{2})$ in the standard rectangular system and relative to this basis we can identify L and \mathbb{Z}^2 and denote $ae + bw$ by (a,b) . The basic inflation shown in Figure 1 gives rise to the map

$$T : x \mapsto 2Rx + (1,0),$$

where R is a reflection in \mathbb{R}^2 through x -axis, i.e. in the new coordinates, $R(1,0) = (1,0)$, $R(0,1) = (1,-1)$.

The various types of points are designated by letter pairs $i\alpha$, where $i \in \{1, \dots, 12\}$ and $\alpha \in \{a, \dots, d\}$ (of which only 36 actually occur). Let $U_{i\alpha}$ be the set of points of

type $i\alpha$. On the basis of this we can make mappings of each point set to other point set.

Define

$$\begin{aligned} h_1 : x &\mapsto Tx + (0, 0), & h_2 : x &\mapsto Tx + (1, 0) \\ h_3 : x &\mapsto Tx + (0, 1), & h_4 : x &\mapsto Tx + (-1, 1) \\ h_5 : x &\mapsto Tx + (-1, 0), & h_6 : x &\mapsto Tx + (0, -1) \\ h_7 : x &\mapsto Tx + (1, -1), & h_8 : x &\mapsto Tx + (2, -1) \\ h_9 : x &\mapsto Tx + (-1, 2), & h_{10} : x &\mapsto Tx + (-1, -1). \end{aligned}$$

Let $f_{i\alpha j\beta}$ be the function which maps $j\beta$ -point set into $i\alpha$ -point set.

[Type 1]

$$\begin{aligned} f_{9a1a} &= h_4 : x \mapsto Tx + (-1, 1), & f_{1a1b} &= h_2 : x \mapsto Tx + (1, 0) \\ f_{9b1a} &= h_9 : x \mapsto Tx + (-1, 2), & f_{1b1b} &= h_1 : x \mapsto Tx + (0, 0) \\ f_{9c1a} &= h_3 : x \mapsto Tx + (0, 1), & f_{4a1b} &= h_5 : x \mapsto Tx + (-1, 0) \\ f_{9d1a} &= h_2 : x \mapsto Tx + (1, 0), & f_{4b1b} &= h_{10} : x \mapsto Tx + (-1, -1) \\ f_{4a1a} &= h_1 : x \mapsto Tx + (0, 0), & f_{4c1b} &= h_6 : x \mapsto Tx + (0, -1) \\ f_{4b1a} &= h_6 : x \mapsto Tx + (0, -1), & f_{4d1b} &= h_7 : x \mapsto Tx + (1, -1) \\ f_{4c1a} &= h_7 : x \mapsto Tx + (1, -1), \\ f_{4d1a} &= h_8 : x \mapsto Tx + (2, -1). \end{aligned}$$

[Type 2]

$$\begin{aligned} f_{12a4a} &= h_1 : x \mapsto Tx + (0, 0), & f_{1a4b} &= h_2 : x \mapsto Tx + (1, 0) \\ f_{12b4a} &= h_4 : x \mapsto Tx + (-1, 1), & f_{1b4b} &= h_1 : x \mapsto Tx + (0, 0) \\ f_{4a4c} &= h_1 : x \mapsto Tx + (0, 0), & f_{1a4d} &= h_1 : x \mapsto Tx + (0, 0) \\ f_{4b4c} &= h_6 : x \mapsto Tx + (0, -1), & f_{1b4d} &= h_5 : x \mapsto Tx + (-1, 0) \\ f_{4c4c} &= h_7 : x \mapsto Tx + (1, -1), \\ f_{4d4c} &= h_8 : x \mapsto Tx + (2, -1). \end{aligned}$$

All points in a sphinx having 2-points in it are mapped as in [Type 1] changing the translation part according to the orientation of the sphinx relative to sphinx 1. Likewise, all points in a sphinx having 4-points in it are mapped as in [Type 2] relative to sphinx 4.

Now we can list the 36×36 matrix(Φ) of affine mappings that make up our substitution system (Figure 4).

We can check that $S(\Phi)$ has PF-eigenvalue 4 and is a primitive matrix and the union of point sets is L. We used Mathematica to check that property (iv) in Theorem 3 is satisfied in Φ^8 (it may actually be satisfied at some lower power). Certainly


```

{{0,h2,0,0,0,0,0,0,h2,0,h1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,h1,0,0,0,0,0},
{0,h1,0,0,0,0,0,0,h1,0,h5,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,h5,0,0,0,0,0},
{0,0,0,0,0,0,h1,h7,0,0,0,0,0,0,0,h1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,h7,0},
{0,0,0,0,0,0,h2,h8,0,0,0,0,0,0,0,h2,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,h8,0},
{0,0,0,0,0,0,h3,h2,0,0,0,0,0,0,0,h3,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,h2,0},
{0,0,0,0,0,0,h9,h3,0,0,0,0,0,0,0,h9,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,h3,0},
{0,0,0,h6,0,h1,0,0,0,0,0,0,h6,0,0,0,0,h1,0,0,0,0,0,0,0,0,0,0,0,0,0,0},
{0,0,0,h1,0,h3,0,0,0,0,0,0,h1,0,0,0,0,h3,0,0,0,0,0,0,0,0,0,0,0,0,0,0},
{h1,h5,0,0,0,0,0,0,h1,0,0,0,0,0,0,0,0,h5,0,0,0,0,0,0,0,0,0,0,0,0,0},
{h6,h10,0,0,0,0,0,0,h6,0,0,0,0,0,0,0,0,h10,0,0,0,0,0,0,0,0,0,0,0,0},
{h7,h6,0,0,0,0,0,0,h7,0,0,0,0,0,0,0,0,h6,0,0,0,0,0,0,0,0,0,0,0,0,0},
{h8,h7,0,0,0,0,0,0,h8,0,0,0,0,0,0,0,0,h7,0,0,0,0,0,0,0,0,0,0,0,0,0},
{0,0,0,0,0,0,h4,0,0,0,0,0,0,h4,0,h1,0,0,0,0,0,h1,0,0,0,0,0,0,0,0,0},
{0,0,0,0,0,0,h1,0,0,0,0,0,h1,0,h7,0,0,0,0,0,h7,0,0,0,0,0,0,0,0,0},
{0,0,0,h4,0,0,0,0,0,h4,h9,0,0,0,0,0,0,0,0,0,0,0,0,0,h9,0,0,0,0,0},
{0,0,0,h5,0,0,0,0,0,h5,h4,0,0,0,0,0,0,0,0,0,0,0,0,h4,0,0,0,0,0},
{0,0,0,h10,0,0,0,0,0,h10,h5,0,0,0,0,0,0,0,0,0,0,0,0,h5,0,0,0,0,0},
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{0,0,0,0,0,0,0,0,0,0,h8,0,0,0,0,0,h7,0,0,0,0,0,h7,h8,0,0,0,0,0},
{0,0,0,0,0,0,0,0,0,0,h7,0,0,0,0,0,h6,0,0,0,0,0,h6,h7,0,0,0,0,0},
{0,0,0,0,0,0,0,0,0,0,h6,0,0,0,0,0,h10,0,0,0,0,0,h10,h6,0,0,0,0,0},
{0,0,0,0,0,0,0,0,0,0,h1,0,0,0,0,0,0,0,h3,0,h1,0,0,0,0,0,h3},
{h4,0,0,0,0,0,0,0,0,0,h6,0,0,0,0,0,0,0,h1,0,h6,0,0,0,0,0,h1},
{h9,0,0,0,0,0,0,0,0,0,h1,h4,0,0,0,0,0,0,0,h3,h9,0,0,0,0,0,h3},
{h3,0,0,0,0,0,0,0,0,0,h2,h3,0,0,0,0,0,0,0,h2,h3,0,0,0,0,0,h2},
{h2,0,0,0,0,0,0,0,0,0,h8,h2,0,0,0,0,0,0,0,h8,h2,0,0,0,0,0,h8},
{0,0,h1,0,0,0,0,0,0,h5,0,h1,0,0,0,0,0,0,h5,0,0,0,0,0,h5},
{0,0,h2,0,0,0,0,0,0,h2,0,0,0,0,0,0,h1,0,0,0,0,0,h1},
{0,0,0,0,0,h6,0,0,0,0,0,0,0,0,0,0,0,h1,0,0,0,0,0,h1,h6},
{0,0,0,0,0,h10,0,0,0,0,0,0,0,0,0,0,0,h5,0,0,0,0,0,h5,h10},
{0,0,0,0,0,h5,0,0,0,0,0,0,0,0,0,0,0,0,h4,0,0,0,0,0,h4,h5},
{0,0,0,0,0,h4,0,0,0,0,0,0,0,0,0,0,0,0,h9,0,0,0,0,0,h9,h4},
{0,0,0,0,0,0,h1,0,0,0,0,0,0,0,0,0,0,h7,0,0,0,0,0,h7,h1,0,0},
{0,0,0,0,0,0,0,h4,0,0,0,0,0,0,0,0,0,0,h1,0,0,0,0,0,h1,h4,0,0}}

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Figure 4: Sphinx matrix function system(Φ)

in Φ^8 there are a large number of modular coincidences. Theorem 1 and 3 says that all 36 point sets are regular model sets in CPS (18).

Chapter 5

The Total Index and Model Sets

5.1 Coset Part and Total Index

In this section we derive another criterion for determining when a partition of a lattice is a partition into Q -adic model sets, the difference this time being that there is no substitution system involved.

We assume that we are given a lattice L in \mathbb{R}^n and an inflation Q on L as in (3). The notation remains the same as before. The main ingredient is a non-negative sub-additive function called the total index which is defined on the subsets of L and its Q -adic completion \overline{L} .

For any subset V of L the *coset part* of V is defined as

$$\mathcal{C}(V) := \bigcup \{ C \mid C \text{ is a coset in } V \}. \quad (35)$$

The key point to remember in what follows is that two cosets in $L(\overline{L})$ are either disjoint or one of them is contained in the other.

Lemma 6 *The coset part of V can be written as a disjoint union of cosets in V .*

PROOF: If V contains no cosets, then the result is clear. Suppose V contains cosets. Let $C_1 = a_1 + Q^{k_1}L$ be a coset in V with k_1 minimal. Consider $V \setminus C_1$. No coset can be partly in C_1 and partly in $V \setminus C_1$. Thus, if $V \setminus C_1$ contains no cosets, then $\mathcal{C}(V) = C_1$. Otherwise let C_2 be a coset $a_2 + Q^{k_2}L$ with k_2 minimal in $V \setminus C_1$. Then $\mathcal{C}(V) \supset C_1 \dot{\cup} C_2$. We continue this process. Since there are only finitely many cosets for $Q^k L$ in L , either we obtain $\mathcal{C}(V) = C_1 \dot{\cup} \cdots \dot{\cup} C_r$ for some r or $\mathcal{C}(V) \supset C_1 \dot{\cup} C_2 \dot{\cup} \cdots$, where $k_1 \leq k_2 \leq \cdots$ is infinite and unbounded. In the latter case, $\mathcal{C}(V) = \bigcup_{i=1}^{\infty} C_i$ is our required decomposition. If not, there is a coset $C = a + Q^k L$ in V such that $C \not\subset \bigcup_{i=1}^{\infty} C_i$. Then there is C_i with $k_{i-1} \leq k < k_i$. This contradicts the choice of C_i . \square

For $V \subset L$, we call a decomposition $\mathcal{C}(V) = \bigcup_i C_i$ of $\mathcal{C}(V)$ into mutually disjoint cosets using the algorithm of Lemma 6, an *efficient* decomposition of V into cosets. Let $[L : C_i]$ be the index of subgroup $Q^k L$ in L , where $C_i = a + Q^k L$, $a \in L$. In this case we call $c(V) := \sum_i [L : C_i]^{-1}$ the *total index* of V . Since any coset is an efficient decomposition of itself, we have $c(V) = \sum_i c(C_i)$. We will see shortly that the total index is finite.

It is useful to note that an efficient decomposition of $\mathcal{C}(V) = \bigcup_i C_i$ of $\mathcal{C}(V)$ into cosets has the following special property: if D is any coset of V then necessarily $D \subset C_i$ for some i .

Lemma 7 *Any two efficient decompositions of $\mathcal{C}(V)$ are the same up to rearrangement of the order of the cosets. In particular the total index is well-defined.*

PROOF: Let $\mathcal{C}(V) = \bigcup C'$ be a second decomposition of $\mathcal{C}(V)$ determined by the same algorithm as in Lemma 6. Then with k_1 as in the Lemma, let D_1, \dots, D_r be all the cosets of V of the form $a + Q^{k_1} L$. These are all disjoint and by the algorithm all of them must be chosen in the decomposition of $\mathcal{C}(V)$, and they all occur before all the others. Thus C_1, \dots, C_r and C'_1, \dots, C'_r are D_1, \dots, D_r in some order. Removing these and continuing in the same way the result is clear. \square

We have similar concepts in \overline{L} . For $W \subset \overline{L}$ we have the coset part $\mathcal{C}^*(W)$ of W and $\mathcal{C}^*(W)$ can be written as a disjoint union of cosets in W . Let $\mathcal{C}^*(W) = \bigcup_i D_i$ where D_i , $i = 1, 2, \dots$, are mutually disjoint cosets in W . We call $c^*(W) := \sum_i [\overline{L} : D_i]^{-1}$ the *total index* of W . This time we do not need to be careful about the way in which the decomposition is obtained since the total index is nothing else than the measure $\mu(\mathcal{C}^*(W))$ of $\mathcal{C}^*(W)$.

Given an efficient decomposition $\mathcal{C}(V) = \bigcup_{i=1} C_i$ into disjoint cosets in L , we define $\overline{\mathcal{C}}(V) := \bigcup_{i=1} \overline{C}_i \subset \overline{L}$. This is actually an open set in \overline{L} . Since $[L : C] = [\overline{L} : \overline{C}]$ we see that $c(V) = c^*(\overline{\mathcal{C}}(V))$. In particular it follows that the total index of any subset V of L is finite and bounded by $\mu(\overline{\mathcal{C}}(V))$.

Lemma 8 *For $X, Y \subset L$ and $X \subset Y$, and any decomposition $\mathcal{C}(X) = \bigcup_i C_i$ into disjoint cosets, $\sum_i c(C_i) \leq c(Y)$. In particular, $c(X) \leq c(Y)$.*

PROOF: Assume first that Y is a single coset C . Then

$$\sum_i c(C_i) = \sum_i c^*(\overline{C}_i) = \sum_i \mu(\overline{C}_i) \leq \mu(\overline{C}) = c^*(\overline{C}) = c(C), \quad (36)$$

since the cosets remain distinct after closing them in \overline{L} .

In the general case, let $\mathcal{C}(Y) = \bigcup_{j=1}^{\infty} C'_j$ be an efficient decomposition of Y . Since $X \subset Y$, each $C_i \subset Y$. In view of the remark above about efficient decompositions, there is for each i a unique j for which $C_i \subset C'_j$. Thus we can arrange the C_i 's so that

$$\mathcal{C}(X) = \bigcup_{j=1}^{\infty} \bigcup_{i \in A_j} C_i \quad (37)$$

where $A_j := \{i \mid C_i \subset C'_j\}$. Now $\bigcup_{i \in A_j} C_i \subset C'_j$, so by the first part of the proof, $\sum_{i \in A_j} c(C_i) \leq c(C'_j)$. Finally

$$c(X) = \sum_j \sum_{i \in A_j} c(C_i) \leq \sum_j c(C'_j) = c(Y). \quad (38)$$

□

5.2 Total Index and Model Sets

Lemma 9 *Let $U_i, i = 1, \dots, m$, be disjoint point sets of the lattice L in \mathbb{R}^n . Let $\Lambda_i = \overline{U_i} \cap L$ and $\mathcal{C}(U_i)$ be the coset part in U_i . Then $\bigcup_{i=1}^m (\Lambda_i \setminus U_i) \subset L \setminus \bigcup_{i=1}^m \mathcal{C}(U_i)$, with equality if $L = \bigcup_{i=1}^m U_i$.*

PROOF For $x \in \bigcup_{i=1}^m \mathcal{C}(U_i)$ there is a coset $C \subset \mathcal{C}(U_i)$ for which $x \in C \subset U_i$. Let $C = a + Q^k L, a \in L$. Suppose x is a limit point of U_j in \overline{L} i.e. $x \in \Lambda_j$ for some $j \neq i$. Then, since $a + Q^k \overline{L}$ is an open neighborhood of x , $(a + Q^k \overline{L}) \cap U_j \neq \emptyset$ i.e. $(a + Q^k L) \cap U_j \neq \emptyset$. But then $U_i \cap U_j \neq \emptyset$, contrary to the assumption. This means $x \notin \bigcup_{i=1}^m (\Lambda_i \setminus U_i)$, proving the first part.

Suppose that $L = \bigcup_{i=1}^m U_i$ and $x \in L$ but $x \notin \bigcup_{i=1}^m \mathcal{C}(U_i)$. Then $x \in U_i$ for some U_i but there is no coset in U_i which contains x . For any $k \in \mathbb{Z}_+$, $B_k(x) := x + Q^k \overline{L}$ is an open neighborhood of x in \overline{L} and $L \cap B_k(x) \not\subset U_i$, by assumption. Since $L = \bigcup_{i=1}^m U_i$, $(L \cap B_k(x)) \cap U_j \neq \emptyset$ for some $j \neq i$. So we can choose $x_k^j \in (L \cap B_k(x)) \cap U_j$. Then we get a sequence $\{x_k^j\}$ convergent to x as $k \rightarrow \infty$. Choosing a subsequence lying entirely in one Λ_j shows that $x \in \Lambda_j$ for some $j \neq i$. Since $x \in U_i$, and U_i, U_j are disjoint, $x \in \Lambda_j \setminus U_j$. □

Theorem 4 *Let $U_i, i = 1, \dots, m$, be disjoint nonempty point sets of the lattice L in \mathbb{R}^n . Let $\mathcal{C}(U_i)$ be the coset part in U_i , $c(U_i)$ the total index of U_i , and W_i the closure of U_i in \bar{L} . Then $\sum_{i=1}^m c(U_i) = 1$ if and only if the sets $U_i, i = 1, \dots, m$, are regular weak model sets in the CPS(18) and $\bar{L} = \bigcup_{i=1}^m W_i$.*

PROOF

(\Rightarrow) Assume that $\sum_{i=1}^m c(U_i) = 1$. Let $U_{m+1} := L \setminus \bigcup_{i=1}^m U_i$. Using Lemma 8 and the fact that $c(L) = 1$, we see that $c(U_{m+1}) = 0$ and $\sum_{i=1}^{m+1} c(U_i) = 1$. For this reason we can assume, in proving that the U_i are weak model sets, that $\bigcup_{i=1}^m U_i = L$ in the first place.

For $j \neq k$ the cosets of $\mathcal{C}(U_j)$ (of which there may be none!) and those of $\mathcal{C}(U_k)$ are disjoint from one another, and the same applies to $\bar{\mathcal{C}}(U_j)$ and $\bar{\mathcal{C}}(U_k)$. Thus

$$\mu\left(\bigcup_{i=1}^m \bar{\mathcal{C}}(U_i)\right) = \sum_{i=1}^m \mu(\bar{\mathcal{C}}(U_i)) = \sum_{i=1}^m c(U_i) = 1,$$

and

$$\mu\left(\bar{L} \setminus \left(\bigcup_{i=1}^m \bar{\mathcal{C}}(U_i)\right)\right) = 0. \quad (39)$$

Now note that $\partial W_j \cap \bigcup_{i=1}^m \bar{\mathcal{C}}(U_i) = \emptyset$ for any j . If not let $a \in \partial W_j \cap \bar{\mathcal{C}}(U_k)$ for some k . Since $\bar{\mathcal{C}}(U_k) \subset \overset{\circ}{W}_k$, we see that $j \neq k$. But $a \in W_j$, so a is a limit point of U_j , and $\bar{\mathcal{C}}(U_k)$ is an open neighborhood of a , so $U_j \cap \bar{\mathcal{C}}(U_k) \neq \emptyset$. This violates the disjointness of the U_i 's. We conclude that $\partial W_j \subset \bar{L} \setminus \left(\bigcup_{i=1}^m \bar{\mathcal{C}}(U_i)\right)$ and hence that

$$\mu(\partial W_j) = 0, \quad (40)$$

for all $j = 1, \dots, m$. Note also

$$\begin{aligned} \Lambda_i \setminus U_i &\subseteq \bigcup_{j=1}^m (\Lambda_j \setminus U_j) \\ &\subset L \setminus \bigcup_{j=1}^m \mathcal{C}(U_j) \quad \text{by Lemma 8} \\ &= L \setminus \bigcup_{j=1}^m (\bar{\mathcal{C}}(U_j) \cap L) = L \setminus \bigcup_{j=1}^m \bar{\mathcal{C}}(U_j). \end{aligned}$$

This shows that

$$\mu(\overline{\Lambda_i \setminus U_i}) \leq \mu\left(\overline{L \setminus \left(\bigcup_{i=1}^m \bar{\mathcal{C}}(U_i)\right)}\right) \leq \mu\left(\bar{L} \setminus \bigcup_{i=1}^m \bar{\mathcal{C}}(U_i)\right) = 0. \quad (41)$$

By Lemma 4(i) and (ii), $\overset{\circ}{W}_i \cap \overset{\circ}{W}_j = \emptyset$ for all $i \neq j$ and $(\Lambda_i \setminus U_i) \subset \bigcup_{j=1}^m \partial W_j$ for all $i = 1, \dots, m$.

Using Lemma 5(i) we obtain that the sets $U_i, i = 1, \dots, m$, are regular weak model sets in the CPS(18).

Remark : Whenever $\overset{\circ}{W}_i \neq \emptyset$, U_i is actually a regular model set. Since $\bigcup_{i=1}^m \overline{\mathcal{C}}(U_i) \subset \bigcup_{i=1}^m W_i$, $\mu(\bigcup_{i=1}^m W_i) = 1$. Thus $\overline{L} \setminus \bigcup_{i=1}^m W_i$ is open of measure 0 and $\overline{L} = \bigcup_{i=1}^m W_i$. This last argument does not require that $\bigcup_{i=1}^m U_i = L$.

(\Leftarrow) Assume that $U_i = \Lambda(V_i) = V_i \cap L$ where $\overline{V_i} \setminus \overset{\circ}{V_i}$ has measure 0 and $\overline{L} = \bigcup_{i=1}^m W_i$. Thus $U_i \subset V_i$ and $W_i := \overline{U_i} \subset \overline{V_i}$. Since L is dense in \overline{L} and for $x \in \overset{\circ}{V_i}$ each ball around x of radius $\epsilon > 0$ contains points of $\overset{\circ}{V_i} \cap L \subset U_i$, it follows that $\overline{U_i} \supset \overset{\circ}{V_i}$. This proves that $\overset{\circ}{V_i} \subset W_i \subset \overline{V_i}$. So $\mu(\overset{\circ}{V_i}) = \mu(W_i)$ and $\mu(W_i \setminus \overset{\circ}{V_i}) = 0$. Now

$$\bigcup_{i=1}^m W_i = \left(\bigcup_{i=1}^m \overset{\circ}{V_i} \right) \cup \left(\bigcup_{i=1}^m (W_i \setminus \overset{\circ}{V_i}) \right).$$

So $\mu(\bigcup_{i=1}^m W_i) = \mu(\bigcup_{i=1}^m \overset{\circ}{V_i})$. Also the disjointness of the U_i gives $\overset{\circ}{V_i} \cap \overset{\circ}{V_j} = \emptyset$ for $i \neq j$ (since L is dense in \overline{L}). Finally

$$1 = \mu\left(\bigcup_{i=1}^m W_i\right) = \mu\left(\bigcup_{i=1}^m \overset{\circ}{V_i}\right) = \sum_{i=1}^m \mu(\overset{\circ}{V_i}) = \sum_{i=1}^m c^*(\overset{\circ}{V_i}) \leq \sum_{i=1}^m c(\overset{\circ}{V_i} \cap L) \leq \sum_{i=1}^m c(U_i) \leq 1.$$

□

Corollary 2 *Let (\tilde{U}, Φ) be a primitive substitution system with inflation Q on the lattice L in \mathbb{R}^n . Suppose that PF-eigenvalue of $S(\Phi)$ is $|\det Q|$ and $L = \bigcup_{i=1}^m U_i$. Then $\sum_{i=1}^m c(U_i) = 1$, where $c(U_i)$ is the total index of U_i if and only if the sets $U_i, i = 1, \dots, m$, are model sets in CPS(18).*

□

PROOF Use Theorem 1 to determine that for all $i, \overset{\circ}{W}_i \neq \emptyset$. Now use Theorem and Remark in the proof.

□.

Chapter 6

Chair Tiling

The two dimensional chair tiling is generated by the inflation rule shown in Figure 5. There are 4 orientations of the chairs in any chair tiling. In [4] it was shown that the chair tiling has an interpretation in terms of model sets based on the lattice \mathbb{Z}^2 and its 2-adic completion as internal space.

In this section we generalize this result to the n -dimensional chair tiling using the results of the last section (see Figure 7 for an example of the 3-dimensional chair). To make things clearer we begin with the case $n = 2$.

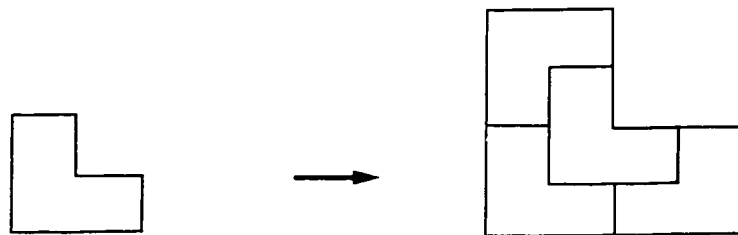


Figure 5: 2-dimensional chair tiling inflation

I. Chair tiling in \mathbb{R}^2

The starting point is to replace each tile by 3 oriented squares. Figure 6 shows the inflation rule, for one chair, in terms of oriented squares. The resulting tiling is a square tiling of the plane in which each of the squares has one of 4 orientations. The centre points of each square form a square lattice which we identify with \mathbb{Z}^2 by assigning coordinates as shown.

Let U_i be the set of centre points corresponding to squares of orientation (i) as given in Figure 6.

We start out from a basic generating set $A_2 := \{(x_1, x_2) | x_i \in \{0, -1\}\}$ and determine the precise maps for the substitution rules of Figure 6.

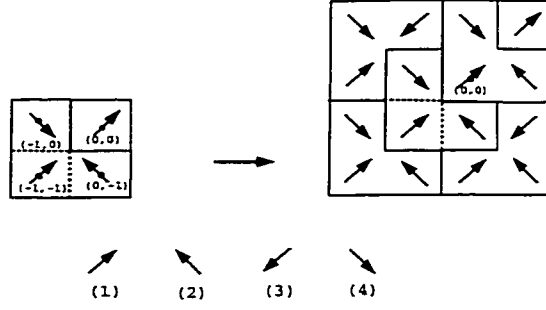


Figure 6: 2-dimensional chair tiling substitution

Letting $e_1 := (0, 0)$, $e_2 := (1, 0)$, $e_3 := (1, 1)$, $e_4 := (0, 1)$, these maps are defined as:

$$\begin{aligned} f_{j,i} : U_i &\rightarrow U_j \text{ by } (x, i) \mapsto (2x + e_j, j) \text{ if } j \neq i \pm 2 \\ f_{i,i}^{(2)} : U_i &\rightarrow U_i \text{ by } (x, i) \mapsto (2x + e_j, i) \text{ if } j = i \pm 2, \end{aligned}$$

where $i, j \in \{1, 2, 3, 4\}$, $x \in \mathbb{Z}^2$, $i \pm 2 := \begin{cases} i + 2 & \text{if } i \leq 2 \\ i - 2 & \text{if } i > 2. \end{cases}$

These are the maps of an affine substitution system Φ . In fact, if we define

$$h_1 : x \mapsto 2x + e_1, \quad h_2 : x \mapsto 2x + e_2, \quad h_3 : x \mapsto 2x + e_3, \quad h_4 : x \mapsto 2x + e_4,$$

then

$$\begin{aligned} f_{1,1} &= h_1, & f_{1,2} &= h_1, & f_{1,1}^{(2)} &= h_3, & f_{1,4} &= h_1 \\ f_{2,1} &= h_2, & f_{2,2} &= h_2, & f_{2,3} &= h_2, & f_{2,2}^{(2)} &= h_4 \\ f_{3,3}^{(2)} &= h_1, & f_{3,2} &= h_3, & f_{3,3} &= h_3, & f_{3,4} &= h_3 \\ f_{4,1} &= h_4, & f_{4,4}^{(2)} &= h_2, & f_{4,3} &= h_4, & f_{4,4} &= h_4, \end{aligned}$$

and

$$\Phi = \begin{pmatrix} \{h_1, h_3\} & \{h_1\} & \{\} & \{h_1\} \\ \{h_2\} & \{h_2, h_4\} & \{h_2\} & \{\} \\ \{\} & \{h_3\} & \{h_3, h_1\} & \{h_3\} \\ \{h_4\} & \{\} & \{h_4\} & \{h_4, h_2\} \end{pmatrix}.$$

Inflating A_2 by the substitutions above we generate the 4 point sets $U_i, i = 1, 2, 3, 4$. The precise description of U_i is as follows :

$$\begin{aligned} U_1 &= \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((0, 0) + 2^k(2, 0) + t(1, 1) + 2^k \cdot 4\mathbb{Z}^2) \\ &\cup \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((0, 0) + 2^k(0, 2) + t(1, 1) + 2^k \cdot 4\mathbb{Z}^2) \cup \bigcup_{t=-\infty}^{\infty} \{t(1, 1)\} \end{aligned}$$

$$\begin{aligned}
U_2 &= \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-1, 0) + 2^k(2, 0) + t(-1, 1) + 2^k \cdot 4\mathbb{Z}^2) \\
&\quad \cup \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-1, 0) + 2^k(0, 2) + t(-1, 1) + 2^k \cdot 4\mathbb{Z}^2) \cup \bigcup_{t=0}^{\infty} \{(0, -1) + t(1, -1)\} \\
U_3 &= \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-1, -1) + 2^k(2, 0) + t(-1, -1) + 2^k \cdot 4\mathbb{Z}^2) \\
&\quad \cup \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-1, -1) + 2^k(0, 2) + t(-1, -1) + 2^k \cdot 4\mathbb{Z}^2) \\
U_4 &= \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((0, -1) + 2^k(2, 0) + t(1, -1) + 2^k \cdot 4\mathbb{Z}^2) \\
&\quad \cup \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((0, -1) + 2^k(0, 2) + t(1, -1) + 2^k \cdot 4\mathbb{Z}^2) \cup \bigcup_{t=0}^{\infty} \{(-1, 0) + t(-1, 1)\}.
\end{aligned}$$

Each of these decompositions is basically into cosets, with the exception of three trailing sets in types 1, 2, and 4 which we will designate by V_1, V_2 , and V_4 respectively.

We can prove the correctness of this as follows:

Let U'_1, U'_2, U'_3, U'_4 be the sets on the right hand sides respectively. Note that

- (i) The generating set A_2 is contained in U'_i adequately, i.e. $(0, 0) \in U'_1$, $(0, -1) \in U'_2$, $(-1, -1) \in U'_1$, $(-1, 0) \in U'_4$
- (ii) Claim that $U'_i \supset \bigcup_{j=1}^4 \Phi_{ij} U'_j, i = 1, 2, 3, 4$.

Check that for any i ,

$$\begin{aligned}
h_i(U'_i) &\subset \bigcup_{\substack{j=1 \\ j \neq i, i \pm 2}}^4 \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-e_i) + 2^{k+1}(2(e_i - e_j)) + \\
&\quad 2t(e_{i \pm 2} - e_i) + 2^{k+1} \cdot 4\mathbb{Z}^2) \cup V_i \\
&\subset U'_i \\
h_{i \pm 2}(U'_i) &\subset \bigcup_{\substack{j=1 \\ j \neq i, i \pm 2}}^4 \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-e_i) + 2^{k+1}(2(e_i - e_j)) + \\
&\quad (2t + 1)(e_{i \pm 2} - e_i) + 2^{k+1} \cdot 4\mathbb{Z}^2) \cup V_i \\
&\subset U'_i
\end{aligned}$$

$$\begin{aligned} h_i(U'_l) &\subset (-2e_l + e_i + 4\mathbb{Z}^2) \cup (-2e_{l\pm 2} + e_i + 4\mathbb{Z}^2) \\ &\subset U'_i, \text{ where } l \neq i, i \pm 2, l \in \{1, 2, 3, 4\} \end{aligned}$$

(iii) $U'_i, i = 1, 2, 3, 4$, are all disjoint.

Indeed within each U'_i , all the cosets and the non-coset part are clearly disjoint. And two cosets or non-coset sets chosen from U'_i and U'_j , where $j \neq i, i \pm 2$, cannot intersect, since they are different by mod 2. Furthermore two of cosets or non-coset sets chosen from U'_i and $U'_{i\pm 2}$ cannot intersect either, since for $a + 2^k \cdot 4\mathbb{Z}^2 \subset U'_i$, $b + 2^l \cdot 4\mathbb{Z}^2 \subset U'_{i\pm 2}$ with $k \leq l$, $a - b \neq 0 \pmod{2^k \cdot 4\mathbb{Z}^2}$.

Now since U'_1, U'_2, U'_3, U'_4 are generated from A_2 by Φ , $U_i \subset U'_i$ for all $i = 1, 2, 3, 4$. Also from $\bigcup U_i = \mathbb{Z}^2$, we get $\bigcup U'_i = \mathbb{Z}^2$. Since all $U'_i, i = 1, 2, 3, 4$, are disjoint, $U_i = U'_i$ for all $i = 1, 2, 3, 4$.

Finally, for any $i = 1, 2, 3, 4$,

$$c(U_i) \geq 2 \cdot \sum_{k=0}^{\infty} \sum_{t=0}^{2^k-1} \frac{1}{(2^k \cdot 4)^2} = 2 \cdot \sum_{k=0}^{\infty} \frac{2^k}{16 \cdot (2^k)^2} = \frac{1}{4}.$$

Thus $\sum_{i=1}^4 c(U_i) = 1$. Theorem 4 shows that $U_i, i = 1, 2, 3, 4$, are regular model sets.

II. Chair tiling in \mathbb{R}^n

In this section we are going to generalize the foregoing to the n -dimensional chair tilings for all $n \geq 2$. The n -chair is an n -cube with a corner taken out of it. The inflation rule, which we spell out algebraically below, is geometrically the obvious generalization of the 2-dimensional case.

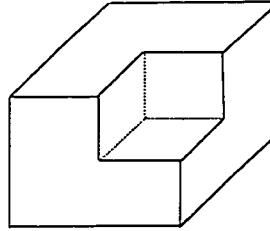


Figure 7: 3-dimensional chair tile

We transform the geometry by replacing each chair by a $2^n - 1$ oriented cubes, as before, and coordinatize the lattice formed by the centres of the cubes, starting from

the basic generating set $A_n := \{(x_1, \dots, x_n) | x_i \in \{0, -1\}\}$. There are 2^n orientations of cubes and hence 2^n types of points (but only $2^n - 1$ of these types appear in the starting set A_n).

For each $k \geq 0$ let $\beta(k)$ be the binary expansion $\epsilon_0 + \epsilon_1 2 + \epsilon_2 2^2 + \dots$ of k , $\epsilon_i \in \{0, 1\}$. We define the basic orientation vectors e_1, \dots, e_{2^n} by

$$e_i := \begin{cases} (\epsilon_0, \dots, \epsilon_{n-1}) & \text{the binary digits of } \beta(i-1) & \text{if } i \leq 2^{n-1}, \\ (1, \dots, 1) - e_{i-2^{n-1}} & & \text{if } i > 2^{n-1}. \end{cases}$$

We determine the sets $U_i, i = 1, \dots, 2^n$, of all i -type points in \mathbb{Z}^n from the points of the basic generating set A_n , using the inflation rules below.

The types of the points of A_n are as follows: for $x = (x_1, \dots, x_n) \in A_n$,

when $x_n = -1$;

$$x \in U_i, \text{ for which } \beta(i-1) = (1, \dots, 1) + x,$$

when $x_n = 0$;

$$\text{if } x = (0, \dots, 0), \quad x \in U_1$$

$$\text{otherwise, } x \in U_{i \pm 2^{n-1}}, \text{ for which } \beta(i-1) = (1, \dots, 1) - ((1, \dots, 1) + x) .$$

The idea of considering our vectors in the form $(1, \dots, 1) + x$ is to make it easy to compare them with the basic orientation vectors.

This conforms with what happens when $n = 2$: there are $2^n - 1$ types in the basic starting set that are in $2^{n-1} - 1$ complementary pairs and 1 pair of vectors $(0, \dots, 0)$ and $(-1, \dots, -1)$ of the same type, namely of type 1.

Define

$$\begin{aligned} f_{j,i} : U_i &\rightarrow U_j \text{ by } (x, i) \mapsto (2x + e_j, j) & \text{if } j \neq i \pm 2^{n-1} \\ f_{i,i}^{(2)} : U_i &\rightarrow U_i \text{ by } (x, i) \mapsto (2x + e_i, i) & \text{if } j = i \pm 2^{n-1}, \end{aligned}$$

where $i, j \in \{1, \dots, 2^n\}$, $x \in \mathbb{Z}^n$, $i \pm 2^{n-1} := \begin{cases} i + 2^{n-1} & \text{if } i \leq 2^{n-1} \\ i - 2^{n-1} & \text{if } i > 2^{n-1} \end{cases}$.

Let Φ be the matrix function system. Define $h_i : x \mapsto 2x + e_i, i \in \{1, \dots, 2^n\}$.

$$\Phi = \begin{pmatrix} \{h_1, h_{1+2^{n-1}}\} \{h_1\} & \dots & \overset{1+2^{n-1}}{\downarrow} \{\} & \dots & \{h_1\} \\ \vdots & & & & \\ \{h_{2^n}\} \{h_{2^n}\} & \dots & \overset{2^n-2^{n-1}}{\downarrow} \{\} & \dots & \{h_{2^n-2^{n-1}}, h_{2^n}\} \end{pmatrix}.$$

Inflating A_n by the maps, we get the precise description of U_i :

$$U_i = \bigcup_{\substack{j=1 \\ j \neq i, i \pm 2^{n-1}}}^{2^n} \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-e_i) + 2^k(2(e_i - e_j)) + t(e_{i \pm 2^{n-1}} - e_i) + 2^k \cdot 4\mathbb{Z}^n) \cup V_i,$$

where

$$V_i = \begin{cases} \bigcup_{t=-\infty}^{\infty} \{t(e_{1 \pm 2^{n-1}} - e_1)\} & \text{if } i = 1 \\ \bigcup_{t=0}^{\infty} \{t(e_i - e_{i \pm 2^{n-1}}) + (-e_{i \pm 2^{n-1}})\} & \text{if } i \neq 1, 1 \pm 2^{n-1} \\ \emptyset & \text{if } i = 1 + 2^{n-1}. \end{cases} \quad (42)$$

The equalities can be proved in the same way as in the 2-dimensional case.

Let U'_i be the set of the right hand side in (42). Note that

(i) The generating set A_n is contained in U'_i adequately, i.e.

$$\begin{aligned} e_1 &\in U'_1 & \text{if } i = 1 \\ -e_{i \pm 2^{n-1}} &\in U'_i & \text{if } i \neq 1, 1 \pm 2^{n-1} \\ -e_{1 \pm 2^{n-1}} &\in U'_1 & \text{if } i = 1 \pm 2^{n-1}. \end{aligned}$$

(ii) Claim that $U'_i \supset \bigcup_{j=1}^{2^n} \Phi_{ij} U'_j, i = 1, \dots, 2^n$.

Indeed for $i \in \{1, \dots, 2^n\}$

$$\begin{aligned} h_i(U'_i) &\subset \bigcup_{\substack{j=1 \\ j \neq i, i \pm 2^{n-1}}}^{2^n} \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-e_i) + 2^{k+1}(2(e_i - e_j)) + \\ &\quad 2t(e_{i \pm 2^{n-1}} - e_i) + 2^{k+1} \cdot 4\mathbb{Z}^n) \cup V_i \\ &\subset U'_i \\ h_{i \pm 2^{n-1}}(U'_i) &\subset \bigcup_{\substack{j=1 \\ j \neq i, i \pm 2^{n-1}}}^{2^n} \bigcup_{k=0}^{\infty} \bigcup_{t=0}^{2^k-1} ((-e_i) + 2^{k+1}(2(e_i - e_j)) + \\ &\quad (2t+1)(e_{i \pm 2^{n-1}} - e_i) + 2^{k+1} \cdot 4\mathbb{Z}^n) \cup V_i \\ &\subset U'_i \\ h_i(U'_l) &\subset (-2e_l + e_i + 4\mathbb{Z}^n) \cup (-2e_{l \pm 2^{n-1}} + e_i + 4\mathbb{Z}^n) \\ &\subset U'_i, \text{ where } l \neq i, i \pm 2^{n-1}, l \in \{1, \dots, 2^n\}. \end{aligned}$$

(iii) $U'_i, i = 1, \dots, 2^n$, are disjoint.

Indeed all cosets and a non-coset set in each U'_i are all disjoint. And two cosets or non-coset sets chosen from U'_i and U'_j , where $j \neq i, i \pm 2^{n-1}$, cannot intersect, since they are different by mod 2. Furthermore two of cosets or non-coset sets chosen from U'_i and $U'_{i \pm 2^{n-1}}$ cannot intersect either, since for $a + 2^k \cdot 4\mathbb{Z}^n \subset U'_i$, $b + 2^l \cdot 4\mathbb{Z}^n \subset U'_{i \pm 2^{n-1}}$ with $k \leq l$, $a - b \neq 0 \pmod{2^k \cdot 4\mathbb{Z}^n}$.

Now since $U'_i, i = 1, \dots, 2^n$, are generated from A_n by Φ , $U_i \subset U'_i$ for all $i = 1, \dots, 2^n$. Also from $\bigcup_{i=1}^{2^n} U_i = \mathbb{Z}^n$, $\bigcup_{i=1}^{2^n} U'_i = \mathbb{Z}^n$. Since all $U'_i, i = 1, \dots, 2^n$, are disjoint, $U_i = U'_i$ for all $i = 1, \dots, 2^n$.

For any $i = 1, \dots, 2^n$,

$$c(U_i) \geq (2^n - 2) \cdot \sum_{k=0}^{\infty} \sum_{t=0}^{2^k-1} \frac{1}{(2^k \cdot 4)^n} = (2^n - 2) \cdot \sum_{k=0}^{\infty} \frac{2^k}{2^{2n} \cdot (2^k)^n} = \frac{1}{2^n}.$$

Thus $\sum_{i=1}^{2^n} c(U_i) = 1$. Theorem 4 shows that $U_i, i = 1, \dots, 2^n$, are regular model sets.

To get a model set interpretation of the chair tiling itself we proceed as follows. We observe that every arrow points to the inner corner of exactly one chair. Let us label each chair by its inner corner point which is at the tip of exactly $2^n - 1$ arrows. These corner points give us 2^n sets X_1, \dots, X_{2^n} according to the type, and all lie in the shift $L' = (\frac{1}{2}, \dots, \frac{1}{2}) + \mathbb{Z}^n$ of our lattice \mathbb{Z}^n . Let $f_i, i = 1, \dots, 2^n$, be $(\frac{1}{2}, \dots, \frac{1}{2}) - e_i$ respectively. Then $U_i + f_i$ is the set of tips of all arrows of type i and $U_i + f_i = L' \cap (V_i + f_i)$, for some $V_i \subset \overline{\mathbb{Z}^n} = (\mathbb{Z}_2)^n$ such that $\overline{V_i}$ compact, $\overset{\circ}{V_i} \neq \emptyset$ and $\mu(\partial V_i) = 0$. Now

$$X_i = L' \cap \left(\bigcap_{j \neq i \pm 2^{n-1}} (V_j + f_j) \right)$$

which is the required regular model set description of X_i , since

$$\partial \left(\bigcap_{j \neq i \pm 2^{n-1}} (V_j + f_j) \right) \subset \bigcup_{j \neq i \pm 2^{n-1}} \partial(V_j + f_j)$$

and $\mu(\partial(V_j + f_j)) = 0$ for all $j = 1, \dots, 2^n$.

From this result we can show that if we mark each chair with a single point in a consistent way, then the set of points obtained from all the chairs of any one type also forms a regular model set, and hence a pure point diffractive set.

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Appendix

A typical sample of material to be studied by diffraction may be thought of (at least in crude terms) as a finite set Λ of points (atoms), x , each of which acts as a scatterer (for the incoming radiation such as X -rays, electrons, neutrons) of certain strength $n(x)$. This gives rise to a measure $\mu_\Lambda = \sum_{x \in \Lambda} n(x) \delta_x$ called the diffractive density of Λ , where δ_x is the delta function such that $\delta_x(f) = f(x)$ with $x \in \Lambda$ and $f \in C_c(\mathbb{R}^3)$, which is the space of continuous \mathbb{C} -valued functions with compact support. Define the measure $\tilde{\mu}$ by $\tilde{\mu}(f) = \mu(\tilde{f})$, where $f \in C_c(\mathbb{R}^3)$ and $\tilde{f}(x) := \overline{f(-x)}$. The diffraction intensity of the sample Λ is, by definition, the volume averaged value of $|\widehat{\mu_\Lambda}|^2$; namely

$$\frac{1}{\text{Vol}(\Lambda)} |\widehat{\mu_\Lambda}(q)|^2 = \frac{1}{\text{Vol}(\Lambda)} \widehat{(\mu_\Lambda \star \tilde{\mu}_\Lambda)}(q),$$

where the $\widehat{}$ indicates the operation of taking Fourier transforms.

This is supposed to describe the intensity per unit volume of the sample at each point $q \in \mathbb{R}^3$. By $\text{Vol}(\Lambda)$ we mean the volume of the region (a sphere, a cube, or whatever) of space that the set Λ of atoms occupies.

Such quantities are only physically meaningful if they reach some stable limit as the sample size $\text{Vol}(\Lambda)$ tends to “infinity”. Thus we are led to determining the autocorrelation measure

$$\gamma := \lim_{\text{Vol}(\Lambda) \rightarrow \infty} \frac{1}{\text{Vol}(\Lambda)} \mu_\Lambda \star \tilde{\mu}_\Lambda$$

and its Fourier transform

$$\widehat{\gamma} = \lim_{\text{Vol}(\Lambda) \rightarrow \infty} \frac{1}{\text{Vol}(\Lambda)} \widehat{(\mu_\Lambda \star \tilde{\mu}_\Lambda)}.$$

Convergence is in terms of the vague topology. Recall that a measure μ is the vague limit of a sequence $\{\mu_n\}$ of measures if for any $f \in C_c(\mathbb{R}^3, \mathbb{R})$, $\{\mu_n(f)\} \rightarrow \mu(f)$.

There is a technical issue here that we will not discuss further : does the shape of the sample matter?

The autocorrelation measure γ is a distribution of positive definite type. This implies that its Fourier transform $\widehat{\gamma}$ is a positive measure. So $\widehat{\gamma_\Lambda}$ converges to a well-defined positive measure $\widehat{\gamma}$, which is called the diffraction measure. $\widehat{\gamma}$ actually

decomposes uniquely into three measures, which are absolutely continuous, singular continuous and pure point measures respectively, i.e. $\widehat{\gamma} = \widehat{\gamma}_{ac} + \widehat{\gamma}_{sing} + \widehat{\gamma}_{pp}$. If $\widehat{\gamma} = \widehat{\gamma}_{pp}$, then we say that $\widehat{\gamma}$ (and Λ) is pure point diffractive. Our primary interest is understanding under what conditions Λ is pure point diffractive. We note that at this point a “physical problem” has turned into a purely mathematical one, and indeed we need no longer restrict ourselves to \mathbb{R}^3 but can work in \mathbb{R}^n .

Let us look at one example of a point set to study the positive diffraction measure. This example is the basis of the diffraction theory for periodic structures (i.e. crystals). Consider a lattice \mathbb{Z}^n in \mathbb{R}^n and define $\rho = \sum_{x \in \mathbb{Z}^n} \delta_x$, where δ_x is the delta function such that $\delta_x(f) = f(x)$ for all $f \in C_c(\mathbb{R}^n, \mathbb{R})$. Let $\rho_r = \sum_{x \in c(r) \cap \mathbb{Z}^n} \delta_x$, where $c(r)$ is the cube $\{(x_1, \dots, x_n) \in \mathbb{R}^n \mid |x_i| \leq r\}$. The autocorrelation of ρ_r is $\rho_r \star \tilde{\rho}_r$, where

$$(\rho_r \star \tilde{\rho}_r)(\varphi) = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \varphi(x+y) d\rho_r(x) d\tilde{\rho}_r(y), \quad \varphi \in C_c(\mathbb{R}^n, \mathbb{R}).$$

Then the volume averaged autocorrelation of ρ is

$$\gamma = \lim_{r \rightarrow \infty} \frac{1}{\text{Vol}(c(r))} \rho_r \star \tilde{\rho}_r.$$

Now

$$\begin{aligned} (\rho_r \star \tilde{\rho}_r)(\varphi) &= \left(\sum_{x \in c(r) \cap \mathbb{Z}^n} \delta_x \right) \star \left(\sum_{y \in c(r) \cap \mathbb{Z}^n} \tilde{\delta}_y \right) (\varphi) \\ &= \sum_{x, y \in c(r) \cap \mathbb{Z}^n} (\delta_x \star \tilde{\delta}_y)(\varphi) \\ &= \sum_{x, y \in c(r) \cap \mathbb{Z}^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \varphi(u+v) d\delta_x(u) d\tilde{\delta}_y(v) \\ &= \sum_{x, y \in c(r) \cap \mathbb{Z}^n} \int_{\mathbb{R}^n} \varphi(x+v) d\tilde{\delta}_y(v) \\ &= \sum_{x, y \in c(r) \cap \mathbb{Z}^n} \varphi(x-y) \\ &= \sum_{x, y \in c(r) \cap \mathbb{Z}^n} \delta_{x-y}(\varphi), \quad \text{where } \varphi \in C_c(\mathbb{R}^n, \mathbb{R}). \end{aligned} \tag{43}$$

Thus

$$\frac{1}{\text{Vol}(c(r))} (\rho_r \star \tilde{\rho}_r)(\varphi) = \frac{1}{(2r)^n} \sum_{x, y \in c(r) \cap \mathbb{Z}^n} \delta_{x-y}(\varphi)$$

$$= \frac{1}{(2r)^n} \sum_{\substack{x, x-z \in c(r) \cap \mathbb{Z}^n \\ z \in \mathbb{Z}^n}} \delta_z(\varphi).$$

Since any $\varphi \in C_c(\mathbb{R}^n, \mathbb{R})$ has a compact support, this sum becomes independent of r once we reach a certain size r_0 (depending on φ). So

$$\sum_{\substack{x, x-z \in c(r) \cap \mathbb{Z}^n \\ z \in \mathbb{Z}^n}} \delta_z(\varphi)$$

is replaced by

$$\sum_{z \in c(r_0)} \left(\sum_{x, x-z \in c(r) \cap \mathbb{Z}^n} 1 \right) \varphi(z).$$

Let

$$v_n(z) := \frac{1}{(2r)^n} \left(\sum_{x, x-z \in c(r) \cap \mathbb{Z}^n} 1 \right).$$

To get the vague limit of $\frac{1}{\text{Vol}(c(r))}(\rho_r \star \tilde{\rho}_r)$, we need only work out $\lim_{n \rightarrow \infty} v_n(z)$. Since z is fixed and $r \rightarrow \infty$, r can be assumed to be very large with respect to z . Let $r_1 = |z|$. From

$$\begin{aligned} (c(r - r_1) \cap \mathbb{Z}^n) &\subset (c(r) \cap \mathbb{Z}^n) \subset (c(r + r_1) \cap \mathbb{Z}^n), \\ \frac{(2(r - r_1))^n}{(2r)^n} &\leq \frac{\sum_{x, x-z \in c(r) \cap \mathbb{Z}^n} 1}{(2r)^n} \leq \frac{(2(r + r_1))^n}{(2r)^n}. \end{aligned}$$

As $r \rightarrow \infty$, $1 \leq \lim_{r \rightarrow \infty} v_r(z) \leq 1$. Thus $\lim_{r \rightarrow \infty} v_r(z) = 1$. Therefore,

$$\begin{aligned} \gamma &= \lim_{r \rightarrow 0} \frac{1}{\text{Vol}(c(r))}(\rho_r \star \tilde{\rho}_r)(\varphi) = \sum_{z \in c(r_0) \cap \mathbb{Z}^n} \varphi(z) \\ &= \sum_{z \in \mathbb{Z}^n} \varphi(z) \\ &= \sum_{z \in \mathbb{Z}^n} \delta_z(\varphi), \end{aligned}$$

since φ has a compact support contained in $c(r_0)$. The diffraction measure which we aimed for is the Fourier transform of this volume averaged autocorrelation. The Poisson summation formula tells us that

$$\widehat{\gamma} = \left(\sum_{z \in \mathbb{Z}^n} \delta_z \right) = \sum_{z \in \mathbb{Z}^n} \delta_z.$$

So this is a pure point diffraction measure of the lattice on \mathbb{R}^n . □