数理科学実践研究レター 2023–3 March 30, 2023

Coordination sequence of a quasicrystal

by

Long Wang

UNIVERSITY OF TOKYO

GRADUATE SCHOOL OF MATHEMATICAL SCIENCES

KOMABA, TOKYO, JAPAN

Coordination sequence of a quasicrystal

Long Wang[1] (Graduate School of Mathematical Sciences, The University of Tokyo)

Abstract
We study the asymptotic behavior of the coordination sequence of a quasicrystal.

準結晶の配位数列

王龍 (東京大学数理科学研究科)

概要
準結晶の配位数列について研究した。$\Lambda = \Lambda(L,\Omega) \subset \mathbb{R}^d$ をモデル集合とし、$x \in \Lambda$ とする. 十分大きいな正整数 n に対して、以下の不等式を満たす定数 c, C が存在する: $c \cdot n^d \leq S_{x,n} \leq C \cdot n^d$.

1 Introduction

In crystallography, the concept of a coordination sequence was introduced and studied for various crystalline structures. Mathematically, coordination sequences can be easily described in the language of graphs. In the case of crystals, a number of methods were proposed that allow one to prove explicit formulas for coordination sequences. A detailed bibliography on these issues can be found in [GSS19]. It is expected that the coordination sequences of crystals are of quasipolynomial type. This conjecture was verified in [NSMN21] very recently. Coordination sequences of quasicrystals remain much less studied. In [SM18], the authors studied the coordination sequence of a Penrose tiling whose asymptotic behavior turned out to be fundamentally new. At present, the problem of describing the coordination sequences of arbitrary quasicrystals is far from being solved. In this note, we study the asymptotic behavior of the coordination sequence of a quasicrystal.

2 Preliminaries

Definition 1. *A Delone set Λ is a discrete subset of $\mathbb{R}^d$ with $R \geq r > 0$, such that*

(1) *for every $x \in \mathbb{R}^d$, there exists $x \neq y \in \Lambda$ with $||x-y|| \leq R$;*

(2) *for each pair $x \neq y \in \Lambda$, $||x-y|| \geq r$.*

A quasicrystal (also known as a Meyer set) Λ is a Delone set $\Lambda \subset \mathbb{R}^d$

(3) *with a finite subset $F \subset \mathbb{R}^d$ such that*

$$\Lambda - \Lambda \subset \Lambda + F.$$

Proposition 2 ([La96])**.** *A Delone set $\Lambda \subset \mathbb{R}^d$ is a quasicrystal, if and only if $\Lambda - \Lambda$ is a Delone set.*

Definition 3. *The model set (also known as a cut-and-project set) $\Lambda(L,\Omega) \subset \mathbb{R}^d$ is associated to data (L,Ω), in which L is a full rank lattice in $\mathbb{R}^{d+k} = \mathbb{R}^d \times \mathbb{R}^k$ with $k \geq 0$, which satisfies*

(i) *No two elements of L have the same image under the projection p_1 onto $\mathbb{R}^d$,*

(ii) *The image of L under the projection p_2 onto $\mathbb{R}^k$ is dense in $\mathbb{R}^k$,*

and Ω is a window in $\mathbb{R}^k$ which is a nonempty bounded open set. Then $\Lambda(L,\Omega)$ is given by

$$\Lambda(L,\Omega) := \{p_1(x) : x \in L \text{ and } p_2(x) \in \Omega\}.$$

Proposition 4 ([Me95, Theorem 1])**.** *A model set $\Lambda(L,\Omega) \subset \mathbb{R}^d$ is a quasicrystal. Conversely, for a quasicrystal $\Lambda \subset \mathbb{R}^d$, there exists a finite set F and a model set $\Lambda(L,\Omega) \subset \mathbb{R}^d$ such that $\Lambda \subset \Lambda(L,\Omega) + F$.*

[1] wangl11@ms.u-tokyo.ac.jp

3 Main result

Given a Delone set $\Lambda \subset \mathbb{R}^d$, and a fixed point $x \in \Lambda$, consider the coordination sequence $(S_{x,n})_{n\in\mathbb{Z}_{>0}}$ defined as follows:

$$S_{x,n} = \#\{y \in \Lambda : \|y - x\| \leq nR\},$$

where # denotes the number of elements in a finite set. Here notice that, by the definition of a Delone set, $\{y \in \Lambda : \|y - x\| \leq nR\}$ is always a finite set.
In this note, we study the asymptotic behaviour of a coordination sequence and obtain the following main result.

Theorem 5. *Let $\Lambda = \Lambda(L, \Omega) \subset \mathbb{R}^d$ be a model set and $x \in \Lambda$ a fixed point. Then*

$$c \cdot n^d \leq S_{x,n} \leq C \cdot n^d$$

for certain positive constants C, c and $n \gg 0$.

Proof. This follows from Proposition 6 and Proposition 7 below. □

Proposition 6. *Let $\Lambda \subset \mathbb{R}^d$ be a Delone set and $x \in \Lambda$ a fixed point. Then*

$$S_{x,n} = O(n^d).$$

Proof. We let

$$W_{x,n} := \{y \in \Lambda : ||y - x|| \leq nR\} \subset \Lambda.$$

Then $S_{x,n} = \#W_{x,n}$, where $W_{x,n}$ is a finite set. We have to show that

$$\#W_{x,n} = O(n^d).$$

For every point $y \in W_{x,n}$, we have the inclusion

$$\begin{aligned} D_y :=& \{z \in \mathbb{R}^d : ||y - z|| \leq r/2\} \\ &\subset \{z \in \mathbb{R}^d : ||x - z|| \leq nR + r/2\}. \end{aligned}$$

For two distinct points $y \neq y' \in W_{x,n}$, we have

$$\operatorname{Int} D_y \cap \operatorname{Int} D_{y'} = \varnothing.$$

Therefore,

$$\#W_{x,n} \leq \frac{\operatorname{Vol}(\{z \in \mathbb{R}^d : ||x - z|| \leq nR + r/2\})}{\operatorname{Vol}(\{z \in \mathbb{R}^d : ||y - z|| \leq r/2\})} = O(n^d).$$

This completes the proof of the proposition. □

Proposition 7. *Let $\Lambda = \Lambda(L, \Omega) \subset \mathbb{R}^d$ be a model set and $x \in \Lambda$ a fixed point. Then*

$$S_{x,n} \geq c \cdot n^d$$

for some positive constant c and $n \gg 0$.

Proof. First we note that for any fixed point $\mathbf{x} \in L$ and $n \gg 0$,

$$S_{\mathbf{x},n}(L) = \#\{\mathbf{y} \in L : \|\mathbf{y} - \mathbf{x}\| \leq nR\} \geq c_0 \cdot n^{d+k}$$

as L is a full rank lattice in $\mathbb{R}^{d+k} = \mathbb{R}^d \times \mathbb{R}^k$. Take a point $x \in \Lambda$ such that $\mathbf{x} = (x, x') \in L$. By the definition of a model set, the projection p_1 onto $\mathbb{R}^d$ is injective on L, and

$$\Lambda = \{p_1(x) : x \in L \text{ and } p_2(x) \in \Omega\}$$

with $\Omega \subset \mathbb{R}^k$ a nonempty bounded open set. Then

$$p_1(\{\mathbf{y} \in L : p_2(\mathbf{y}) \in \Omega, \|\mathbf{y} - \mathbf{x}\| \le R\}) \subset \{y \in \Lambda : \|y - x\| \le R\}.$$

Since $p_1|_L$ is injective, it suffices to show that

$$\#\{\mathbf{y} \in L : p_2(\mathbf{y}) \in \Omega, \|\mathbf{y} - \mathbf{x}\| \le nR\} \ge c \cdot n^d$$

for some positive constant c and $n \gg 0$. Note that $\Omega \subset \mathbb{R}^k$ is bounded, so we can take an open ball in $\mathbb{R}^k$ with radius R_0 that contains Ω. Thus, for $n \gg 0$, we have $nR \gg R_0$, and

$$\#\{\mathbf{y} \in L : p_2(\mathbf{y}) \in \Omega, \|\mathbf{y} - \mathbf{x}\| \le nR\} \ge c \cdot n^d$$

for some positive constant c. □

Remark 8. *The proof of Proposition 7 uses the structure of model sets in an essential way. Currently we do not know whether Proposition 7 holds for quasicrystals (or even more generally, for Delone sets) as Proposition 6 does. If this is the case, then Theorem 5 holds for quasicrystals.*

Remark 9. *Let $\Lambda \subset \mathbb{R}^d$ be a quasicrystal and $x \in \Lambda$ a fixed point. One can also consider the following refined coordination sequence $(s_{x,n})_{n \in \mathbb{Z}_{>0}}$ where*

$$s_{x,n} := \{y \in \Lambda : (n-1)R < \|y - x\| \le nR\}.$$

We do not know whether it holds that

$$c \cdot n^{d-1} \le s_{x,n} \le C \cdot n^{d-1}$$

for some positive constants C, c and $n \gg 0$.

Acknowledgement The author thanks Takafumi Mase, Junichi Nakagawa, Yusuke Nakamura, Atsushi Shiho, and the referee for beneficial suggestions, discussions and comments. He is grateful to the support from Leading Graduate Course for Frontiers of Mathematical Sciences and Physics.

References

[GSS19] C. Goodman-Strauss and N. J. A. Sloane, *A coloring-book approach to finding coordination sequences*, Acta Cryst. (2019). A**75**, 121–134.

[La96] J. C. Lagarias, *Meyer's concept of quasicrystal and quasiregular sets*, Commun. Math. Phys. **179** (1996), 365–376.

[Me95] Y. Meyer, *Quasicrystals, Diophantine approximation and algebraic numbers*, in *Beyond quasicrystals*, 3–16, Springer, 1995.

[NSMN21] Y. Nakamura, R. Sakamoto, T. Mase and J. Nakagawa, *Coordination sequences of crystals are of quasi-polynomial type*, Acta Cryst. (2021). A**77**, 138–148.

[SM18] A. Shutov and A. Maleev, *Coordination numbers of the vertex graph of a Penrose tiling*, Acta Crystallogr. Sect. (2018). A**74**, 112–122.