Aperiodic Order
Part 1

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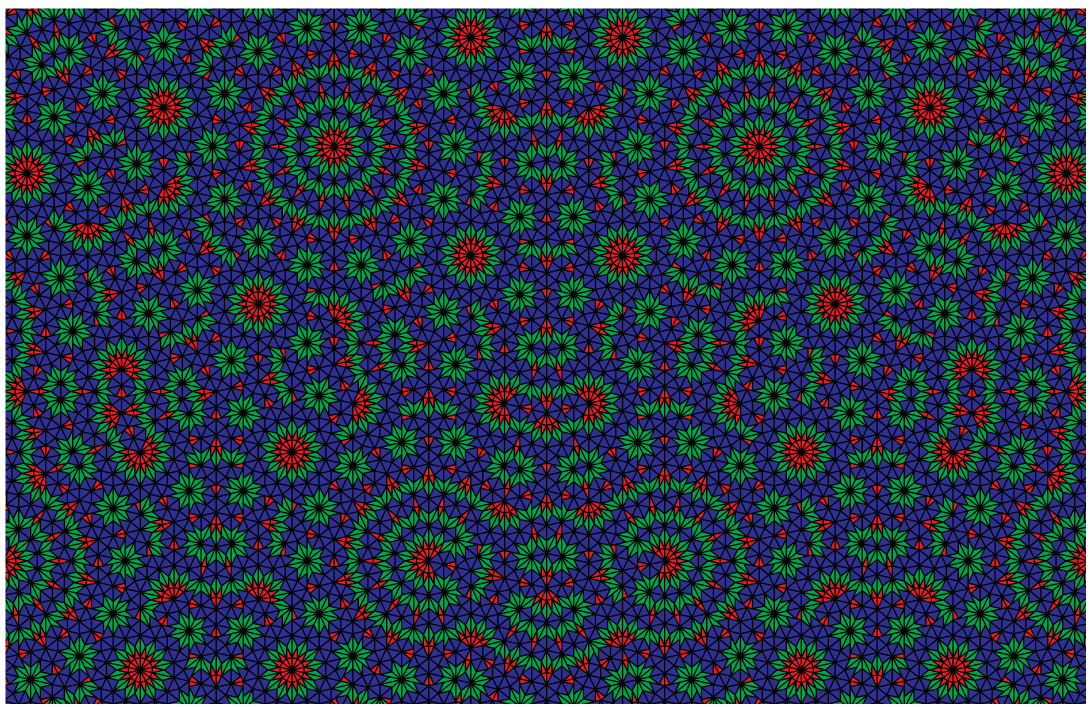
`http://mcs.open.ac.uk/ugg2/ltcc/`



1.1 What is Aperiodic Order?

- What is order?
  - Symmetry
  - Group theory
  - Dynamical systems
  - Harmonic analysis
  - Spectral theory
- Crystals as paradigm of order in nature
- What is a crystal?
  - Diffraction
  - Crystallographic restriction
  - Complete classification of periodic crystal structures
- Aperiodic crystals
  - Incommensurate crystals
  - Quasicrystals

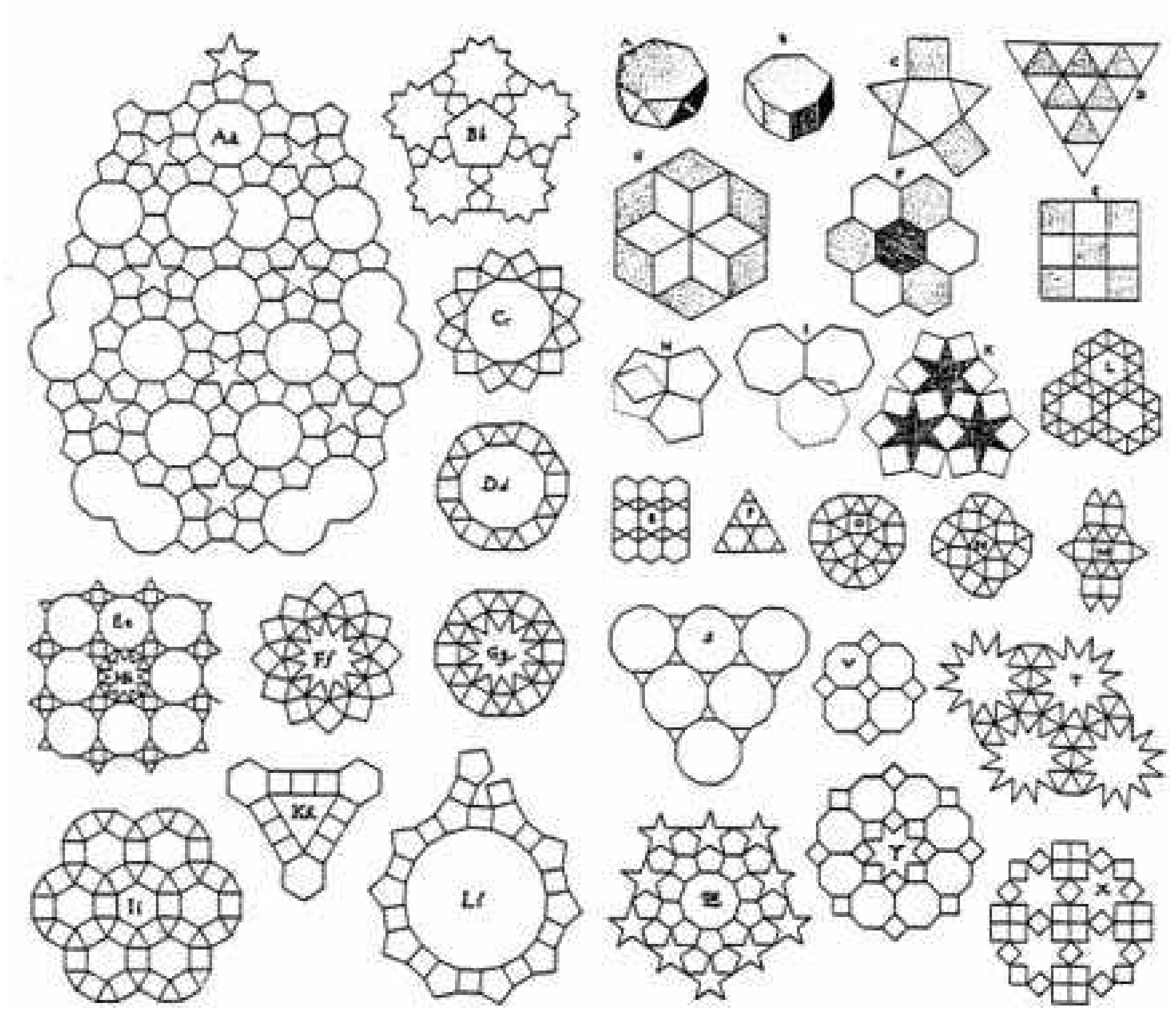
1.2 A few historical remarks

- Geometric patterns in medieval Islamic art
- Johannes Kepler (1571–1630)
- Hao Wang (1961)
- Undecidability of the domino problem: Robert Berger (1966)
- Model sets: Yves Meyer (1970)
- Roger Penrose (1974)
- Ammann, deBruijn, Kramer, . . .
- Discovery of quasicrystals by Dan Shechtman (1982)
- Shechtman receives Nobel prize in Chemistry (2011)

1.2 A few historical remarks

An example of Islamic art from Bukhara, Uzbekistan

1.2 A few historical remarks



Kelper's sketches in Harmonices Mundi Libri V (1619)

1.2 A few historical remarks

Roger Penrose and his rhombus tiling in the foyer of the Mitchell Institute for Fundamental Physics and Astronomy at Texas A&M University

1.2 A few historical remarks

Dan Shechtman, Nobel Prize in Chemistry 2011

1.3 Point sets

A set consisting of one point is called a *singleton set*, and countable unions of singleton sets are called *point sets*.

A point set $\varLambda \subseteq \mathbb{R}^d$ is *discrete* if each element $x \in \varLambda$ has an open neighbourhood $U = U(x) \subseteq \mathbb{R}^d$ that does not contain any other point of $\varLambda$. For each $x \in \varLambda$, there is an $r > 0$ such that $B_r(x)$ (open ball of radius r around x) satisfies $B_r(x) \cap \varLambda = \{x\}$.

$\varLambda$ is *uniformly discrete* if there is an open neighbourhood U of $0 \in \mathbb{R}^d$ such that $(x + U) \cap (y + U) = \varnothing$ holds for all distinct $x, y \in \varLambda$.

Here, $x + U := \{x + u \mid u \in U\}$ and, more generally, we define the *Minkowski sum* and *difference* of two arbitrary sets $U, V \subseteq \mathbb{R}^d$ as

$$U \pm V := \{u \pm v \mid u \in U, \, v \in V\}.$$

1.3 Point sets

A point set $\varLambda \subseteq \mathbb{R}^d$ is called *locally finite* if, for all compact $K \subseteq \mathbb{R}^d$, the intersection $K \cap \varLambda$ is a finite set (or empty).

A point set $\varLambda \subseteq \mathbb{R}^d$ is *relatively dense* if a compact $K \subseteq \mathbb{R}^d$ exists such that $\varLambda + K = \mathbb{R}^d$.

A point set $\varLambda \subseteq \mathbb{R}^d$ is a *Delone set* (Delaunay set), if it is both uniformly discrete and relatively dense.

A point set $\varLambda \subseteq \mathbb{R}^d$ is a *Meyer set*, if $\varLambda$ is relatively dense and $\varLambda - \varLambda$ is uniformly discrete.

A *cluster* of a point set $\varLambda \subseteq \mathbb{R}^d$ is the intersection $K \cap \varLambda$ for some compact $K \subseteq \mathbb{R}^d$.

A point set $\varLambda \subseteq \mathbb{R}^d$ has *finite local complexity* (FLC) w.r.t. to translations when the collection $\{(t + K) \cap \varLambda \mid t \in \mathbb{R}^d\}$, for any given compact $K \subseteq \mathbb{R}^d$, contains only finitely many clusters up to translations.

1.3 Point sets

Relation between different properties of point sets:

$$\Lambda \text{ Meyer } \implies \Lambda \text{ FLC and Delone } \implies \Lambda \text{ Delone}$$

Lemma: Let $\Lambda \subseteq \mathbb{R}^d$ be a Delone set, such that $\Lambda - \Lambda \subseteq \Lambda + F$ for some finite set $F \subseteq \mathbb{R}^d$.
Then Λ is a Meyer set.

Proof: Λ Delone $\implies$ Λ relatively dense
We need to show that $\Lambda - \Lambda$ is also uniformly discrete
Let $\Delta := \Lambda - \Lambda$, then

$\Lambda - \Lambda$ uniformly discrete $\iff$ 0 is isloated point in $\Delta - \Delta$

Now, $\Delta - \Delta \subseteq (\Lambda + F) - (\Lambda + F) \subseteq \Delta + (F - F) \subseteq \Delta + F'$
which is locally finite since F' is finite

$\implies$ 0 is isolated point in $\Delta - \Delta$ ■

Lagarias showed that the converse is true in $\mathbb{R}^d$ (and more generally), but the argument is more involved.

1.4 Lattices

A point set $\varGamma \subseteq \mathbb{R}^d$ is called a *lattice* in $\mathbb{R}^d$ if there exist d vectors $b_1, \dots, b_d$ such that

$$\varGamma \;=\; \mathbb{Z}b_1 \oplus \cdots \oplus \mathbb{Z}b_d \;:=\; \left\{ \sum_{i=1}^{d} m_i b_i \;\middle|\; \text{all } m_i \in \mathbb{Z} \right\},$$

together with the requirement that its $\mathbb{R}$-span $\langle \varGamma \rangle_{\mathbb{R}} = \mathbb{R}^d$. The set $\{b_1, \dots, b_d\}$ is called a *basis* of the lattice $\varGamma$.

$\varLambda \subseteq \mathbb{R}^d$ is a *crystallographic point packing* in $\mathbb{R}^d$ if there is a lattice $\varGamma$ in $\mathbb{R}^d$ and a finite set $F \subseteq \mathbb{R}^d$ with $\varLambda = \varGamma + F$.

The factor group $\mathbb{R}^d/\varGamma$ of a lattice $\varGamma \subseteq \mathbb{R}^d$ is compact. A set of representatives that is relatively compact and measurable is called a *fundamental domain* $\mathrm{FD}_{\varGamma}$ of $\varGamma$. If $\{b_1, \dots, b_d\}$ is a basis of $\varGamma$, a natural choice is

$$\mathrm{FD}_{\varGamma} \;=\; \left\{ \sum_{i=1}^{d} \alpha_i b_i \;\middle|\; 0 \le \alpha_i < 1 \text{ for all } i \right\}.$$

Its volume $\mathrm{vol}(\mathrm{FD}_{\varGamma}) = |\det(b_1, \dots, b_d)|$ does not depend on the choice of $\mathrm{FD}_{\varGamma}$.

1.4 Lattices

Lemma: Any lattice $\Gamma \subseteq \mathbb{R}^d$ is a Meyer set. Consequently, it is also a Delone set of finite local complexity.

Proof:

Γ lattice $\implies \Gamma - \Gamma = \Gamma \quad$ (Γ is a group)

It is sufficient to show that Γ is relatively dense and uniformly discrete

Choose $K \subseteq \mathbb{R}^d$ to be the closed parallelotope spanned by the d basis vectors

$\Gamma + K = \mathbb{R}^d \implies$ relative denseness

any open ball $\subseteq K \implies$ uniform discreteness ∎

1.4 Lattices

Let $\varLambda$ be a point set in $\mathbb{R}^d$. An element $t \in \mathbb{R}^d$ is a *period* of $\varLambda$ when $t + \varLambda = \varLambda$. The set $\mathrm{per}(\varLambda) := \{t \in \mathbb{R}^d \mid t + \varLambda = \varLambda\}$, called the *set of periods* of $\varLambda$, is a subgroup of $\mathbb{R}^d$.

A point set $\varLambda \subseteq \mathbb{R}^d$ is called *periodic* (of *rank* m) when $\mathrm{per}(\varLambda) \subseteq \mathbb{R}^d$ is non-trivial (with $1 \leq m = \dim\langle \mathrm{per}(\varLambda)\rangle_{\mathbb{R}} \leq d$), and *non-periodic* when $\mathrm{per}(\varLambda) = \{0\}$. The set $\varLambda$ is called *crystallographic* when $\mathrm{per}(\varLambda)$ is a lattice in $\mathbb{R}^d$, and *non-crystallographic* otherwise.

If $\varGamma$ is a lattice in $\mathbb{R}^d$, its *dual lattice* $\varGamma^*$ is defined as

$$\varGamma^* = \{y \in \mathbb{R}^d \mid \langle x|y\rangle \in \mathbb{Z} \text{ for all } x \in \varGamma\},$$

where $\langle x|y\rangle$ is the scalar product in $\mathbb{R}^d$. If $\{b_1, \dots, b_d\}$ is a lattice basis of $\varGamma$, the vectors b_i^* satisfying $\langle b_i^*|b_j\rangle = \delta_{i,j}$ for $1 \leq i, j \leq d$ form a lattice basis of $\varGamma^*$, called the *dual basis*.

1.4 Lattices

Proposition: A locally finite point set $\varLambda \subseteq \mathbb{R}^d$ is crystallographic if and only if there is a lattice $\varGamma \subseteq \mathbb{R}^d$ and a finite point set $F \subseteq \mathbb{R}^d$ such that $\varLambda = \varGamma + F$.

Proof:

If $\varLambda = \varGamma + F$, then $\varLambda$ is locally finite

Clearly, $\varGamma \subseteq \mathrm{per}(\varLambda)$ is a discrete subgroup of $\mathbb{R}^d$
$\implies \mathrm{per}(\varLambda)/\varGamma$ is a finite group

$\mathbb{R}^d/\mathrm{per}(\varLambda)$ compact $\implies \mathrm{per}(\varLambda)$ lattice $\implies \varLambda$ crystallographic

Conversely, assume that $\varLambda$ is crystallographic,
with lattice of periods $\varGamma := \mathrm{per}(\varLambda)$

Choose a fundamental domain K of $\varGamma$, so $\mathbb{R}^d = \bigcup_{t \in \varGamma} (t + K)$

Define $F := K \cap \varGamma$ finite $\implies \varLambda = \varGamma + F$ ∎

1.5 Crystallographic restriction

Lemma: Consider a lattice $\varGamma \subseteq \mathbb{R}^d$. If $R \in \mathrm{O}(d)$ satisfies $R\varGamma \subseteq \varGamma$, one has $R\varGamma = \varGamma$. The corresponding characteristic polynomial $P(\lambda) = \det(R - \lambda\mathbf{1})$ has integer coefficients only, so that $P(\lambda) \in \mathbb{Z}[\lambda]$.

Proof:

For any $S \subseteq \mathbb{R}^d$, define $S_r := S \cap \overline{B_r(0)}$

$R\varGamma \subseteq \varGamma \implies (R\varGamma)_r \subseteq \varGamma_r$ but $\mathrm{card}(R\varGamma)_r = \mathrm{card}\varGamma_r$

$\implies (R\varGamma)_r = \varGamma_r$ for all $r > 0 \implies R\varGamma = \varGamma$

Basis $\{b_1, \dots, b_d\}$ of $\varGamma = \mathbb{Z}b_1 + \dots + \mathbb{Z}b_d$

$R\varGamma = \varGamma \implies$ each b_i mapped onto linear combination of b_j

$Rb_i = \sum_{j=1}^{d} b_j a_{ji} \implies RB = BA \implies R = BAB^{-1}$ ($\det(B) \neq 0$)

$A \in \mathrm{GL}(d, \mathbb{Z})$, and R and A share characteristic polynomial

$\implies P(\lambda)$ has integer coefficients ■

1.5 Crystallographic restriction

Corollary: A lattice $\Gamma \subseteq \mathbb{R}^d$ with $d = 2$ or $d = 3$ can have n-fold rotational symmetry at most for $n \in \{1, 2, 3, 4, 6\}$.

Proof:

For $d = 2$, rotation matrix $R_\varphi = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}$

$$P(\lambda) = \lambda^2 - \operatorname{tr}(R_\varphi)\lambda + \det(R_\varphi)$$

$$\operatorname{tr}(R_\varphi) = 2\cos\varphi \in \mathbb{Z} \implies |\cos\varphi| \in \{0, \tfrac{1}{2}, 1\}$$

$$\implies \varphi \in \tfrac{\pi}{3}\mathbb{Z} \cup \tfrac{\pi}{2}\mathbb{Z} \implies n \in \{1, 2, 3, 4, 6\}$$

For $d = 3$, $R \in \mathrm{SO}(3)$ can be written (by Euler's theorem)

as $R = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Characteristic polynomial of R is $(1 - \lambda)P(\lambda)$

$\implies$ same restriction ■

1.6 Cyclotomic fields

Let $\xi_n \in \mathbb{C}$ be a primitive nth root of unity (with $n > 2$), so $\xi_n^m = 1$ precisely when $n|m$.

The *cyclotomic field* $\mathbb{Q}(\xi_n)$ is a field extension of $\mathbb{Q}$ of degree $\phi(n)$, where ϕ is Euler's totient function

$$\phi(n) := \mathrm{card}\{1 \leq k \leq n \mid \gcd(k, n) = 1\}.$$

$\mathbb{Z}[\xi_n]$ is the ring of integers $\mathbb{Q}(\xi_n)$, it is a $\mathbb{Z}$-module of rank $\phi(n)$.

$\mathbb{Z}[\xi_n]$ is a Principal Ideal Domain for several important values of n (including all $n < 23$), though this is not true in general.

The maximal real subfield of $\mathbb{Q}(\xi_n)$ is $\mathbb{Q}(\xi_n + \bar{\xi}_n)$, with relative degree 2 (for $n > 2$). Its ring of integers is $\mathbb{Z}[\xi_n + \bar{\xi}_n]$.

1.6 Cyclotomic fields

The polynomial $x^n - 1$ (with $n \geq 1$) has a unique factorisation (in $\mathbb{Q}[x]$) into integer polynomials that are irreducible over $\mathbb{Q}$,

$$x^n - 1 = \prod_{\ell | n} Q_\ell(x),$$

where $Q_\ell(x) \in \mathbb{Z}[x]$ has degree $\phi(\ell)$ and is called the ℓ-th *cyclotomic polynomial*. The polynomials are recursively defined this way, via the Euclidean algorithm. Explicitly, they are given by

$$Q_\ell(x) = \prod_{\xi} (x - \xi) = \prod_{k | \ell} (x^k - 1)^{\mu(\ell/k)},$$

where ξ runs over the $\phi(\ell)$ distinct primitive ℓ-th roots of unity, and μ denotes the Möbius function.

1.7 Algebraic numbers

A real algebraic integer $\alpha > 1$ is called a *Pisot–Vijayaraghavan number*, or *PV number* for short, if all its algebraic conjugates (apart from α itself) lie inside the open unit disk.

Example: The golden ratio $\tau = (1+\sqrt{5})/2 \approx 1.618$ is an algebraic unit of degree 2, as a root of $x^2 - x - 1 = 0$. Its algebraic conjugate is $\tau' = (1-\sqrt{5})/2 = 1 - \tau \approx -0.618$, so τ is a PV number.

A real algebraic integer $\alpha > 1$ is called a *Salem number*, if all its algebraic conjugates (apart from α itself) lie inside the closed unit disk, with at least one conjugate on the unit circle.

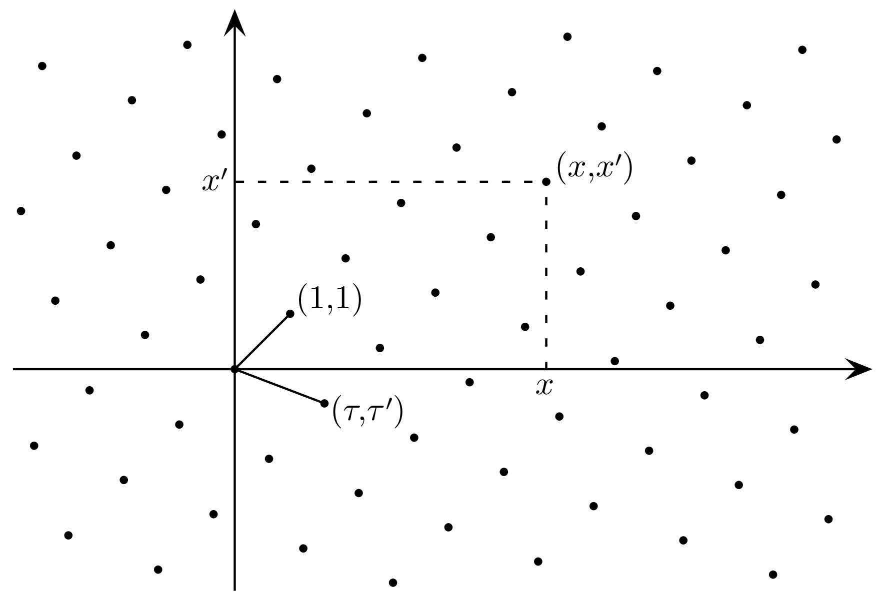
Theorem (Lagarias): If $\varLambda \subseteq \mathbb{R}^d$ is a Meyer set with $\alpha\varLambda \subseteq \varLambda$ for some $\alpha > 1$, then α is a PV or a Salem number.

1.8 Minkowski embedding

We consider the example of $\mathbb{Z}[\tau] = \{m + n\tau \mid m, n \in \mathbb{Z}\}$.

Algebraic conjugation $x \mapsto x'$ in $\mathbb{Q}(\sqrt{5}\,)$ is defined by $\sqrt{5} \mapsto -\sqrt{5}$ and its extension to a field automorphism.

The *diagonal embedding* $\mathcal{L} = \big\{(x, x') \mid x \in \mathbb{Z}[\tau]\big\}$ defines a lattice in $\mathbb{R}^2$, generated by the vectors $(1, 1)$ and (τ, τ').



The Minkowski embedding of real algebraic integers of rank m into $\mathbb{R}^m$ is defined analogously in terms of algebraic conjugates.

1.9 Lattice projections

Lemma: Let Γ be a lattice with a point symmetry group that contains an element of order p^r, with p a prime and $r \geq 1$. Then, the minimal dimension of Γ is $d = \phi(p^r) = p^{r-1} \cdot (p-1)$.

Theorem: Consider a locally finite planar point set with n-fold symmetry that is constructed from a lattice in $\mathbb{R}^d$ by a symmetry-preserving (partial) projection. Then, $d \geq \phi(n)$, with the lower bound being sharp.