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QUASICRYSTALS: STATE OF THE ART AND OUTLOOKS

Mathematical aspects of quasicrystals

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Abstract

A two-dimensional model of a quasi-crystal is the Penrose tiling (1974), which is an aperiodic "disjoint" covering of the plane generated by two rhombi R_{36° and R_{72° with equal side lengths. It is crucial that the areas' ratio is irrational

$$\varphi = \frac{\text{area}\, R_{72^\circ}}{\text{area}\, R_{36^\circ}} = \frac{1+\sqrt{5}}{2}\,(\text{golden ratio})\,(\varphi^2 - \varphi - 1 = 0),$$

which in turn reveals a local five-fold symmetry, forbidden for crystals. Recent advances on "Wang tiles", that is square tiles that cover the plane but cannot do it in a periodic fashion, are due to Jeandel and Rao (An aperiodic set of 11 Wang tiles, Advances in Combinatorics, pp 1–37, 2021), giving a definitive answer to the problem raised by Hao Wang in 1961. Other recent applications to variational problems in Homogenization are also mentioned (Braides et al. in C R Acad Sci Paris 347(11–12):697–700, 2009).

Keywords Penrose tilings · Quasi-periodic 2d lattices · Quasicrystals · Homogenization

1 Introduction

The mathematical theory of quasi-periodic crystals, after the discovery of natural quasicrystals (Bindi et al. 2009), has become an important area of investigation both in theoretical and experimental sciences (see Bindi 2008; Bindi and Stanley 2020; Bindi and Parisi 2023; van Smaalen 2023).

In this note, we present some basic mathematical ideas about tilings in the plane $\mathbb{R}^2$, starting with the concepts of regular and semi-regular, or periodic and aperiodic, tiles.

In Sect. 2, we describe Wang's conjecture and some recent advances (2021).

In Sect. 3, we examine Penrose tilings, which can be seen as two-dimensional models for quasicrystals. We shall provide details in the case where the prototiles, three rhombi $R_{\frac{\pi}{7}}, R_{\frac{2\pi}{7}}$ and $R_{\frac{3\pi}{7}}$, produce a seven-fold symmetry.

In Sect. 4, we recall the Fibonacci sequence and in Sect. 5, we mention recent works regarding calculus of variations (in particular, the homogenization of Penrose tilings).

2 Wang tiles

For $0 < \alpha < 90$, we denote by R_{α° the planar rhombus with an acute angle of α degrees. A *tiling* (or tessellation) is a covering of a portion $S \subseteq \mathbb{R}^2$ by non-overlapping polygonal (or more generally, compact) shapes called tiles, which may differ in shape, size and orientation. Each tile is the projection of a d-dimensional face of a D-dimensional hypercube ($d < D$) onto Euclidean d-space.

A tiling is *periodic* if it is invariant under two given linearly independent directions (in other words, shifting the pattern without rotating it produces the same tiling).

One long-standing problem has been that of constructing semi-regular tilings from regular ones. Starting from

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1960, the problem arose on whether there existed “tilesets” admitting *only* non-periodic tilings. Such sets are said to be *aperiodic*.

Remark It is not difficult to tesselate $\mathbb{R}^2$ non-periodically, using only one triangle with angles 75°–75°–30°.

In 1961, Wang conjectured that every tileset that realizes a tiling of $\mathbb{R}^2$ must also admit a periodic tiling of $\mathbb{R}^2$. In 1966, his student Berger disproved the conjecture, by finding a set of more than 20,000 square tiles that cover the plane but cannot do it in a periodic way. The prototiles he employed are Wang tiles, namely square tiles with coloured edges. Wang tiles are juxtaposed so that adjacent edges share the same colour. Wang was motivated by his interests in mathematical logic.

The number of tiles needed was drastically reduced in 1996, when an aperiodic tileset of only 13 Wang tiles was discovered. At the same time, it has been shown that it is impossible to obtain aperiodic Wang tilings consisting of 4 tiles or less (1987).

In a 2021 paper published in Advances in Combinatorics Jeandel and Rao (2021) settled the matter for good, they found an aperiodic Wang tiling made of 11 pieces and 4 colours, and showed there cannot exist aperiodic tilings with fewer than 11 Wang tiles.

3 Penrose tilings

The main discovery regarding aperiodic tilings is due to Penrose, who showed how to tessellate $\mathbb{R}^2$ in a non-periodic fashion using two rhombi (R_{36° and R_{72°). The Penrose tiling exhibits a five-fold symmetry, and can be seen as a two-dimensional model of a quasi-crystal.

Its prototiles are a “thin” rhombus R_{36° and a “fat” rhombus R_{72°, both with *unit* edges (Fig. 1).

Since the edge length is 1, we have:

$$\text{area } R_{36^\circ} = \sin 144^\circ = 2\sin 72^\circ \cos 72^\circ$$

and

$$\text{area } R_{72^\circ} = \sin 72^\circ = 2\sin 36^\circ \cos 36^\circ,$$

so that

$$\frac{\text{area } R_{72^\circ}}{\text{area} R_{36^\circ}} = \frac{1}{2\cos 72^\circ} = \varphi = \frac{1+\sqrt{5}}{2}$$

where φ is the golden ratio: an irrational solution to $x^2 - x - 1 = 0$. The solutions to $x^7 - 1 = 0$ are $1, e^{i\frac{2\pi}{7}}, e^{i\frac{4\pi}{7}}, e^{i\frac{6\pi}{7}}, e^{i\frac{8\pi}{7}}, e^{i\frac{10\pi}{7}}, e^{i\frac{12\pi}{7}}$ and their sum is zero:

$$\cos\frac{2\pi}{7} + \cos\frac{4\pi}{7} + \cos\frac{6\pi}{7} = -\frac{1}{2}.$$

Using elementary formulas, such as

$$\cos\alpha\cos\beta\cos\gamma = \frac{\cos(\alpha+\beta+\gamma)+\cos(-\alpha+\beta+\gamma)+\cos(\alpha-\beta+\gamma)+\cos(\alpha+\beta-\gamma)}{4}$$

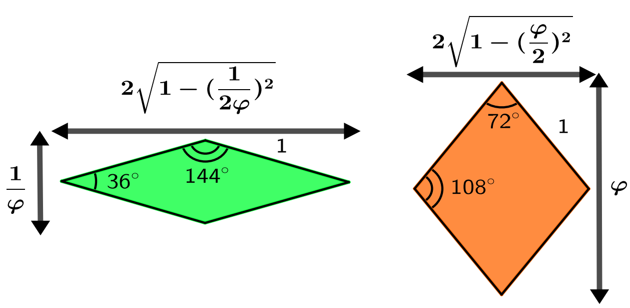

Fig. 1 Penrose prototiles ($\varphi = \frac{1+\sqrt{5}}{2}$)

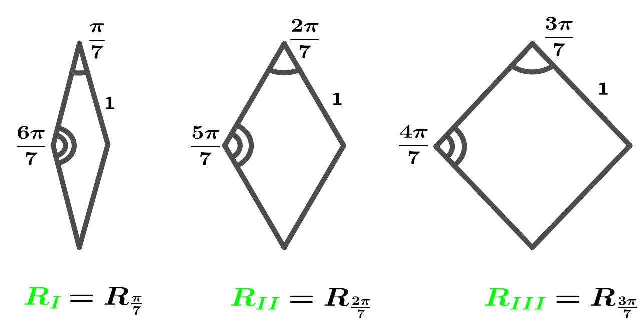

Fig. 2 Prototile rhombi of seven-fold tilings

we have

$$\cos\frac{2\pi}{7}\cos\frac{4\pi}{7}+\cos\frac{4\pi}{7}\cos\frac{6\pi}{7}+\cos\frac{6\pi}{7}\cos\frac{2\pi}{7}=-\frac{1}{2}$$

and

$$\cos\frac{2\pi}{7}\cos\frac{4\pi}{7}\cos\frac{6\pi}{7}=\frac{1}{8}.$$

In particular

$$\left(x-2\cos\frac{2\pi}{7}\right)\left(x-2\cos\frac{4\pi}{7}\right)\left(x-2\cos\frac{6\pi}{7}\right)$$
$$=x^3+x^2-2x-1.$$

A tiling with a seven-fold symmetry can be obtained using the three rhombi $R_{\frac{\pi}{7}}, R_{\frac{2\pi}{7}}, R_{\frac{3\pi}{7}}$ (Fig. 2).

A quasi-periodic 7-fold rhombic tiling, whose basic shapes are rhombi with acute angles of $\frac{\pi}{7}$, $\frac{2\pi}{7}$ and $\frac{3\pi}{7}$ radians, enjoys the property that (e.g. $R_{\frac{2\pi}{7}}$) the prototiles can be arranged to form a seven-pointed star, hence producing 7-fold rotational symmetry.

As in case of pentagonal symmetry, where the length of the long diagonal of $R_{\frac{2\pi}{5}}$ equals the golden ratio $\varphi=2\cos\frac{\pi}{5}$, here the length of the long diagonal of $R_{\frac{2\pi}{7}}$ equals $\phi=2\cos\frac{\pi}{7}$.

Similar to the five-fold case, the ratio of the areas of the 3 prototile rhombi (or their reciprocals) are the irrational solutions to the algebraic equation:

$$x^3+x^2-2x-1=0,$$

namely

$$\psi_1=2\cos\frac{\pi}{7}, \psi_2=2\cos\frac{4\pi}{7}, \psi_3=2\cos\frac{6\pi}{7}.$$

Actually

$$\frac{\text{area } R_{\frac{2\pi}{7}}}{\text{area } R_{\frac{\pi}{7}}}=-\psi_3, \frac{\text{area } R_{\frac{3\pi}{7}}}{\text{area } R_{\frac{2\pi}{7}}}=\psi_1, \frac{\text{area } R_{\frac{\pi}{7}}}{\text{area } R_{\frac{3\pi}{7}}}=-\psi_2.$$

Quasicrystals consist of long-range ordered, but aperiodic arrangements of atoms. They reveal periodicity only in high-dimensional hyperspaces, and no translational invariance.

Important for quasicrystals are the so-called *rational* approximant phases, which are periodic structures close to aperiodic quasicrystalline ones, and which can be described as projections of the quasicrystalline hyper-structure along *rational* directions in hyperspace with a *rational* slope approximating the golden ratio.

The method of hyperdimensional constructions and their projection to lower dimensions to obtain quasi-periodic structures are a powerful tool. By suitable rational approximation of irrational quantities, intrinsic in the projection matrices, periodic structures are related to "perfect" Penrose tilings modulo certain "defects". One such example are "phasons" which, when inserted regularly in Penrose lattices, change them into periodic approximants.

4 Fibonacci chain

This is a basic representation of an aperiodic system in $\mathbb{R}$. Let us recall the Fibonacci numbers $(F_k)_{k\in\mathbb{N}}$:

$1, 1, 2, 3, 5, 8, 13, 21, 34, 55, \dots,$

where each number is the sum of the two integers preceding it, according to the inductive definition

$$\begin{cases} F_1=F_2=1 \\ F_{k+2}=F_{k+1}+F_k. \end{cases}$$

It is well known that

$$\lim_{k\to\infty}\frac{F_{k+1}}{F_k}=\varphi=\frac{\sqrt{5}+1}{2}.$$

The Fibonacci tiling is obtained by projection from a 2D periodic structure, and represents an aperiodic covering of $\mathbb{R}$ generated by two segments L (long) and S (short), whose lengths have ratio $\frac{|L|}{|S|}=\varphi$. The segments are juxtaposed as follows: as the length of the chain tends to ∞, the ratio between the number of L edges and S edges contained in the chain tends to the golden ratio φ (Fig. 3).

The chain does not have a translational symmetry, but has a clear "local" order. For example, there are no consecutive short segments SS, and no triples LLL. The projection acts from a 2d periodic lattice onto a straight line with slope φ, a physical line.

To find a rational approximant, one defines an irrational "strip" which contains the lattice points that will be projected onto the physical line, thus filling the Fibonacci sequence.

In order to obtain a periodic 1d sequence that will approximate the Fibonacci chain, the irrational strip is replaced by a

$\#L/\#S$	chain
1	L
1	LS
2/1	LSL
3/2	LSLLS
5/3	LSLLSLSL
8/5	LSLLSLSLLSLLS
13/8	LSLLSLSLLSLLSLSLLSLSL

Fig. 3 Approximants of the Fibonacci chain

suitable rational one. This "cut-and-project" construction was introduced by Harald Bohr for almost periodic functions.

Bohr introduced the notion of a hyperspace and showed that quasi-periodic functions arise as restrictions of high-dimensional periodic functions to an irrational slice.

The difference between the Fibonacci algorithm and the approximant method becomes clearer once we look at their respective recursive formulas:

$$w_{n+2} = w_{n+1} + w_n$$

and

$$w_{n+2} = w_{n+1} + w.$$

5 Homogenization of Penrose tilings

The homogenization theory deals with the description of the macroscopic properties of media with fine microstructure and has important applications to the study of the properties of composite materials. Originally (∼ 1970) it was introduced in case of periodic structures, when the period is "small" with respect to the size of the region in which the system is to be studied.

The main problem consisting in going back from the microscopic quantities to the macroscopic ones, which are measurable.

The problem of homogenization of integral energies goes back to E. Sanchez Palencia, I. Babuska, E. De Giorgi-S. Spagnolo, F. Murat-L. Tartar, P. Marcellini for which we quote the reference books (Bensoussan et al. 1978) and Dal Maso (1993).

Functionals of the form ($\Omega \subset \mathbb{R}^2$)

$$F_\varepsilon(u) = \int_\Omega f\left(\frac{x}{\varepsilon}, Du(x)\right) \mathrm{d}x$$

for $u \in W^{1,2}(\Omega;\mathbb{R}^m)$, a Sobolev space of L^2 functions with gradient in L^2, are considered and some natural limit as $\varepsilon \to 0$ is described as

$$F_H(u) = \int_\Omega f_H(Du(x))\, \mathrm{d}x$$

with explicit expression for f_H due to periodicity.

In other words, we are performing the asymptotic analysis of fast-oscillating integral functionals depending on a small-scale parameter ε, as ε goes to zero.

Let us concentrate here to the special case $f(x,\xi) = \sum_{i,j=1}^2 a_{ij}(x)\xi_i\xi_j$

$$F_\varepsilon(u) = \int_\Omega \sum_{i,j} a_{ij}\left(\frac{x}{\varepsilon}\right) u_{x_i} u_{x_j}\, \mathrm{d}x$$

where $[a_{ij}(x)]$ is a bounded symmetric matrix, such that (for a $\lambda > 0$)

$$\lambda \mid \xi \mid^2 \leq \sum_{i,j} a_{ij}\xi_i\xi_j \quad \forall \xi \in \mathbb{R}^2$$

and we suppose $a_{ij}(x)$ is Y-periodic where $Y = \{x \equiv (x_i) \in \mathbb{R}^2 : 0 < x_i < \overline{y}_i\}$ and $\overline{y} = (\overline{y}_i)$, $\overline{y}_i > 0$ is fixed in $\mathbb{R}^2$ namely, $\forall x$

$$a_{ij}(x + \overline{y}) = a_{ij}(x) \quad \forall i, j$$

If $\Omega \subset \mathbb{R}^2$ is bounded, there exists, for any $\varphi \in L^2(\Omega)$ and $\varepsilon > 0$ a unique solution u_ε to the minimum problem

$$\int_\Omega \left\{ f\left(\frac{x}{\varepsilon}, Du_\varepsilon\right) - \varphi(x)u_\varepsilon \right\} \mathrm{d}x = \text{minimum}$$

such that $u_\varepsilon = 0$ are on the boundary $\partial\Omega$. (Dirichlet problem).

It can be proved that there exists a *constant* symmetric positive-definite matrix $[\alpha_{ij}]$ such that u_ε converges in L^2 as $\varepsilon \to 0$ to the solution u of the minimum problem

$$\int_\Omega \left\{ \sum_{i,j} \alpha_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} - \varphi(x)u \right\} \mathrm{d}x = \text{minimum}$$

and $u = 0$ on $\partial\Omega$.

The interesting fact is that the matrix α_{ij} is *different* from

$$\frac{1}{\mathrm{meas}(Y)} \int_Y a_{ij}(x)\, \mathrm{d}x.$$

Recently (Braides et al. 2009), a homogenization theorem was proved for energies which follow the geometry of an a-periodic Penrose tiling.

The authors consider mixtures of two linear conducting materials with different dieletric constants depending on the type of tiles. The coefficient $a = a(y)$ only takes two values $\alpha, \beta \in \mathbb{R}$ depending on the tile type y (see Braides et al. 2009). One can prove a homogenization-type theorem for energies that abide by the geometry of an aperiodic Penrose tiling. The result is obtained by showing that the already-existing general homogenization theorems can be applied. The method applies to general quasicrystalline geometries.

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Data availability Data are available.

Declarations

Conflict of interest The authors declare no conflict of interest.

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