Shapes of crystals

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On a game board, form a shape using A identical pieces. The *perimeter* is the number of outer edges, i.e. edges which are not shared by two pieces. The number A is the *area* of the shape.



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Aim of the game : find the shape which, for a given area, minimizes perimeter.

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Image: A matrix

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These are three *discrete* isoperimetric problems.

Here are a few solutions of isoperimetric games.



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Theorem

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R.J. Haüy (1784) proposed that matter should be formed of tiny polyhedra glued together. This was naive, but the idea of microscopic periodicity was a good one, and finally was confirmed experimentally in 1912.



Proposition

Crystallographic restriction. In 2 or 3 dimensions, if a periodic array of points is stabilized by a rotation or screw rotation, the rotation angle must be a multiple of $\pi/3$ or $\pi/2$.

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Proof (*Hauÿ*, 1822). In a basis of translation vectors stabilizing the array, the matrix of the rotation has integral entries. Its trace is an integer. Or, in an arbitrary basis, the trace of a rotation with angle θ equals $1 + 2\cos(\theta)$. Thus $\cos(\theta) = 1, \frac{1}{2}, 0, -\frac{1}{2}, -1, \theta = 0, \frac{\pi}{3}, \frac{\pi}{2}, \frac{2\pi}{3}, \pi$.

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During 200 years, crystallographers have taken this rule for granted. It has been confirmed by *diffraction patterns* (obtained using X-rays), which reflect the crystal's symmetry.



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A crystal is a solid whose diffraction pattern is made of distinct spots.

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Quasiperiodicity can produce crystals. A phenomenon in 3-space is *quasiperiodic* if it is the trace, on a 3-dimensional vector subspace, of a higher dimensional periodic phenomenon.

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The same process applied in dimension 6 generates non periodic tilings of 3-dimensional space, whose diffraction patterns are made of spots, and which admit screw rotations with angle $2\pi/5$. These are good candidates for models of *quasicrystals*.