SYMMETRIES OF QUASICRYSTALS

by

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Abstract

We consider tiling models of "round quasicrystals" which would have diffraction patterns which are fully rotation invariant – rings instead of Bragg peaks. They can be distinguished from glasses by self-similarity of the pattern of radii of the rings.

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Quasicrystals were discovered by Schectman et al[1] due to the unusual 10-fold rotational symmetry exhibited in certain directions by their (electron) diffraction patterns, a symmetry which is well known to be impossible for ordinary crystals. An early model to explain this symmetry was put forward by Levine and Steinhardt[2], based on an observation of Mackay[3] that a particle configuration associated with a (3-dimensional version of) a planar Penrose tiling (Fig. 1) would have diffraction patterns with just such a forbidden symmetry. (The *qualitative* features of the diffraction patterns are independent of precisely how scatterers would be associated with each type of tile, as long as no accidental symmetries are introduced by their placement.)

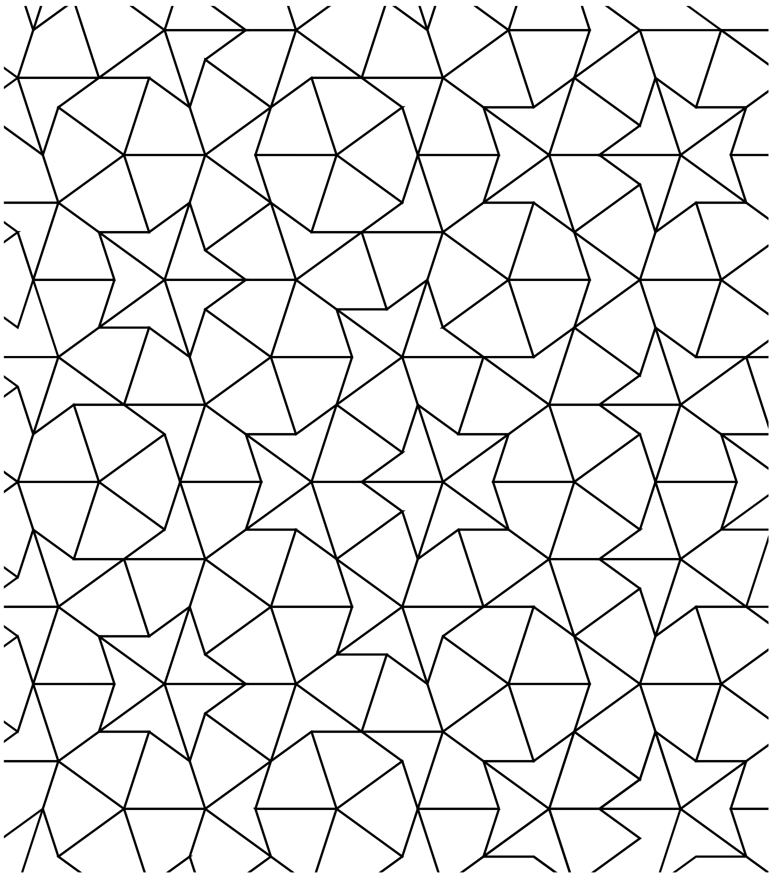
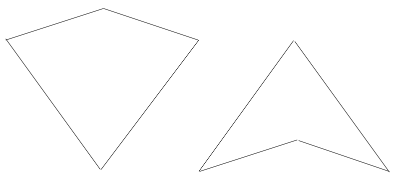


Figure 1. A Penrose tiling

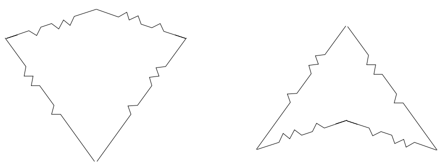
There was some confusion at first due to the "local 5-fold symmetry" of the Penrose tilings; the Penrose tilings have arbitrarily large regions with centers of 5-fold rotational symmetry. Any such symmetry in the real-space pattern of the scatterers will produce the same rotational symmetry in the diffraction pattern in certain directions. But it was eventually realized that the key feature of the Penrose tilings is their "statistical 10-fold symmetry" – the fact that every finite pattern of tiles in the tiling appears in 10 different rotational orientations with the same frequencies, the *equality* of the frequencies giving rise to the 10-fold rotational *symmetry* of the diffraction patterns[4,5]; diffraction is only sensitive to such frequencies, and the well known transference, of a real-space symmetry of the pattern of scatterers to a symmetry in the diffraction intensity, is only a special case of this.

The other crucial feature in this modelling was that the Penrose tilings, and its various "aperiodic" analogues in 2 and 3 dimensions, have "matching rules", which means that when the matching rules are used to make a tiling from the tiles, the only tilings *possible* are the desired ones. Matching rules govern how the boundaries of tiles may abut; Fig. 2 shows the two basic quadrilateral shapes (the "kite" and "dart") for Penrose tiles, and Fig. 3 shows how they can be modified by matching rules so as to restrict how edges of tiles may abut in a tiling. (If the Penrose matching rules are not enforced, the quadrilateral Penrose tiles could be used to make uninteresting tilings.) The restricted tilings made using matching rules can be thought of, at least heuristically, as energy ground states – abutting tiles having "low energy" when their boundaries match and having "high energy" otherwise; an allowed tiling (as opposed to a tiling made without respect to the matching rules) is clearly a lowest energy configuration.



kite dart

Figure 2. The kite and dart



kite dart

Figure 3. The modified kite and dart

Many generalizations of the Penrose tilings were produced over the years using a projection technique due to N.G. de Bruijn[6]. This technique proved able to produce tilings, some with matching rules, with other forbidden rotational symmetries[(7)].

A new phenomenon, not possible from tilings made by a projection technique, was exhibited by the planar "pinwheel" tilings[(8)], and the recently published[(9)] 3-dimensional "quaquaversal" tilings (Figs. 4,5), based on generalizing a different feature of the Penrose tilings – the fact that they have a *hierarchical structure*. Such tilings can be made using "inflation", that is, using rules for dividing tiles into smaller versions of themselves. Fig. 6 shows the inflation rule for pinwheel $(1, 2, \sqrt{5}$ right) triangles. A pinwheel tiling can be made by starting with a $1, 2, \sqrt{5}$ right triangle, dividing it, then expanding about some point by a linear factor of $\sqrt{5}$, as shown. Then apply the division rule to each of the 5 triangles thus produced and expand the result about some point, getting 25 triangles, etc. The Penrose tilings can also be obtained by an inflation rule instead of matching rules, but we will not show this because it is a bit more complicated[10].

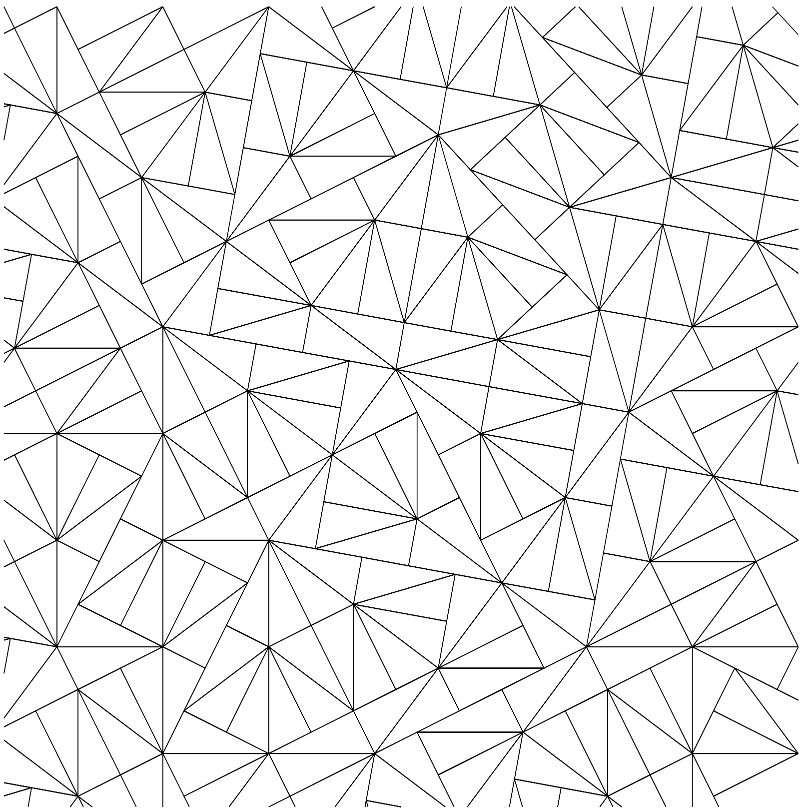


Figure 4. A pinwheel tiling

So the Penrose tilings can be thought of as produced in any of three essentially different ways – by enforcing matching rules, or by a projection technique, or by an

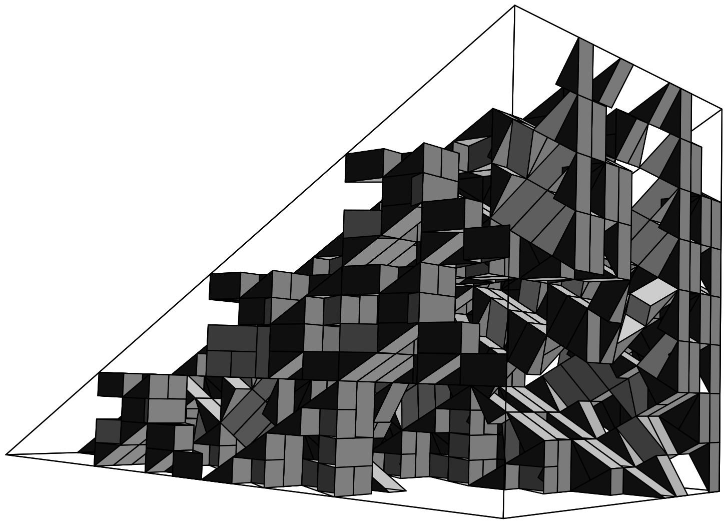


Figure 5. A quaquaversal tiling

inflation process. The pinwheel and quaquaversal tilings can be produced either by matching rules or an inflation process[8,11], but not by projection. (It is necessary that the tilings used to model materials be enforced by matching rules if one wants the structure to be thought of as an energy ground state.)

The new feature that the pinwheel and quaquaversal tilings have in common is that they give rise to diffraction patterns which are *fully rotation invariant*[12,9,5]; the diffraction consists of uniform rings rather than isolated Bragg peaks. (It is not known if the rings are sharp or diffuse.) In accordance with the above this just corresponds to the fact that any finite structure in such a tiling appears in that tiling with the same frequency (density) in all rotational orientations.

The value of this rotational symmetry of these tilings is that it points to a possibility not previously known. Given diffraction data from bulk material which is rotation invariant (made of rings), it has been natural to suppose the material *must be* either a conglomerate of randomly oriented microcrystals (like a powder) or a glass, i.e. a frozen liquid. These new models point to the *possibility* that the material could be a single quasicrystal – a fully deterministic structure.

We emphasize that although the above tiling models (pinwheel and quaquaversal) of what might be called "round quasicrystals" are to some extent closely related to the older models built on Penrose-like tilings, there are two points worth noting. First, it is not possible to make a model of a round quasicrystal using projection techniques, which have been much more widely used than inflation techniques. And second, the very possibility of round quasicrystals is not well known, so that diffraction data showing rings could easily be misinterpreted as indicating something other than a fully deterministic (quasicrystalline) structure.

A possible way to distinguish such a quasicrystal from a glass would be to examine the radial part of the diffraction data. We use the ergodic theory framework for diffraction[13,5] as it is particularly convenient for symmetries. In this way the frequencies associated as above with the structure of scatterers give rise to a probability distribution on a space X of such structures together with unitary representations, of any spatial transformations under which the frequencies are invariant, on the Hilbert space $\mathcal{H}$ of square integrable functions on X. Furthermore such symmetries lead to symmetries of the spectral projections of translations. Specifically, for the pinwheel we know that the frequencies are fully rotation invariant, and so the spectral projections E_s of translations are invariant in the sense that for any rotation R^Θ of Euclidean space we have $E_{R^\Theta s} = U^\Theta E_s U^{-\Theta}$, where U^Θ is the natural unitary representation on $\mathcal{H}$ of the rotation R^Θ. Diffraction intensities are given by formulas of the form $I(s)ds = d\!<\!f, E_s f\!>$ where $f \in \mathcal{H}$ incorporates the structure of the charge density of a single scatterer[13,5]. Therefore $I(R^\Theta s)ds = d\!<\!U^\Theta f, E_s U^\Theta f\!>$. If the charge density is rotation invariant then $U^\Theta f = f$ and the diffraction intensity is rotation invariant: $I(R^\Theta s)ds = I(s)ds$.

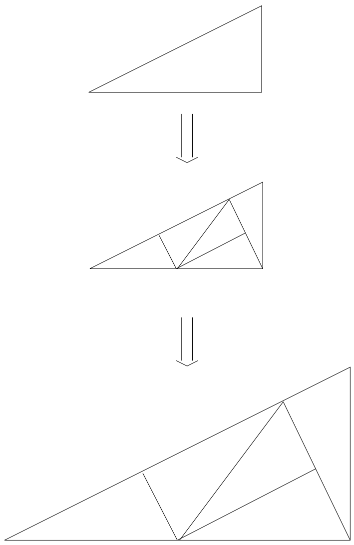


Figure 6. The pinwheel substitution

The pinwheel frequencies are also invariant under inflation (as is true for the frequencies of any tiling made by inflation), so the same argument now shows that $I(\kappa s)ds = d\!<\!U^\kappa f, E_s U^\kappa f\!>$ where κ is the similarity of Euclidean space used in the inflation and U^κ is the unitary representation of this transformation$^{(14)}$. (For the pinwheel, $\kappa s = \sqrt{5}s$.) But there is now a difference from rotations since the charge density cannot be invariant under the similarity transformation κ (or f be invariant under U^κ). So all we can hope to see as evidence of the inflation symmetry is a self-similarity of the radii of the rings in the diffraction pattern, not a self-similarity in the full diffraction intensity function. (In other words the support of the diffraction intensity is self-similar, not the actual values of the intensity.)

In summary, quasicrystals with a hierarchical structure exhibit a self-similarity in the (support of the) radial part of their diffraction, and this could be used to distinguish "round quasicrystals" from glasses. Distinguishing them from conglomerates of randomly oriented microcrystals is presumably easier.

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