Deformed Model Sets & Distorted Penrose Tilings

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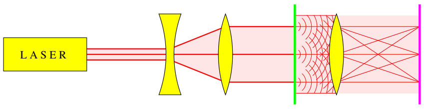
Abstract

On this poster, we show how the mathematical concept of a deformed model set can be used to gain insight into the diffraction pattern of quasicrystalline structures. We explain what a deformed model set is, what its characteristic features are and how it relates to certain disorder phenomena in solids. We then apply this concept to distorted Penrose tilings, *i.e.*, Penrose tilings where we apply size-effect-like distortions. While the size effect in crystals only operates on the diffuse scattering, there is also an intensity transfer on the Bragg peaks in distorted Penrose tilings. The persistence of pure point diffraction in distorted Penrose tilings can be explained by interpreting such tilings as deformed model sets.

1 Crystallography

Crystallography is the (experimental) science of determining the arrangement of atoms in a solid, usually through the analysis of the diffraction pattern of the solid in question. For this, the solid/sample is targeted by a beam of some type, either X-rays, neutrons or electrons.



Macroscopic properties – especially mechanical, thermal and electrical properties – are not only determined by the "ideal ordering" of the atoms in a solid, but often depend highly on disorder phenomena, defects *etc.*, as is well-known for semiconductors.

2 Disorder

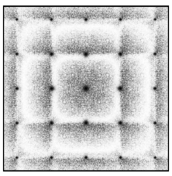
The (possible) "ideal" positions of the atoms of a solid form a point set. There are two basic scenarios of disorder for such a (general) point set:

- The (possibly different) atoms are distributed at random on the point set in question. This is a model for a random solid solution/an alloy. The diffraction spectrum consists (almost surely) of two terms: the first one describes the diffraction spectrum of a system where the scattering amplitudes have been replaced by their mean (which for lattices and model sets is pure point diffractive), while the second term is a homogeneous diffuse background which is proportional to the mean square difference of the scattering amplitudes.
- The atoms are displaced randomly from their ideal positions. This is, *e.g.*, used to describe the effect of thermal motion in a solid ("Debye-Waller effect"). The diffraction spectrum consists (almost surely) of two terms: firstly, the diffraction pattern of the original structure is reduced by an envelope function, which is 1 at the origin and tends to 0 at high angles. Secondly, an absolutely continuous spectral component is added such that one gets "lots" of diffuse scattering in regions where the intensities of the Bragg peaks are reduced "a lot" due to thermal motion.

3 Size Effect in Crystals

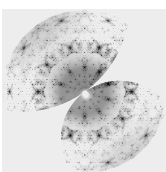
One may also consider the following two cases of disorder, which yield modulations in the diffuse scattering while the Bragg peaks are unchanged in the lattice case:

- The distribution of the atoms (on the ideal lattice positions) is determined by the neighbourhoods. One obtains a periodic modulation of the diffuse scattering which is symmetric around Bragg peaks.
- The atoms are displaced according to their neighbourhood, *i.e.*, relaxations take place locally such that neighbouring atoms tend to move apart if they are both "large", or closer together if they are both "small". For crystals, this *size effect* (re-)distributes the diffuse intensity such that there is more intenisty on one side (either the small or the large angle side) of each Bragg peak and less on the other.



4 Diffraction Pattern of $Al_{71}Co_{13}Ni_{16}$

M.A. Estermann, K. Lemster, T. Haibach and W. Steurer (2000) measured the diffraction pattern of a decagonal quasicrystal.



Not only does the diffuse scattering show the asymmetry known from the size effect, but also the intensities of Bragg peaks themselves show modulations. How can one explain this behaviour?

5 Quasicrystals and Model Sets

Model sets (also called *cut and project sets*) are a possible mathematical description of quasicrystals.

Model sets are defined within a *cut and project scheme* $(\mathbb{R}^d, H, \tilde{L})$: The *physical* (or *direct space*) is given by $\mathbb{R}^d$, the d-dimensional Euclidean space. We denote the *internal space* by H, which is often also given by a Euclidean space $H = \mathbb{R}^m$ (for some m). In the product space $\mathbb{R}^d \times H$, a lattice $\tilde{L}$ is given such that

- the canonical projection $\pi : \mathbb{R}^d \times H \to \mathbb{R}^d$ is one-to-one (wherefore $\pi : \tilde{L} \to L = \pi(\tilde{L})$ is a bijection).
- the canonical projection $\pi_{\text{int}} : \mathbb{R}^d \times H \to H$ into the internal space has dense image ($L^\star = \pi_{\text{int}}(\tilde{L})$ is dense in H).

This situation is schematically summarised as follows:

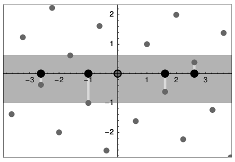
$$\begin{array}{ccccc} \mathbb{R}^d & \xleftarrow{\pi} & \mathbb{R}^d \times H & \xrightarrow{\pi_{\text{int}}} & H \\ \cup & & \cup & & \cup\ \text{dense} \\ L & \xleftrightarrow{1-1} & \tilde{L} & \longrightarrow & L^\star \end{array}$$

Note that we can define the so-called *star map* $^\star : L \to H,\ x \mapsto x^\star = \pi_{\text{int}}(\pi^{-1}(x))$.

Given a cut-and-project scheme $(\mathbb{R}^d, H, \tilde{L})$ and a non-empty compact set $W \subset H$ in the internal space with $\text{cl}(\text{int}\, W) = W$ (the set W is called a *window*), we define the set

$$\Lambda(W) = \{x \in L \mid x^\star \in W\}.$$

Then, a translate (in the direct space) of $\Lambda(W)$ is called a *model set*; if, in addition, the Haar measure of the boundary ∂W is zero, we deal with a *regular model set*.



Fundamental in the theory of model sets is the following theorem.

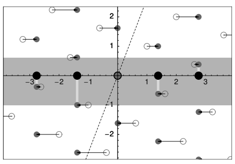
Theorem. *Regular model sets are pure point diffractive, i.e., their diffraction pattern consists of Bragg peaks only.* □

6 Deformed Model Sets

Let $\theta : H \to \mathbb{R}^d$ be a continuous map and $\Lambda(W)$ a regular model set. Then we can define the set

$$\Lambda_\theta(W) = \{x + \theta(x^\star) \mid x^\star \in W\}.$$

We call $\Lambda_\theta(W)$ a *deformed model set* if it is still a Delone set.



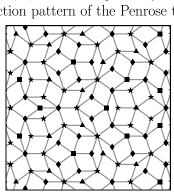
One obtains the following theorem.

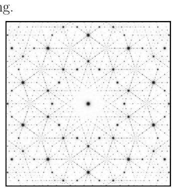
Theorem. *Deformed model sets are pure point diffractive, i.e., their diffraction pattern consists of Bragg peaks only.* □

7 Penrose Tiling

The rhombic Penrose tiling can be defined within the following cut and project scheme: The direct space is $\mathbb{R}^2$, the internal space is $\mathbb{R}^2 \times \mathsf{C}_5$ and $L = \mathbb{Z}[\xi_5]$ (the 5th cyclotomic integers). The star map consists of the Galois automorphism of $\mathbb{Z}[\xi_5]$ sending ξ_5 to ξ_5^2 and a homomorphism $\varrho : \mathbb{Z}[\xi_5] \to \mathsf{C}_5$ defined by $\varrho(h+j\cdot\xi+k\cdot\xi^2+\ell\cdot\xi^3) = (h+j+k+\ell) \bmod 5$.

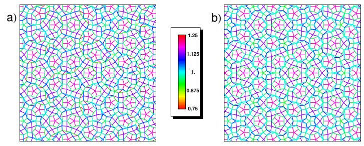
The window consists of two types of connected window-components: a small and a big pentagon. The small pentagons yield the "square" respectively "triangle" vertices in the following figure, while the big pentagons yield the "diamond" and "star" vertices. They correspond to positions $x \equiv 1, 4, 2, 3 \bmod 5$ respectively. On the right, we show the (pure point) diffraction pattern of the Penrose tiling.





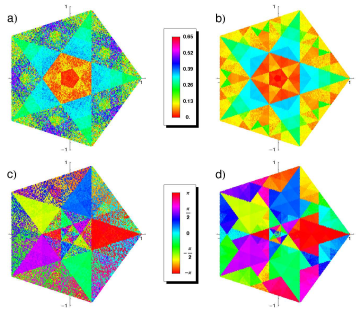
8 Distorted Penrose Tiling

We have carried out a Monte Carlo simulation, where a Hooke's law spring is assumed to act along each rhombus edge. The equilibrium length of the springs is given by 1.15 for "square-diamond" respectively "triangle-star" edges, while it is 0.85 for "diamond-star" edges. The outcome of this MC simulation is depicted on the left in the following figure, while on the right we have averaged over 500 outcomes of the MC simulation.

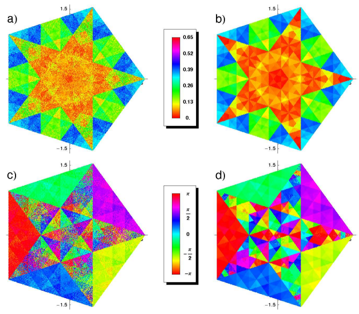


9 Results

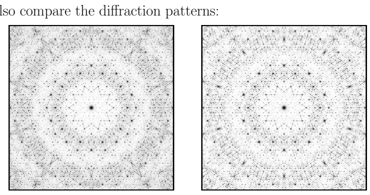
To judge if the distortion can be described as deformed model set, we plot the displacement in the distorted Penrose tiling as function of the internal coordinate. Moreover, we look at the absolute value and the direction of the displacement seperately. The outcome after the averging procedure is shown on the right hand side. We first look at the small pentagons:



For the big pentagons, the situation is the following:



We also compare the diffraction patterns:



Our findings can be summarised as follows:

- Especially the averaged distorted Penrose tiling is rather well described as a deformed model set.
- The diffraction patterns show size-effect-like features, also for the Bragg peaks.
- The description as deformed model set explicitly explains the intensity transfer on the Bragg peaks.

We hope that this work helps the reader to gain some insight and is of general use in the structure determination of quasicrystals.

References

- B. Sing and T.R. Welberry, *Deformed model sets and distorted Penrose tilings*, Z. Kristallogr. **221** (2006) 621–634; mp_arc/06-199.
- T.R. Welberry and B. Sing, *Deformed Penrose tilings*, Philosophical Magazine, accepted for publication.
- Also see references therein.