

## Session VIII - Thursday, September 3 - morning

## PL7

#### VISIBLE LATTICE POINTS AND WEAK MODEL SETS

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Recently, the dynamical and spectral properties of square-free integers, visible lattice points and various generalisations have received increased attention; see [1,3] and references therein. One reason is the connection with Sarnak's conjecture on the `randomness' of the Möbius function, another the explicit computability of correlation functions as well as eigenfunctions for these systems. Here, we use the set V of points (x,y) of the square lattice  $Z^2$  that are visible from the origin as a paradigm. Clearly, these are just the pairs with coprime corrdinates; see Fig. 1 for an illustration.

By the Chinese Remainder Theorem, V has holes of arbitrary size and it is classic that the natural density exists and is equal to  $6/^{-2}$ . It turns out that V has positive topological entropy equal to its density [4] and one thus might expect to leave the realm of pure point spectrum. However, V has pure point dynamical and diffraction spectrum [1,4]; see Fig. 1 and note that the disk areas represent the intensities. In fact, it is a major step to characterise the hull, i.e. the lattice translation orbit closure of V in the local topology. One can further show that the patch frequencies exist and this gives rise to a translation-invariant Borel probability

measure on the hull. Our main result is that the corresponding measure theoretic dynamical system is isomorphic to a Kronecker system. Moreover, both the dynamical and the diffraction spectra are given by the points of  $Q^2$  with square-free denominator. It turns out that all the examples mentioned above are weak model sets (the corresponding windows may have empty interior and a boundary of positive Haar measure) and it is thus natural to have a look at this abstract class of cut-and-project sets.

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Figure 1. Central patch of V (left) and the diffraction of V restricted to the square  $[0,2]^2$  (right).

Krystalografická společnost

#### S8-L1

#### A DECORATED SILVER MEAN TILING WITH MIXED SPECTRUM

#### Franz Gähler

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There are many inflation tilings with a pure-point and a continuous part in their dynamical or diffraction spectrum, also higher-dimensional ones [1,2]. Most are generated by a constant length inflation, and are thus lattice based. Here, we describe a procedure to construct a mixed-spectrum, almost 2-1 extension of any pure-point inflation tiling, and illustrate it with the well-known silver mean tiling, constructing thus a mixed-spectrum tiling based on a quasiperiodic tiling.

The starting point is the observation that many of the mixed-spectrum examples have a symmetry in their inflation rules [3]. All tiles come in geometrically equal pairs, and tiles within a pair are distinguished by the presence or absence of a bar. Swapping the bar status of all tiles is a symmetry, which commutes with the inflation. Wiping out all bars defines a factor map which is 2-1 almost everywhere. Provided the maximal equicontinuous factors (MEF) of both the barred and the unbarred tiling are the same, the factor map from the barred tiling to its MEF is then 2-1 almost everywhere, which implies that its spectrum is mixed [4].

This picture suggests how to construct mixed-spectrum inflation tilings in a systematic way. Starting with our favourite pure-point inflation tiling, we split each tile type into a pair, one with and one without a bar, and assign the bars in the inflation rule such that i) the bar swap symmetry is observed, ii) the resulting inflation is primitive, and iii) the barred and the unbarred tiling have the same MEF. As there are many ways to assign the bars, often there are such solutions.

We illustrate the procedure with the silver mean tiling, for which we introduce a suitably twisted version with bar swap symmetry. By general arguments, it is in fact true that the spectrum carried by the kernel of an almost 2-1 map to a pure-point factor must be pure. The factor map from the barred to the unbarred tiling is such a map, wherefore the spectrum in the odd sector with respect to the bar swap must be pure, either absolutely continuous or singular continuous. To discriminate between the two, we compute the autocorrelation of the twisted silver mean tiling with a decoration which is odd under the bar swap. This autocorrelation does not tend to zero for a series of distances tending to infinity, which by the Riemann— Lebesgue lemma implies that its Fourier transform, the diffraction spectrum, must have a singular component. As the diffraction spectrum is contained in the dynamical spectrum, the latter thus has a singular continuous component in the odd sector, so that it must be purely singular continuous there.

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S8-L2

## MULTIDIMENSIONAL PERIOD DOUBLING STRUCTURES

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**Figure 1**. 3D period doubling structure: isometric projection of generation 4 displaying three-fold and mirror symmetry.

We briefly review the connection of the period doubling sequence to the period doubling route to chaos [1, 2]. We develop the formalism necessary to generalize the period doubling sequence to arbitrary dimension by straightforward extension of the substitution and recursion rules [3, 4]. We discuss the symmetries of the structures (see e.g. Fig. 1). We show that the period doubling structures of arbitrary dimension are pure point (i.e. Bragg) diffractive [5, 6].

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S8-L3

### A SUBSTITUTION TILING WITH DENSE TILE ORIENTATIONS AND 7-FOLD ROTATIONAL SYMMETRY

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Planar tilings have been a focus of study not only for their interesting algebraic and geometric properties, but also because these serve as models for aperiodic crystal structures. In this talk, a construction of a vertex-to-vertex planar

tiling with 7 - fold rotational symmetry via substitution will

be presented. Substitution is defined on a prototile set con-

sisting of a regular heptagon and triangles. For the tiling to be vertex-to-vertex, rules are imposed by placing arrows on the sides of each prototile. It will be shown that the 7-fold tiling has dense tile orientations. Moreover, properties pertaining to areas of the prototiles will be discussed.

#### S8-L4

## PUSHING THE BOUNDARIES OF CRYSTALLOGRAPHY: DEBYE-WALLER FACTOR REDEFINED

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The main purpose of crystallography is to solve and refine crystal structures based on measured diffraction data. Complex crystal structures require big datasets consisting also of weak peaks. By using powerful synchrotron facilities and modern detectors it is possible to collect diffraction patterns with a very high dynamic range. It is, however, a big challenge to properly process the measured data. One of many corrections applied during structure refinement process is the Debye-Waller (D-W) factor correction. It compensates for the perturbations arising from thermal vibrations (phononic term) or flips (phasonic term) of atoms. The D-W factor can be also generalized to a statistical interpretation [1, 2]. The general formula for D-W factor is  $\exp[-k^2 ]^2$ , where k is the scattering vector and is a variance of the distribution of atomic arrangement (both is physical or perpendicular space).

In our presentation we discuss the limitations of the D-W factor in terms of structure refinement and propose a way to improve the results of such analysis. We prove that the D-W factor substantially limits the range of diffraction data possible to use in a refinement process. It works correctly only for small values of the exponential in the abovementioned formula. For real crystals (including quasicrystals), satisfactorily good results are only obtained for strong reflections with intensities higher than 1% in rel-

ative scale. Peaks with intensities  $10^{-4}$ - $10^{-3}$  are refined rather incidentally (see *e.g.*[3]). This means that including weak reflections in a refinement procedure frequently makes the refinement results worse.

We show how to improve the use of D-W factor. Our calculations are performed for a simple 1D model quasicrystal – the Fibonacci chain. Both the model choice and its low dimensionality do not affect our concluding remarks. For the Fibonacci chain we modelled the fluctuations in physical as well as perpendicular space. We claim, that redefinition of the D-W factor by either including higher-order moments of the statistical distribution or replacing the Gauss function with more appropriate functions essentially allows also weak peaks to be included in the refinement. Our results are general and can be applied for structural investigations of perfect crystals, including quasicrystals, but also any systems with defects or highly disordered.

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