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**Superquasicrystals with 8-, 10- and 12-fold point symmetries**

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We present several limit-quasiperiodic structures with 8-, 10- and 12-fold point symmetries. These structures are generated with inflation procedures as in the case of the Penrose patterns. Yet they are the first structures ever known with limit-quasiperiodic order and non-crystallographic point symmetries, and we categorize them as superquasicrystals [K. Niizeki and N. Fujita, J. Phys. A: Math. Gen. 38 L199 (2005)]. Their internal space structures are not as simple as quasicrystals, because the atomic-surfaces depend on the lattice points of the relevant hyperlattices. We numerically investigate such atomic-surfaces by mapping the real-space structure into the internal space. The structure factors are also calculated, in which successive generations of super-quasilattice reflections are clearly observed.

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Keywords: limit-quasiperiodic; non-crystallographic point symmetry; inflation rule; self-similarity

## 1. Introduction

In modeling two-dimensional (2D) quasicrystals (QC's), it is very common to use the Penrose patterns as well as their associates. These geometrical models normally have quasiperiodic structures with non-crystallographic point groups (NCPG's), among which  $D_8$ ,  $D_{10}$  and  $D_{12}$  are especially important regarding real world QC's. In the common scheme of constructing

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such a structure, one considers a 4D periodic structure (called hypercrystal) and takes its section along a 2D subspace  $E_2$ . The hypercrystal is a periodic arrangement of atomic-surfaces (AS's) on the relevant 4D hyperlattice, which is determined by the NCPG. It is also important that a QC have self-similarities closely connected to the NCPG.[1, 2] The similarity ratios are given by quadratic irrationals such as  $\tau = 1 + \sqrt{2}$ ,  $(1 + \sqrt{5})/2$  and  $2 + \sqrt{3}$  associated with the groups  $D_8$ ,  $D_{10}$  and  $D_{12}$ , respectively. This property provides an alternative way of constructing QC's by inflation rules.

Recently, the above setup has been extended to limit-quasiperiodic structures with NCPG's.[3] Although such structures resemble the quasiperiodic counterparts in many ways, they exhibit markedly different characteristics. We call such structures *superquasicrystals* (SQC's) because of their inherent hierarchical superstructures.[3] So far only few concrete examples have been known for this type of structures. Hence, it is our purpose to present here several new SQC's with the NCPG's  $D_8$ ,  $D_{10}$  and  $D_{12}$ . The theoretical framework of Ref.[3] is used to describe the structures and to compute their properties (e.g. structure factors) numerically. The inflation rules for generating these SQC's have been obtained by trial and error, while general guidelines for constructing similar structures await further investigations.[4]

## 2. Structures in real space

FIG.1 presents three SQC's with the point groups  $D_8$ ,  $D_{10}$  and  $D_{12}$  shown as planar aperiodic tilings involving finite kinds of polygonal tiles. These SQC's, denoted as  $T_8$ ,  $T_{10}$  and  $T_{12}$ , are generated by repeating the inflation rules indicated by thicker lines in the figure, hence they are self-similar. They are reported here for the first time except for  $T_8$ , which has been reported in Ref.[3]. Each structure consists of a discrete set of points located at the vertices as well as at the centers of every regular decagon or dodecagon for  $T_{10}$  or  $T_{12}$ , respectively. No lattice point is assumed at the center of an octagon for  $T_8$ . It is remarkable that every tile is symmetrically decorated in the inflation procedure of each SQC as shown in FIG.1. No inflation rule with this property is known for the case of QC's.

In a QC or SQC tiling with the NCPG  $D_p$  ( $p = 8, 10$  or  $12$ ), the edges of the tiles are given by normalized vectors,  $\mathbf{e}_j = (\cos(j\theta_p), \sin(j\theta_p))$  with  $j = 0, \dots, p-1$  and  $\theta_p = 2\pi/p$ ; these vectors represent the vertices of a  $p$ -gon centered on the origin. It is important to note that only four of them are linearly independent with respect to integer coefficients, and in

the following we shall take the first four members as the basis set. The lattice points of the structure are given as a discrete subset,  $\Sigma_0$ , of the module  $\Lambda := \{n_0\mathbf{e}_0 + n_1\mathbf{e}_1 + n_2\mathbf{e}_2 + n_3\mathbf{e}_3 \mid n_j \in \mathbf{Z}\}$ ; thus each point in  $\Lambda$  is specified by the four indices  $n_j$ . It is known that the module  $\Lambda$  is  $\tau$ -scale invariant (i.e.  $\tau\Lambda = \Lambda$ ) where  $\tau$  is the quadratic irrational associated with the NCPG. This property of  $\Lambda$  is of primary importance because it is essentially the origin of the self-similarity of QC's.[1, 2, 5]

The module  $\Lambda$  can be described as a projection of the relevant 4D hyperlattice,  $\hat{\Lambda}$ , onto the 2D subspace  $E_2$ . For each of the three NCPG's, only the primitive hyperlattice is relevant. These hyperlattices together with their generators are

$$\text{the octagonal lattice } (D_8) : (\mathbf{e}_j, (-)^j \mathbf{e}_j),$$

$$\text{the decagonal lattice } (D_{10}) : (\mathbf{e}_{2j}, \mathbf{e}_{4j}),$$

$$\text{the dodecagonal lattice } (D_{12}) : (\mathbf{e}_j, (-)^j \mathbf{e}_j),$$

respectively, where  $j = 0, 1, 2$  and  $3$ .[1, 6]

An inflation rule specifies a subset  $\Sigma_1$  of  $\Sigma_0$  such that it is geometrically similar to  $\Sigma_0$ ;  $\Sigma_1$  is represented as  $\Sigma_1 = \sigma(\Sigma_0)$  with  $\sigma$  being a similarity transformation associated with the inflation rule. Then  $\Sigma_1$  is a discrete subset of the module  $\Lambda_1 := \sigma(\Lambda)$ , which is generally a similar submodule of  $\Lambda$ .  $\sigma$  can have either of the forms:  $\nu$  (type I) and  $\nu\sigma_p$  (type II), where  $\nu (\in \mathbf{Z}[\tau] := \{m + n\tau \mid m, n \in \mathbf{Z}\})$  is just a scaling factor and  $\sigma_p$  is the basic similarity transformation specified by the condition,  $\sigma_p(\mathbf{e}_j) := \mathbf{e}_j + \mathbf{e}_{j+1}$ .[3] In our specific examples, the generators,  $\sigma(\mathbf{e}_j)$ , of  $\Lambda_1$  can be inferred from the edge vectors of the inflated tiling, and this infers the explicit forms of  $\sigma$  for the three SQC's to be  $\sigma_8$ ,  $(1 + \tau)\sigma_{10}$  and  $(1 + \sqrt{3})\sigma_{12}$  for  $p = 8, 10$  and  $12$ , respectively. Since  $\sigma(\mathbf{e}_j)$ 's belong to  $\Lambda$ , they are indexed with the bases  $\mathbf{e}_j$  of  $\Lambda$ , i.e.  $\sigma(\mathbf{e}_j) = m_{ij}\mathbf{e}_i$ . This defines the  $4 \times 4$  transformation matrix  $M = (m_{ij})$ , which are

$$M_8 = ((1, 1, 0, 0)^t, (0, 1, 1, 0)^t, (0, 0, 1, 1)^t, (-1, 0, 0, 1)^t),$$

$$M_{10} = ((3, 1, 2, -1)^t, (1, 2, 2, 1)^t, (-1, 2, 1, 3)^t, (-3, 2, -1, 4)^t) \text{ and}$$

$$M_{12} = ((2, 3, 1, -1)^t, (1, 2, 2, 1)^t, (-1, 1, 3, 2)^t, (-2, -1, 3, 3)^t),$$

for the present SQC's,  $T_8$ ,  $T_{10}$  and  $T_{12}$ , respectively.

In the 4D language,  $\sigma$  is lifted to a 4D bi-similarity transformation  $\hat{\sigma} = \sigma \oplus \sigma^\perp$  where  $\sigma^\perp$  is the conjugate transformation in the internal space.[3] The submodule  $\Lambda_1$  is then

lifted to  $\hat{\Lambda}_1 = \hat{\sigma}\hat{\Lambda}$ , which is generally a sublattice (or superlattice) of  $\hat{\Lambda}$ . The index  $k := [\hat{\Lambda} : \hat{\Lambda}_1] \equiv |\det M|$  gives the number of sublattices, being congruent to  $\hat{\Lambda}_1$ , into which  $\hat{\Lambda}$  is divided.[2, 3] By inspecting the transformation matrix  $M_8$ , one may find that the sublattice  $\hat{\Lambda}_1$  of  $\hat{\Lambda}$  for  $T_8$  is formed by the lattice vectors whose indices satisfy  $n_0 + n_1 + n_2 + n_3 \equiv 0 \pmod{2}$ , and that  $\hat{\Lambda}$  is divided into two (i.e.  $k = 2$ ) sublattices which are indicated by the values of  $n_0 + n_1 + n_2 + n_3 \pmod{2}$ . Similarly, for  $T_{10}$ ,  $\hat{\Lambda}$  is divided into five (i.e.  $k = 5$ ) sublattices indicated by the values of  $n_0 - n_1 + n_2 - n_3 \pmod{5}$ , which is zero for  $\hat{\Lambda}_1$ . Finally, for  $T_{12}$ , it turns out that there are four (i.e.  $k = 4$ ) relevant sublattices,  $\hat{\Lambda}_{00}$ ,  $\hat{\Lambda}_{10}$ ,  $\hat{\Lambda}_{01}$  and  $\hat{\Lambda}_{11}$ , where  $\hat{\Lambda}_{pq}$  is specified by the values of  $p := n_1 + n_2 \pmod{2}$  and  $q := n_0 + n_2 + n_3 \pmod{2}$ .[2] The sublattice  $\hat{\Lambda}_1$  is identified as  $\hat{\Lambda}_{00}$ . We notice that  $k = (|\sigma||\sigma^\perp|)^2$  where  $|\sigma|$  (resp.  $|\sigma^\perp|$ ) stands for the scale factor of the similarity transformation  $\sigma$  (resp.  $\sigma^\perp$ ).

An important property of the similarity transformation  $\sigma$  is its Pisot property represented as  $|\sigma^\perp| < 1$ . This is a sufficient condition for the inflation rule to produce a structure which is point diffractive.[3] Then, the criterion for distinguishing a QC and an SQC arises as follows. On the one hand, a QC is obtained iff  $k = 1$  and hence  $\hat{\Lambda}_1 = \hat{\Lambda}$ . On the other hand, an SQC is obtained iff  $k > 1$  and hence  $\hat{\Lambda}_1$  is a proper sublattice of  $\hat{\Lambda}$ . This implies that the self-similarity of an SQC corresponds to taking successive generation of proper sublattices,  $\hat{\Lambda}_n := \hat{\sigma}^n \hat{\Lambda}$  ( $n = 1, 2, \dots$ ). It follows that  $\hat{\Lambda}$  is divided with respect to  $\hat{\Lambda}_n$  into  $k^n$  residue classes  $R_n := \hat{\Lambda}/\hat{\Lambda}_n$ , and we may assign to each lattice point of  $\hat{\Lambda}$  an infinite series of residue classes to which it belongs at successive generations. The latter series can be seen as a “decimal fraction” associated with each lattice point. Note that we have just introduced into  $\hat{\Lambda}$  a hierarchical superlattice structure for the SQC. Such a structure is named in Ref.[3] a *super-Bravais-lattice*, which is mathematically an inverse system.[7]

AS's are no longer uniform for an SQC because of the hierarchical structure in  $\hat{\Lambda}$ . For every lattice point, an AS is uniquely determined, yet it can be different for another lattice point; there can be an infinite kinds of AS's for a single SQC. So far, very little is known about the general construction principle of such AS's. It is, however, instructive to consider averaged AS's over sublattices of  $\hat{\Lambda}$ .[3] Each averaged AS is given by mapping the relevant subset of the lattice points of the SQC into the internal space. In FIG.2 several averaged AS's calculated in this way are shown for  $T_8$ ,  $T_{10}$  and  $T_{12}$ . A detailed analysis strongly indicates that the boundaries of the AS's have fractal nature.

## 3. Structure factors

As in the case of a QC, the structure factor  $S(\mathbf{Q})$  of an SQC consists only of Bragg peaks, whose positions are given by the relevant Fourier module.  $S(\mathbf{Q})$  is divided into superlattice reflections  $S_n(\mathbf{Q})$ ,  $n = 0, 1, 2, 3, \dots$ , derived from the hierarchical superlattice structure of the SQC. The Fourier module for the main reflections  $S_0(\mathbf{Q})$ ,  $\Lambda_0^*$ , coincides with that of a QC with the same hyperlattice, and is inferred from the reciprocal of the basis vectors of  $\hat{\Lambda}$ . It follows that  $\Lambda_0^* = \Lambda/2$ ,  $(2/5)\Lambda_1$  or  $\Lambda/\sqrt{3}$  for  $D_8$ ,  $D_{10}$  or  $D_{12}$ , respectively.

The Fourier module  $\Lambda_n^*$  associated with the  $n$ -th order superlattice  $\hat{\Lambda}_n$  is defined by the projection of the reciprocal lattice,  $\hat{\Lambda}_n^*$ , of  $\hat{\Lambda}_n$  onto  $E_2$ . The following relations are important:  $\Lambda_{n+1}^* = \sigma^{-1}\Lambda_n^*$  and  $\sigma^2\Lambda = \sqrt{k}\Lambda$ . [3] By combining the latter two, one can readily show that  $\Lambda_n^* = (1/\sqrt{k})\sigma\Lambda_{n-1}^* = \dots = (1/\sqrt{k})^n\sigma^n\Lambda_0^*$ . The infinite series of the Fourier modules,  $\Lambda_n^*$ 's, is an increasing series, and the Fourier module of the SQC is equal to the limiting set:  $\Lambda_\infty^* := \cup_{n=0}^\infty \Lambda_n^*$ .

It is more convenient to represent  $\Lambda_\infty^*$  as the sum of the increments  $\Delta_n := \Lambda_n^* - \Lambda_{n-1}^*$ ,  $n = 1, 2, 3, \dots$ , which are disjoint; namely,  $\Lambda_\infty^* = \Lambda_0^* + \Delta_1 + \Delta_2 + \dots$ . Then the  $n$ -th order superlattice reflections,  $S_n(\mathbf{Q})$  ( $n \geq 1$ ), are supported on the subset  $\Delta_n$ . Therefore, the Bragg peaks for an SQC should be indexed by five integers where the fifth integer specifies the order  $n$  of the superlattice. [3]

The structure factors of  $T_8$ ,  $T_{10}$  and  $T_{12}$  are calculated by taking a periodic approximant with large enough unit cell. We use an inflated square (for  $T_8$  or  $T_{12}$ ) or 2-fold hexagonal (for  $T_{10}$ ) tile as the unit cell. The Bragg peaks supported on  $\Delta_n$  for different  $n$  can be distinguished and are shown by distinct symbols in FIG.3. The results demonstrate the existence of superlattice reflections  $S_n(\mathbf{Q})$ , which is a peculiar feature to the SQC's. The superlattice reflections are damped rapidly as  $n$  is increased, implying that the non-uniformity of the AS's for the SQC's becomes weak as the order of superlattice increases. It is also an interesting point to elucidate whether this rapid damping is universal for all SQC's generated with inflation rules.

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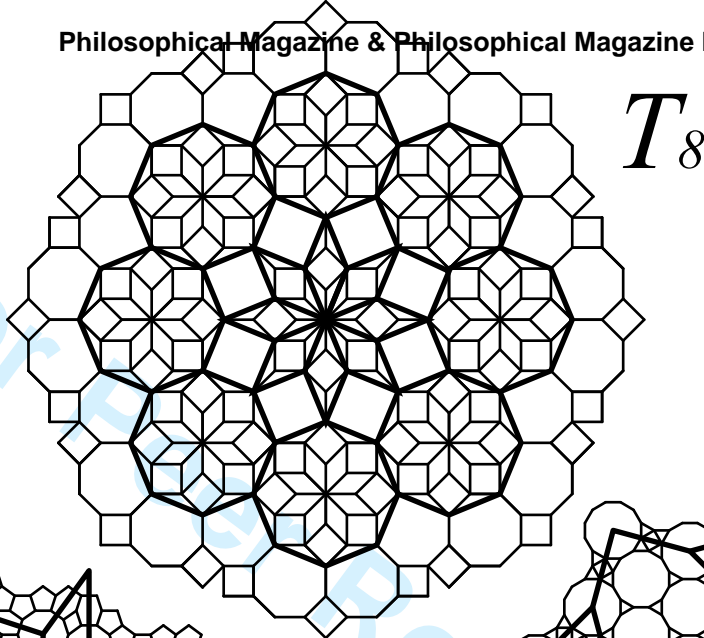


FIG. 1: Symmetrical patches of the three 2D SQC's,  $T_8$ ,  $T_{10}$  and  $T_{12}$ . The inflation rules are shown by thicker lines in each tiling; the inflation rule of the obese rhombus in  $T_{10}$  is shown separately.  $T_8$  involves three kinds of tiles, {rhombus, square, regular octagon}, while  $T_{10}$  five, {rhombi (acute, obese), regular pentagon, 2-fold hexagon, regular decagon}, and  $T_{12}$  four, {equilateral triangle, square, 3-fold hexagon, regular dodecagon}.

FIG. 2: Averaged AS's for  $T_8$ ,  $T_{10}$  and  $T_{12}$ . The average is taken over  $\Sigma_0$  (the whole lattice points of the SQC's) as well as its subsets  $\Sigma_{1,\alpha}$  originating from the first order sublattices of  $\hat{\Lambda}$  congruent with  $\hat{\Lambda}_1$ ; different sublattices are distinguished by  $\alpha$ . The subsets  $\Sigma_{1,1}$  and  $\Sigma_{1,4}$  of  $T_{10}$  interchange via the 10-fold rotation, so that the relevant averaged AS's have 5-fold symmetry. The same holds for  $\Sigma_{1,2}$  and  $\Sigma_{1,3}$ . The subsets  $\Sigma_{1,01}$ ,  $\Sigma_{1,10}$  and  $\Sigma_{1,11}$  of  $T_{12}$  iterate by three-cycle via the 12-fold rotation, so that the relevant averaged AS's have 4-fold symmetry.

FIG. 3: The structure factors of the SQC's, (a)  $T_8$ , (b)  $T_{10}$  and (c)  $T_{12}$ . Only a  $1/p$  ( $p = 8, 10$  and  $12$ ) sector with the origin at the left end is shown. The cutoff is set to 0.0001 (0.01%) of the strongest spot at the origin. The area of a spot is proportional to the Fourier intensity. In each case, a wide view and a magnified view of the boxed part are shown separately. In the wide view, the main reflections are shown by open circles, while superlattice reflections by black spots. In the magnified view, different patterns are used for superlattice reflections of different orders, where the size of the spots are somewhat emphasized.

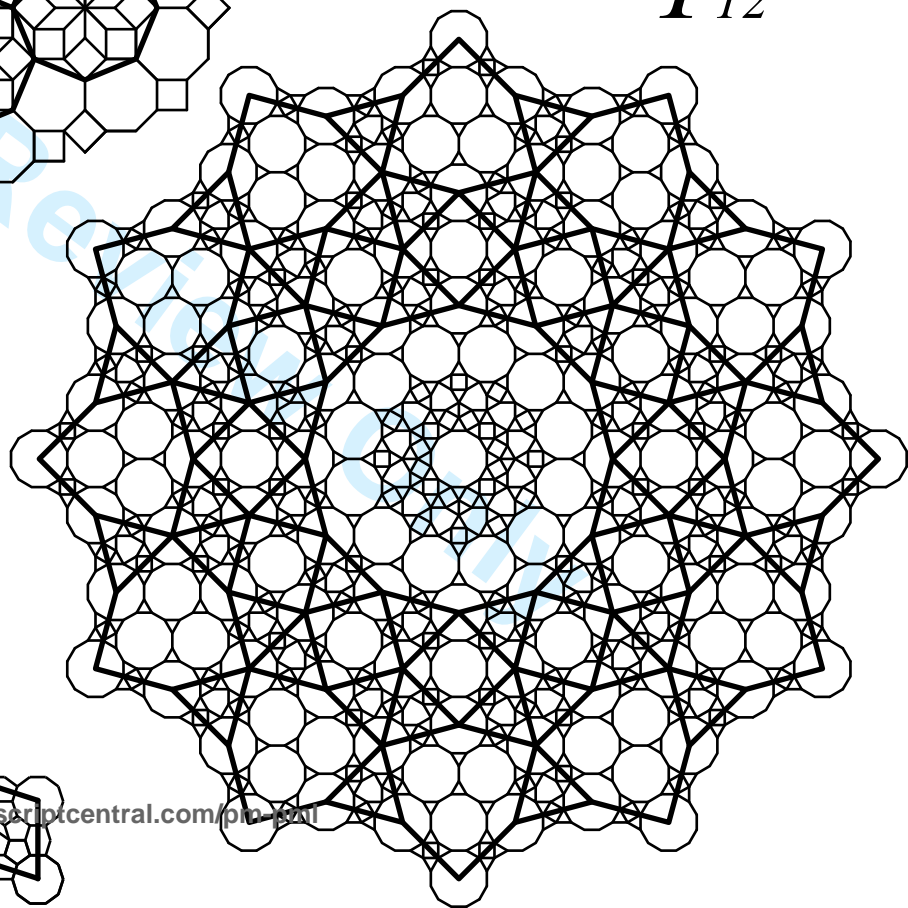
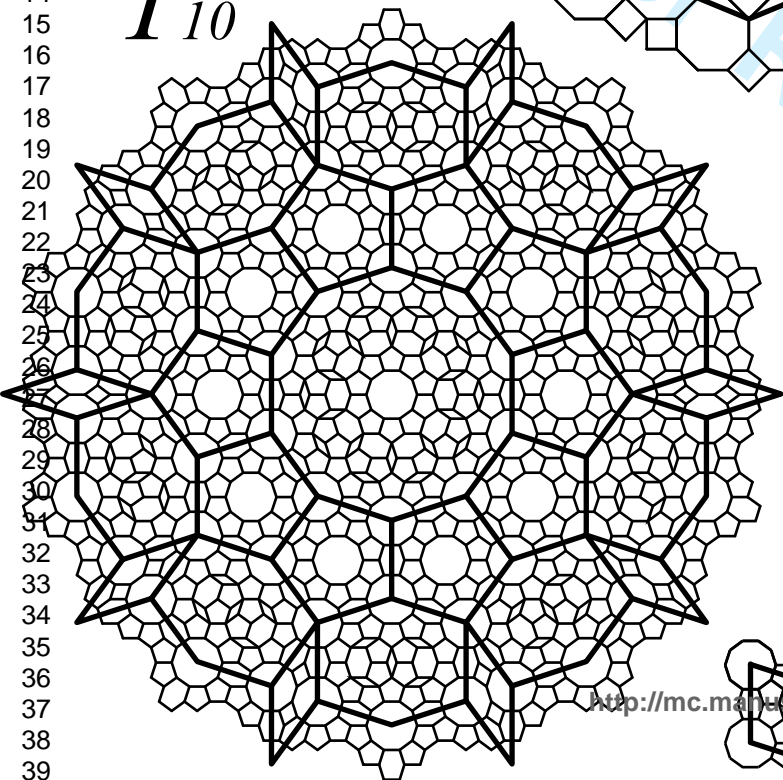
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$T_8$

$T_{12}$

$T_{10}$

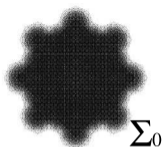


$T_8$

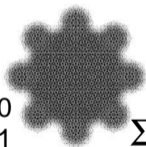
$T_{10}$

$T_{12}$

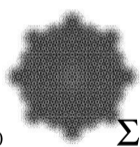
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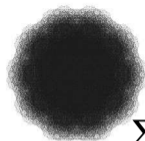
$\Sigma_0$



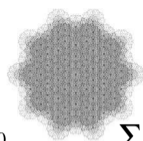
$\Sigma_{1,0}$



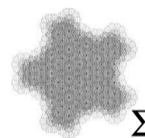
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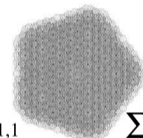
$\Sigma_0$



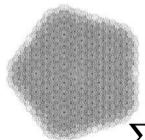
$\Sigma_{1,0}$



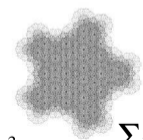
$\Sigma_{1,1}$



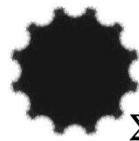
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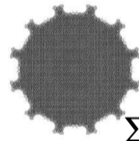
$\Sigma_{1,3}$



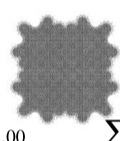
$\Sigma_{1,4}$



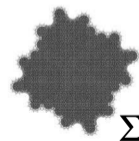
$\Sigma_0$



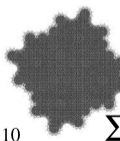
$\Sigma_{1,00}$



$\Sigma_{1,01}$



$\Sigma_{1,10}$



$\Sigma_{1,11}$

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