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Structure of decagonal quasicrystals described by clusters

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The cluster model offers a new approach to the structure of quasicrystals. The model assumes that the whole structure can be covered by only one structure unit – the cluster. However, because quasicrystals are not periodic, clusters must overlap each other. The first known cluster is G33 proposed by Gummelt. Another type of cluster is the kite cluster – it is the smallest possible cluster that can cover the whole Penrose tiling. There are three different kite clusters: 17-atom K17, 7-atom K7 and 4-atom K4 discussed in the paper.

Key words: *quasicrystal; cluster; structure factor*

1. Introduction

The discovery of quasicrystals [1] forced scientists to review their knowledge of the structure of the solid matter. Quasicrystals produce the forbidden, 5-fold diffraction pattern. In 70', Penrose[**] proved that it is possible to cover the whole plane non-periodically using only two elements: thick and thin rhombuses. Atoms put in the corners of those rhombuses gave a 5-fold, crystalline diffraction pattern. To commemorate this breakthrough, the first quasicrystalline structure model was named the Penrose tiling.

At the same time another model of quasicrystals has been developed – the high -dimensional "cut and project" model [2–4]. Atoms of quasicrystals are put, in this model, in the vertices of regularly arranged 5D hyper-cubes. Despite some non-physical assumptions, the model produces very accurate results and is quite easy to handle with. Another model – the statistical one [5, 6], using only physical probability distributions, describes quasicrystals as good as the "cut and project" model.

In 1996 Gummelt [7] showed that it is possible to cover the whole plane with only one unit structure – the cluster. To do this, different clusters must overlap each other.

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Although the cluster model is difficult from the mathematical point of view, physicists willingly use it as it is the most physical model of all [7–12]. Clusters seem to be the most natural form of solidified atoms; the overlapping can be treated as sharing atoms between different clusters; finally, the arrangement of atoms in a cluster can keep the 5-fold symmetry.

For the model structures each approach can be transformed into another. This paper concentrates on the cluster model; however, to describe it as effectively as possible, other models are used as well.

2. Geometrical properties of clusters

Gummelt's cluster (G33) consists of 33 atoms arranged in a circular figure of the radius of 5.044. The atoms filling up the cluster lie in the vertices of rhombuses of the Penrose tiling. The length of the edges of the rhombuses is assumed to be equal to 1. The main part of each cluster occupies a thick rhombus inflated τ^2- times (Fig. 1). The Penrose tiling can be covered by clusters by replacing each thick rhombus by a cluster. The area of the G33 which surrounds the thick rhombus lying in its centre overlaps every other rhombus of the Penrose tiling which lies in the vicinity of the one replaced by the cluster. Because the overlapped area is large, up to 5 clusters can cover the same area of the Penrose tiling.

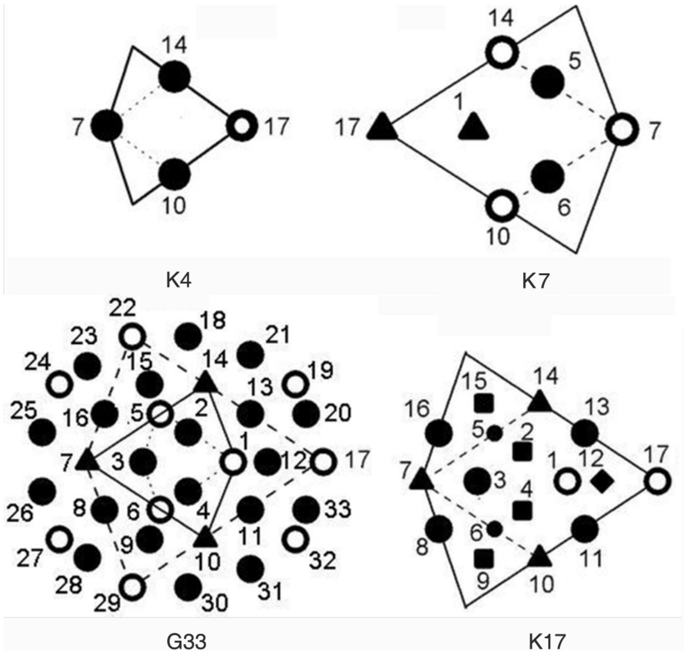

Fig. 1. The family of kite clusters and G33. Different types of atoms are marked with different shapes

There are some points in G33 that can be removed without damaging the Penrose structure. When all such points are removed, the rest will form the K17 kite-cluster (Fig. 1). The K17 cluster, recently discovered by us [9], consists of 17 points arranged within the area of a kite. The main part of a K17 occupies, as in G33, a thick rhombus inflated τ^2 times. To two sides of the thick rhombus are attached to halves of a thin rhombus. The Penrose tiling can be covered by K17 by replacing each thick rhombus with this cluster. The area surrounding the main thick rhombus in K17 cluster is considerably smaller than it was in G33. This results in a lower value of the coverage coefficient and higher number of independent atoms which can decorate K17. This cluster can be decorated by 6 different atoms – marked with various shapes in Fig. 1.

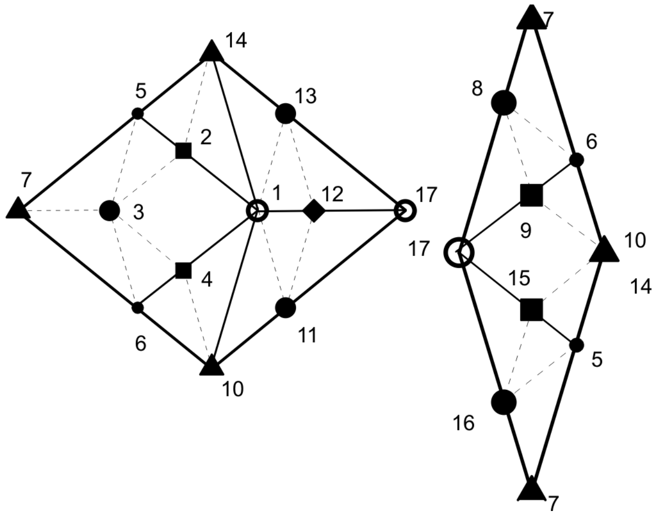

Fig. 2. Thick and thin rhombuses decorated as K17

Figure 2 shows the K17 cluster transformed into the rhombuses. Transformation into rhombuses has numerous advantages. Rhombuses never overlap – which makes statistical calculations very easy; properties of rhombuses are well known; the structure factor for freely decorated rhombuses was already derived and can be used for cluster decoration as well [7].

One of the most important properties of clusters is the concentration of decorating atoms defined as a ratio of the number of specific atoms to the number of all atoms filling up the structure. It is well known that the number of thick rhombuses is τ-times larger than the number of thin rhombuses. So, if there are n_{Sj} atoms of type j in a thin rhombus, there must be also τn_{Lj} atoms of this kind in a thick rhombus. If we have a structure built of N_S thin rhombuses, the number of atoms of j type is equal to $N_S(n_{Sj} + \tau n_{Lj})$. Following the same procedure, we can get the whole number of all decorating atoms in the Penrose tiling as equal to $N_S(n_S + \tau n_L)$, where n_S and n_L are the number of all atoms decorating thin and thick rhombuses, respectively. Concentration c_j can be then calculated as:

$$c_j = \frac{n_{S\,j} + \tau n_{L\,j}}{n_S + \tau n_L} \tag{1}$$

The concentrations of all atoms decorating the K17 cluster are given in Table 1.

Table 1. Groups of atoms of various types decorating clusters K17, K7, K4 and G33

K17		K7		G33		K4	
Atom No.	C_{17} [%]	Atom No.	C_7 [%]	Atom No.	C_{33} [%]	Atom No.	C_4 [%]
1, 17	13.0	7, 10, 14	27.6	1, 5, 6, 17, 19, 22, 24, 27, 29, 32	27.6	17	27.6
5, 6	14.6						
7, 10, 14	10.6	1, 14	34.2	7, 10, 14	10.6	7, 10, 14	72.4
3, 8, 11, 13, 16	23.6			2, 3, 4, 8, 9, 11, 12, 13, 15, 16, 18, 20, 21, 23, 25 26, 28, 30, 31, 33	61.8		
12	9.0	5, 6	38.2				
2, 9, 4, 15	29.2						

Cluster K17 is based on the thick rhombus which is divided two times in accordance with the inflation rules. If the inflation rules were used only once, seven-atom K7 cluster would be formed. A thick rhombus itself can be also treated as a 4-atom K4 cluster. The whole family of kite clusters is presented in Fig. 1. We can also easily transform a K17 cluster into a K7 or K4 one by removing from the K17 atoms which are not present in the cluster we want to get. We need to remove atoms number 2, 3, 4, 8, 9, 11, 12, 13, 15 and 16 to transform K17 into K7 and additionally atoms 1, 5 and 6 if we want to obtain the K4 cluster. We can explore all the needed properties and relations for K17 and use them for both K7 and K4. For instance, we do not need to look for new overlapping rules for K7 and K4. They must be identical to the inflation rules of K17. We don't need to check which atoms are of the same kind. If atoms 7, 14 and 10 are of the same kind in the K17 cluster, so they are in K7 and in K4. Finally, this procedure also speeds up statistical calculation. The concentrations of atoms of K7 and K4 clusters are collected in Table 1.

3. The "cut and project" method

The idea of the "cut and project" method is to fill up the 5D space with atoms regularly arranged in the vertices of 5D hyper-cube. The 5D space is then divided into 2 subspaces: 2D physical space – in which we can observe quasicrystals, and 3D perpendicular space. Now, we choose one elementary 5D cell and through its vertices we provide the planes parallel to the physical space. Only these atoms matter which are inside the space limited by the set of the most exterior planes. This space is called the projection strip. Projection of atoms lying inside the projection strip onto the physical space gives the Penrose tiling. Projection onto the perpendicular space gives the so called atomic surface, which can be considered as a probability distribution of atoms building the quasicrystal. For the Penrose tiling, the atomic surface consists of 4 pentagons (shown in Fig. 4) separated along the $z_{\perp}$ axis. Projections of all atoms are collected on these pentagons. The probability density in every point of the atomic surface is constant – the pentagons are “flat”.

4. Structure factor for the clusters transformed into rhombuses

The detailed derivation of the structure factor for the rhombus model can be found in [6]. At this point, we focus on the final results of these calculations. The structure factor for the freely decorated rhombuses is a sum of structure factors derived separately for thin and thick rhombuses:

$$F\left(n_x,m_x,n_y,m_y\right)=\sum_{j=1}^{n_L}F_{Lj}\left(n_x,m_x,n_y,m_y\right)+\sum_{j=1}^{n_S}F_{Sj}\left(n_x,m_x,n_y,m_y\right) \tag{2}$$

The sums go over the cluster atoms decorating the rhombuses. Structure factor for the thick rhombus:

$$F_{Lj}\left(n_x,m_x,n_y,m_y\right)=Cf_a p_j \mathrm{re}$$

$$\times\left[p_j\sum_{\alpha=0}^{4}\exp i\left(k_x\Delta x_{j,\alpha}+k_y\Delta y_{j,\alpha}+\phi_j\right)\iint_{\Delta_{2\alpha}}\exp i\left(\chi_x u_x+\chi_y u_y\right)\mathrm{d}u_x\,\mathrm{d}u_y\right]$$

where:

$$\chi_x=\left(n_x-m_x\tau\right)k_x,\qquad \chi_y=\left(n_y-m_y\tau\right)k_y$$

$$k_x=\frac{2\pi}{5}\left(n_x+\frac{m_x}{\tau}\right),\qquad k_y=\frac{2\pi}{5}\tau\sqrt{\tau+2}\left(n_y+\frac{m_y}{\tau}\right)$$

n_x, n_y, m_x, m_y are the indices of the diffraction peaks (k_x, k_y), f_a is the atomic scattering factor, Δx, Δy – decorating the rhombus coordinates given in relation to the position of atoms number 17; $\Delta_{2\alpha}$ – the triangular probability distribution of the rhombuses in the Penrose tiling written in the physical space (u_x, u_y) – details in [6]; α – orientation of rhombuses, C – normalization constant, p_j – occupation probability, τ – a golden value equal to ca. 1.618.

5. Statistical distribution of clusters

Some clusters cannot be transformed into rhombuses. In such a case another approach must be applied – we need to combine the cluster model, the statistical model and “cut and project” model. If we knew the distribution of cluster’s atoms we might compute the Fourier transform over this distribution and get the structure factor for the clusters.

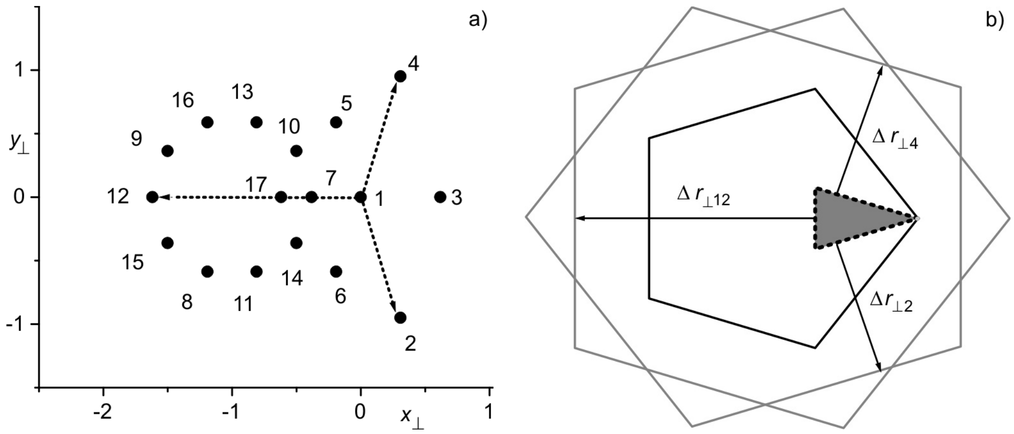

Fig. 3. Cluster K17 written in the perpendicular space (a), and determination of the probability distribution for the K17 cluster (b)

For the calculations we take the largest kite cluster – K17 and choose the coordinates of the atom No. 1 as a reference point. The projection of atoms of the K17 cluster onto the perpendicular space is presented in Fig. 3a. Dotted arrays connect atom 1 and its furthest neighbours. Atoms 2, 4 and 12 limit the shape of the distribution of atoms No. 1 (Fig. 3b). The area of the distribution (P_{K17}) equals 0.1551. We can use this value to calculate the coverage coefficient δ. We define it as a ratio of the area of the distribution of all cluster’s atoms to the area of the atomic surface P_{AS} which is equal to ca. 17.205. The area of the distributions of all atoms in clusters is equal to P_{K17} multiplied by the number of atoms (17 for K17 and 33 for G33) and by 10 orientations (P_{K17} is calculated for a specific orientation, whereas every K17 can also be found rotated by the angle of $\alpha\times 2\pi/5$, $\alpha = 0, 1, \ldots, 9$)

$$\delta = \frac{10NP_{\Delta}}{P_{PA}} \approx \frac{NP_{\Delta}}{1.7205} \tag{3}$$

The coverage coefficients are equal to 2.98 and 1.53 for G33 and K17, respectively. These results mean that every point of the Penrose tiling and the atomic surface is taken, on average, by 2.98 G33 clusters or by 1.53 K17 clusters. Having the shape of the distribution of atom number 1 and the perpendicular relative coordinates of all other atoms, we can fill up the atomic surface with the distributions of all cluster’s atoms (Fig. 4). In order to determine which atoms overlap, we need to rotate the distributions by the angle of $\alpha\times 2\pi/5$, $\alpha = 0, 1, \ldots, 9$. After rotation, we combine all overlapping triangles. The results are shown in Fig. 5. Because the atomic surface is symmetrical, we can reduce it to only two pentagons. Atomic surface has been divided into 7 separated parts.

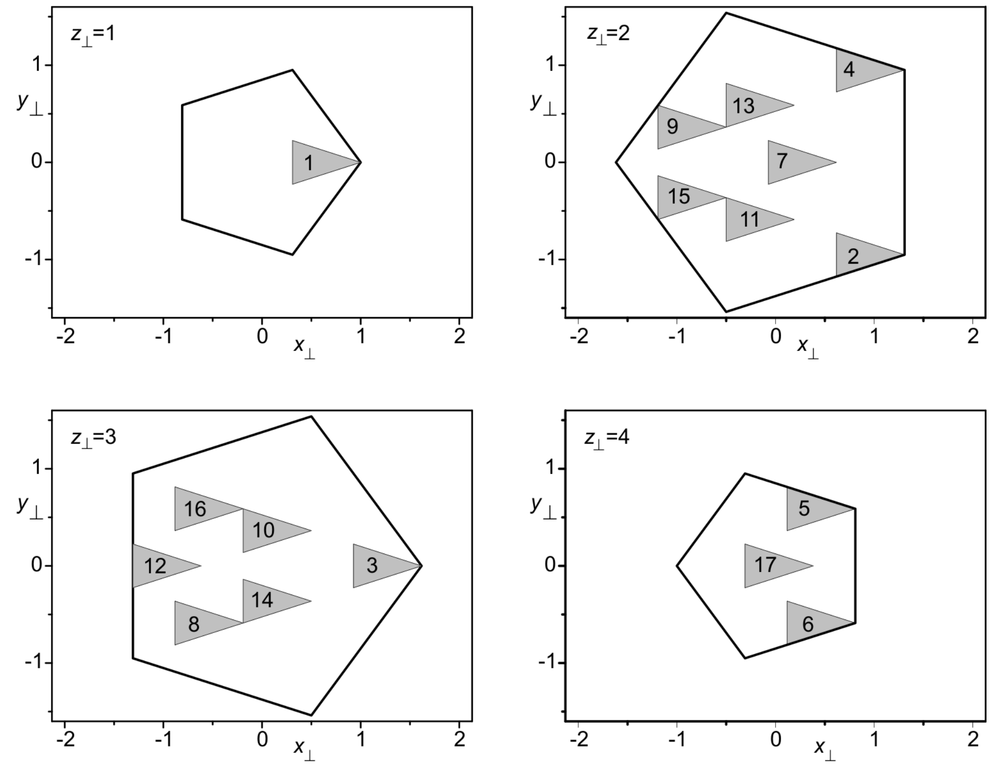

Fig. 4. Arrangement of the distributions of all atoms decorating the K17 cluster within the atomic surface

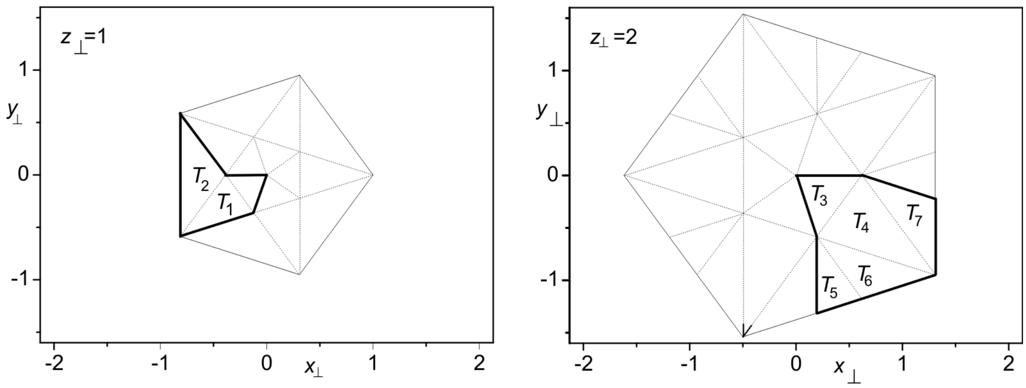

Fig. 5. Atomic surface division. Each area relates to another atom type of K17

Table 2 contains the coordinates of the vertices, the areas and indicates which atoms build these parts. The results are consistent with Table 1 with two exceptions.

There are two more independent types of atom in Table 2 when compared with Table 1. Atoms 2 plus 9 never overlap 4 plus 15. Their positions in clusters are symmetrical and because of that we assume that they must be of the same kind. Additionally, atoms 1 and 17 are separated, because their triangle distributions do not overlap – they don't need to be of the same kind. This is the major difference between the cluster and rhombus models. In the rhombus model we had to assume these two atoms to be equal. The source of this difference lies in the empty vertices of kite clusters. When we transform clusters into the rhombuses we have to put atom number 17 into these vacant spots.

Table 2. Numerical description of the atomic surface divided into separated parts assigned to various types of atoms decorating the K17 cluster

	Atom No.	Vertex 1	Vertex 2	Vertex 3	Area	Concentration C_{17} [%]
T_{1A}	1	$\{0, 0\}$	$\{2\cdot(2-\tau), 0\}$	$\{2\tau-3, \tau-2\}$	0.069	13
T_{1B}	17	$\{\tau, 1-\tau\}$	$\{2(2-\tau), 0\}$	$\{2\tau-3, \tau-2\}$	0.155	
T_2	5, 6	$\{2(2-\tau), 0\}$	$\{\tau, \tau-1\}$	$\{\tau, 1-\tau\}$	0.251	14.6
T_3	7, 10, 14	$\{0, 0\}$	$\{2(\tau-1), 0\}$	$\{2-\tau, 1-\tau\}$	0.182	10.6
T_4	3, 8, 11, 13, 16	$\{\tau+1, -1\}$	$\{2(\tau-1), 0\}$	$\{2-\tau, 1-\tau\}$	0.406	23.6
T_5	12	$\{2-\tau, 1-\tau\}$	$\{2-\tau, \tau-3\}$	$\{2(\tau-1), 2(1-\tau)\}$	0.155	9.0
T_6	2, 9	$\{2-\tau, 1-\tau\}$	$\{\tau+1, -1\}$	$\{2(\tau-1), 2(1-\tau)\}$	0.251	14.6
T_7	4, 15	$\{2(\tau-1), 0\}$	$\{\tau+1, 3-2\tau\}$	$\{\tau+1, -1\}$	0.251	14.6

The area of each separated part of the atomic surface is proportional to the number of atoms belonging to the area. This gives us another opportunity for calculating the concentration of each atom – as a ratio of the area of a specific j atom P_j to the area of the atomic surface: $c_j = P_j/P_{\mathrm{AS}}$. This equation leads to the results which are consistent with ones got by means of equation (1) – compare tables 1 and 2.

6. Structure factor for the cluster model

Having the atomic surface divided into the separated parts connected to different types of atoms we can calculate the Fourier transform over each of these parts. As a result we get a structure factor for the cluster model.

$$F(\chi_x, \chi_y) = C \cdot \mathrm{re}\left[\sum_{t=1}^{t_{\max}} f_{t,a} \sum_{j=1}^{2} \exp(\mathrm{i}\varphi_j) \sum_{\alpha=0}^{4} \iint_{T_{t,j,\alpha}} \exp \mathrm{i}(\chi_x u_x + \chi_y u_y)\, \mathrm{d}u_x\, \mathrm{d}u_y\right] \tag{4}$$

The meaning of symbols used in this equation is described in Section 4. Equation (4) gives much less flexibility than (2). It should be used when a transformation into rhombuses is not possible.

7. Conclusions

The cluster model offers a new approach to the structure of quasicrystals. The model assumes that the whole structure can be covered by only one structure unit – the cluster. However, because quasicrystals are not periodic, clusters must overlap each other.

This model is more and more popular among the physicists. It gives a simple unit structure which can hold the symmetry of the diffraction pattern. Cluster is also more stable than rhombus form from the energetic point of view.

The first known cluster is G33 proposed by Petra Gummelt [7]. Another type of cluster is the kite cluster – it is the smallest possible cluster that can cover the whole Penrose tiling. There are three different kite clusters: 17-atom K17, 7-atom K7 and 4-atom K4.

The most important property of any cluster is the number of independent atoms that can decorate this cluster. In case of G33, there are 3 independent atoms which cover the plane with the relative concentration 62:28:11. In the case of kite clusters we have 6 independent atoms in K17 (29:24:15:13:11:9), 3 in K7 (38:34:28) and 2 in K4 (76:24). The relative concentration of atoms filling-up the kite-clusters is similar to the relative concentration of the atoms building the quasicrystalline stable compounds, for instance: composition of $Al_{71}TM_{29}$ [13, 14] versus (38 + 34):28 in the K7. Kite-clusters can be then used as a very good initial model for the further refinement. Another important property of clusters is the value of the coverage coefficient. The higher value it has, the more intensively clusters overlap which has an effect on the number of independent atoms. Application of kite-clusters to the real decagonal quasicrystals has been already proved and will be presented elsewhere [15].

To get some valuable theoretical properties of clusters we can transform them into rhombuses or use the “cut and project” method. Both methods impose their own limitation on clusters. The “cut and project” method allows decorating only in Penrose’s positions, the rhombus method not always can be used – some clusters cannot be transformed into rhombuses.

Acknowledgements

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