A hexagonal golden–mean tiling

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Aperiodic tilings with rotational symmetries ‘forbidden’ in periodic systems have garnered much attraction in crystallography. However, quasicrystals and quasicrystalline arrangements are not solely defined by exhibiting these symmetries. In fact, there is a great potential in exploring multi–length–scale aperiodic tilings with rotational symmetries commensurate with periodicity (2–, 3–, 4– and 6–fold), in particular, investigating the interface between periodic and aperiodic structures which share these rotational symmetries. Motivated by this, we introduce a new multi–length–scale, 6–fold aperiodic tiling.

Aperiodic tilings have proved to be an essential tool in understanding, modelling, and representing quasicrystalline structures. However, there are limited examples which explore aperiodic tilings exhibiting rotational symmetries commensurate with periodic real–space structures i.e. 2–, 3–, 4–, and 6–fold [1–4]. This is despite the fact quasicrystals are not restricted to exhibiting ‘forbidden’ symmetries only [5], and the obvious benefits of studying the transition between periodic and aperiodic structures (facilitated by a sharing of rotational symmetries).

As such, we introduce the classification of a two–length–scale 6–fold aperiodic tiling. We discuss the tiling in terms of the multigrid method, substitution rules, vertex and edge matching rules, and its perpendicular–space structure.

Grid dualization

We create a 6–fold tiling skeleton using a generalisation of the multigrid method [6, 7], which we briefly explain here. A regular multigrid is a superposition of m distinct grids, or parallel lines with equal spacing, where no more than two lines intersect at a given point (a singular multigrid permits more than two). Each of the m grids is orthogonal to a grid vector \( g_m \). A tiling can be constructed by taking the dual of the multigrid, where each intersection point of the grids corresponds to a tile. The tile edges are formed by the tiling vectors \( t_m \) associated with the grids which form the intersection point. We note that the grid and tiling vectors do not need to be identical in magnitude, only in orientation [7]. Alternatively, the dual can be calculated by considering each closed polygon in the multigrid. These correspond to single vertices in the tiling defined at position \( P = \sum_{m} n_m t_m \), where \( n_m \) is the number of lines in the \( m \)th grid separating the polygon from the origin [8].

We start by describing our tiling vectors, \( t_m \), which are shown in Figure 1(a) and are split into two sets. Set \( L \) is defined by \( t_m = (\tau \cos \theta, \tau \sin \theta) \) for \( m = 1, 3, 5 \) and set \( S \) as \( t_m = (\cos \theta, \sin \theta) \) for \( m = 2, 4, 6 \), where \( \theta = \frac{m\pi}{3} \) and \( \tau = \frac{1 + \sqrt{5}}{2} \), the golden mean. The ratio of the magnitude of the vectors in sets \( L \) and \( S \) is therefore \( \tau : 1 \), respectively.

Our multigrid is then constructed considering a set of grid vectors \( g_m \) which are identical in orientation to \( t_m \) yet with modified magnitudes. We design \( g_m \) so that the
FIG. 1: (a) The tiling vectors for each of the sets, $L$ and $S$. Set 2 (blue) is $\tau$-deflated with respect to set 1 (black). (b) The grid vectors for each of the sets. Set 1 (black) is $\tau$-deflated with respect to Set 2 (blue). (c) The hexagrid, where a black circle indicates the origin.

magnitude ratio of sets $L$ and $S$ in grid–space is 1:$\tau$ (an inversion of the tiling vector magnitude ratio), demonstrated in Figure 1(b). If we maintain the $t_m$ magnitude ratio for $g_m$, then the number of $S$ tiles will exceed the number of $L$ tiles: smaller separations in the corresponding grids produce a denser set of intersections, hence leading to more tiles. However, we wish to follow the convention in golden–mean quasicrystals that the frequency of larger ‘building blocks’ is greater than the smaller building blocks by some factor of $\tau$. For example, there are $\tau$ more large segments than small in the Fibonacci chain [9, 10], $\tau^2$ more $L^2$ tiles than $S^2$ tiles in the Fibonacci square grid [11], and the frequency of ‘fat’ to ‘skinny’ rhombuses in the Penrose tiling is $\tau$:1 [12]. Our choice allows us to guarantee more $L$ tiles than $S$, with the exact frequency relationship between tiles discussed in the next section.

The resultant regular multigrid formed by $g_m$ is shown in Figure 1(c), which we call a ‘hexagrid’. We note that the hexagrid is essentially the combination of two $\tau$-scaled kagome lattices with a common origin, i.e., the black circle shown in Figure 1(c). As the kagome lattice has a group symmetry of $p6m$ [12], both the hexagrid and its dual has 6-fold rotational symmetry around this origin. We discuss the effects of shifting the grids of the hexagrid in a later section. Figure 2(a) shows a portion of the resultant tiling after calculating the dual of the hexagrid. Its centre of 6-fold symmetry is marked as a black circle. There are three basic types of rhombic tiles, shown in Figure 2(b) and labelled as large, $L$, small, $S$, and parallelogram, $P$.

To demonstrate the long–range order of the tiling point–set, we calculate its Fourier transform. To do so, we define a set of reciprocal space basis vectors such that $t_i \cdot q_i' = 2\pi \delta_{ii'}$, where $\delta_{ii'}$ is the Kronecker delta, and $t_i$ and $q_i'$ are the real and reciprocal space vectors. If each position is described by a delta function so that the density is $p(r) = \sum_{k=1}^{N} \delta(r - x(k))$, then the Fourier transform of the density is $p(r) = \sum_{k=1}^{N} \exp(-i q \cdot x(k))$. The inset of Figure 2(a) shows the resultant pattern where circle size is relative to spot intensity, and the pattern is normalized by the central spot.

**Substitution rules**

The hexagonal tiling can also be generated considering substitution rules for the 3 basic tiles shown in Figure 2(b). In fact, it is necessary to expand the total set of proto–tiles to contain 8 distinct tiles: 3 large, 3 small, and 2 parallelogram tiles. Figure 3(a) shows the set of proto–tiles, coloured uniquely and labelled numerically according to their tile type, and, Figure 3(b) shows...
FIG. 3: (a) The tiles used in substitution, which are labelled and numbered according to their geometry. (b) Substitution rules for each of the tiles. (c) A patch of the hexagonal tiling constructed through substitution with 8 coloured tiles.

We can calculate the tile frequencies across the tiling by inspection of the components of the eigenvector of the largest eigenvalue of the substitution matrix, $M$ [11]. The substitution rules for each tile are read descending each column, where values indicate how many tiles (in the corresponding rows) are contained within the substitute:

$$M = \begin{pmatrix}
L_1 & L_2 & L_3 & P_1 & P_2 & S_1 & S_2 & S_3 \\
1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 1 & \frac{1}{2} & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & \frac{1}{2} & 0 & 0 & 1 & 0 \\
2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 2 & 2 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 
\end{pmatrix}$$

where the tile labels are given as headings in the rows and columns. The largest eigenvalue of the matrix is $\lambda_1 = \tau^2$, giving the eigenvector $u_1$, which is proportional to:

$$u_1 = \begin{pmatrix}
L_1 \\
L_2 \\
L_3 \\
P_1 \\
P_2 \\
S_1 \\
S_2 \\
S_3 
\end{pmatrix} = \begin{pmatrix}
2\tau^2 \\
\tau^2 \\
\tau^2 \\
4\tau \\
4\tau \\
2 \\
1 \\
1 
\end{pmatrix}$$
so that there are an equal number of S2 and S3 tiles, yet twice as many S1 tiles, and so on. The tile frequencies are then simply calculated by dividing $u_1$ by the total of its components ($12\tau+8$) and given as a percentage:

$$F \approx \begin{pmatrix}
L_1 & 19.1 \\
L_2 & 9.5 \\
L_3 & 9.5 \\
p_1 & 23.6 \\
p_2 & 23.6 \\
s_1 & 7.2 \\
s_2 & 3.6 \\
s_3 & 3.6
\end{pmatrix}$$

so that the sum of the L tile frequencies is $\tau^2$ greater than the sum of the S tile frequencies, as expected from our design of the magnitude of $g_m$.

**Vertex and edge matching rules**

The hexagonal tiling has 32 allowed vertex configurations, which are shown in Figure 4(a), where the columns are indexed numerically, and the rows are grouped by the coordination number of each vertex. The exact fraction of the vertices across the infinite tiling are given in Table I, which has the same layout as Figure 4(a).

The vertices are enforced with edge matching rules (and vice-versa), which are shown in Figure 4(b) as arrows, triangles, and circles decorating the edges of the tiles. The edge rules are rotationally asymmetric, which is an important factor to consider when arbitrarily decomposing tiles; as previously mentioned, the substitutions of the tiles are rotationally asymmetric. Therefore, a tile’s orientation (considering the edge matching rules) should be factored in before the decomposition. Asterisked vertices in Figure 4(a) are examples which highlight the importance of discerning unique vertices. Each vertex may look graphically similar if their individual tiles are rotated by $180^\circ$, but the edge-matching/vertex combination would be incorrect for the tiling we have described – leading to a ‘dead-end’, or, a site where continued defect-free growth of the tiling is stopped.

**Grid shifts and symmetry**

After defining substitution, vertex, and edge matching rules, we can discuss the effects of applying shifts to the individual grids of the hexagrid. When constructing the Penrose tiling by the dual of a pentagrid, arbitrary shifts of $\gamma_m$ can be applied to the $m$ individual grids along the direction of their grid vector, such that there is a total shift vector $\vec{\gamma} = (\gamma_0, ..., \gamma_4)$. If the sum of $\vec{\gamma}$ is an integer, we obtain Penrose tilings [13]. For non-integer
sум, we find ‘generalised’ tilings which do not satisfy the vertex/matching rules of the Penrose tiling, and are not self-similar through tile substitution [14].

For the hexagrid, we find that to satisfy our substitution and vertex/matching rules, the \( L \) and \( S \) grid-sets are explicitly required to form two \( p6m \) kagome-like structures. As such, each grid-set must independently meet one of two simple conditions: either that the sum of their shifts must equal an integer, or, that each of their shifts is an integer. So long as both grid-sets meet either of these conditions, the tiling can be defined by the rules we have described. Arbitrary non-zero shifts which do not satisfy these conditions distort the kagome lattice-like grids into a more general trihexagonal structure with \( p3 \) symmetry [12], regardless of whether the total sum of shifts is an integer. This in turn changes the intersection behaviour in grid-space, giving generalised-type tilings. A few examples of applying arbitrary grid shifts and the resultant duals are shown in Supplementary Figure 2.

Applying shifts under the aforementioned conditions removes the common origin of 6-fold rotational symmetry shown in Figures 1(a) and 3(c). However, the resultant tilings are statistically indistinguishable after 6-fold rotations. Therefore, they still exhibit overall 6-fold symmetry [15–17].

**High-dimensional projection**

We can also analyse the hexagonal tiling considering a higher-dimensional space: vertices of certain aperiodic tilings can be considered as a subset of lattice points occupying an \( n \)-D superspace [7, 18]. The \( n \)-D superspace can be split into complementary spaces, physical (par-) and perpendicular (perp-). The lattice points projected onto par-space produce the tiling, whereas the points projected onto perp-space are referred to as the ‘window’.

The tiling is composed of 6 vectors, which can be regarded as non-linearly independent when spanning the tiling in 2-D. However, these vectors can also be considered as projections of 6 linearly independent vectors which describe a 6-D lattice (similarly, the hyperplanes of the hexagrid). We can therefore follow the convention of splitting a 6-D space into a 2-D par-space, and an orthogonal 4-D perp-space. A subset of the 6-D lattice points \( n = (n_1, n_2, n_3, n_4, n_5, n_6) \) labelled with integers \( n_m \) (i.e., as with the dual-grid method above) are projected onto the 2-D par space to create the tiling, while

|   | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| C | \( \frac{1}{12 \tau^6} \) | \( \frac{1}{12 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | \( \frac{\sqrt{5}}{4 \tau^4} \) | \( \frac{\sqrt{5} \tau}{4 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | -   | -   | -   |
| D | \( \frac{\sqrt{5}}{4 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | \( \frac{1}{2 \tau^4} \) | \( \frac{3}{2 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | -   | -   |
| E | \( \frac{\sqrt{5}}{4 \tau^4} \) | \( \frac{\sqrt{5}}{2 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | \( \frac{\sqrt{5}}{4 \tau^4} \) | -   | -   | -   | -   | -   | -   |
| F | \( \frac{1}{4 \tau^4} \) | \( \frac{1}{2 \tau^4} \) | \( \frac{1}{4 \tau^4} \) | \( \frac{\sqrt{5}}{2 \tau^4} \) | \( \frac{1}{12 \tau^8} \) | \( \frac{\sqrt{5}}{4 \tau^8} \) | \( \frac{1}{12 \tau^{10}} \) | \( \frac{\sqrt{5}}{4 \tau^8} \) | \( \frac{1}{4 \tau^8} \) | -   |

**TABLE I:** Fraction of vertex configurations in the infinite tiling. Rows and columns are as Figure 4(a).
the projection onto 4-D perp-space construct the windows.

We can represent the 4-D perp-space structure by following Socolar’s description of the dodecagonal tiling [19]. First, the 4-D perp-space is split into two 2-D subspaces. We define the first sub-space, $E^\perp$, as being panned by $e_1^\perp \equiv (101010)$ and $e_2^\perp \equiv (010101)$, such that the subset of projected 6-D vertices only intersect with planes defined by $n \cdot e_1^\perp = i$ and $n \cdot e_2^\perp = j$, where $i$ and $j$ are integers. The points occupy the second 2-D sub-space, $\tilde{E}$, defined by the projection $n \cdot \tilde{t}_m$, where $\tilde{t}_m$ are the 6-D vectors projected onto $\tilde{E}$: $\tilde{t}_m = (\cos \theta, \sin \theta)$, where $\theta = \frac{\pi(m+3)}{3}$ for $m = 1, 3, 5$, and $\tilde{t}_m = (\tau \cos \theta, \tau \sin \theta)$, where $\theta = \frac{\pi j}{3}$ for $j = 2, 4, 6$. $\tilde{t}_m$ are shown in Figure 5(a). We can then view the $\tilde{E}$ points which intersect planes in $E_\perp$ corresponding to the above condition for $i$ and $j$.

For the hexagonal tiling, we find that the 4-D perp-space can be represented by nine 2-D spaces, where $i, j$ are only equal to $\pm 1, 0$. Figure 5(b) shows the perp-space planes, where the rows correspond to $i$, and the columns $j$. The planes are subdivided to indicate the perp-space regions which encompass points corresponding to specific vertices in the tiling. Examples are numbered, indicating which vertex-type the region corresponds to, referring to the labelling system in Figure 5(a) and Table I. The sum of each vertex region, as a ratio of the total area of all regions, corresponds to the fractions in Table I. The regions are coloured only for clarity, as opposed to any analytical significance.

**Conclusions**

Using a generalisation of the multigrid method as a starting point, we have rigorously defined a new golden-mean aperiodic tiling with 6-fold symmetry. Two grid sets forming $\tau$-scaled kagome lattices can be used as a ‘hexagrid’, the dual of which forms our tiling. Under certain conditions, applying shifts to the hexagrid modifies the central symmetric point of the resultant dual without loss of the overall 6-fold symmetry. Our statistical analyses of the substitution and vertex rules provided a deep understanding of the infinite tiling both in parallel, and perpendicular space.

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