Topological Properties of Aperiodic Monotiles: Exploring More Inflation Rules

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Abstract: Recently discovered aperiodic monotiles form a set of novel quasi-crystal structures with conceivable implications in solid state physics. This paper explores the physical implications of the Turtle tile, the sibling tile of the Hat tile which displays graphene-like properties. Tight binding model simulations were used to extract spectral characteristics from the disordered monohedral lattice. The fractal nature of aperiodic Turtle tiling is hinted at in its density of states, spectral band structure and k-space diagram. While the observed features are inconsistent with the expected graphene patterns, the model predicts possible unconventional superconductivity. More lattice geometries using these unique shapes are to be investigated.

I. INTRODUCTION

Quasi-crystals are a relatively novel concept in condensed matter physics which bridge the gap between amorphous chaos and crystalline order. Albeit rare, this class of solids displays an intriguing non-periodic ordering at the atomic level [1]. Symmetries in these quasi-lattices lead to exotic electronic, vibrational, optical and other topological phenomena of high research interest. David Smith (*et al.*)'s recently discovered set of aperiodic monotiles [2] exhibits such behaviours. The most notable of these shapes is the *hat*, which shows graphene-like properties according to a paper published by Schirmann *et al.* [3]. To further explore these promising geometries, I analyzed the Turtle tile under a variety of inflation methods using Python scripts.

This paper reports the intrinsic properties of infinite aperiodic monotile lattices and their potential applications in solid state engineering. Up next, Section II contextualizes the "einstein tiling problem" and thus birth of infinite aperiodic monotilings. Section III then states the originality of this project. Section IV presents the results of this study, followed by reflections on their significance (Section V). Finally, Section VI concludes the paper with potential outlooks.

II. BACKGROUND

An aperiodic monotile is a shape which tiles an infinite plane, but never periodically. Until recently, research on this open problem, dubbed "Hilbert's Einstein Tile", had produced no convincing candidates and remained largely unsolved. However, amateur mathematician David Smith unexpectedly stumbled upon the elusive shape when he sketched it during his open ended investigation of shapes and their tiling properties[2]. Indeed, the simple polykite ("hat" in Fig. 1) seemingly manages to avoid the simple repetition of translational symmetry. Henceforth, we shall call this tile the **Hat**.

A. The Hat Tile Continuum

The discovery of the hat was only a part of a bigger picture; it belonged to a continuous set of 14-sided polygons. This family of aperiodic shapes can be characterized by two positive integers $0 \leq a, b \leq 1$ which alternate over the 14 edges (see Fig. 2). Every shape of this set is thus denoted as $Tile(a, b)$, and their angles never change. Figure 1 illustrates a few significant members of the set. At the extremities, the "chevron" and "comet", along with the equilateral Tile(1,1), are the only members that admit periodic tilings. Now, while the hat's physical properties have previously been studied, other members of the family may also hold interesting properties.

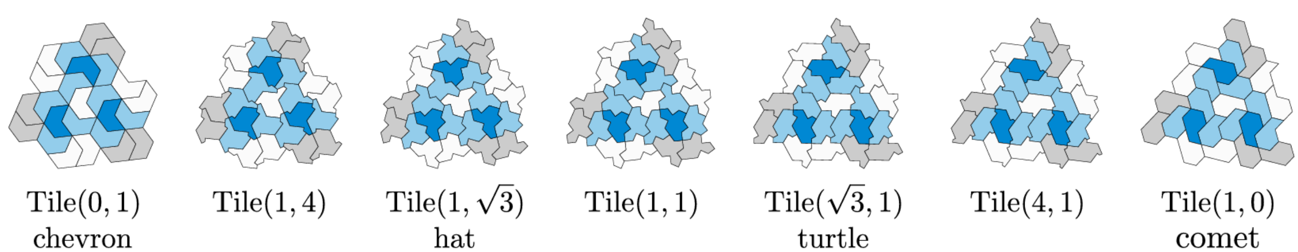


FIG. 1: Selected samples from the infinite aperiodic monotile set. In dark blue, an instance of the tile's reflection, each surrounded by a congruent "shell" of three of their unreflected counterpart (light blue). These clusters are an important feature of aperiodic monohedral tilings.

B. The Vampire Einstein Problem

The "vampire einstein problem" again requires aperiodic monohedral tiling over a plane, but with the added restriction of not using any tile reflections (like a vampire!). Under these new conditions, a small modification 2 to the previously mundane Tile(1,1) provides an aperiodic, homochiral monohedral tiling [4]. Simply put, homochirality is defined as uniform 'handedness' over a space, or the fact that no euclidean transformation can superpose mirrored images such as your left and right hands. By imposing an arbitrary curvature on Tile(1,1), we construct a new "Spectre" tile, which solves the vampire einstein problem.

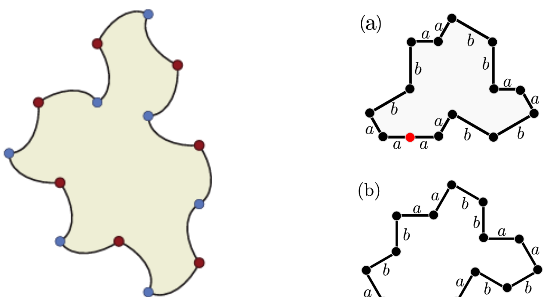


FIG. 2: Left: Modified equilateral Tile(1,1) called the "Spectre", with arbitrarily curved edges. It's ghostly resemblance is more apparent when rotated by -90°. **a)** Hat Tile$(1,\sqrt{3})$ with appropriate edge length. **b)** Pre-Spectre Tile(1,1) with obviously equilateral sides. The red circle indicates an additional vertex that occurs at the intersection of some neighbouring tiles. It also splits the $2a$ long side.

C. Proving Aperiodicity: Polykite Metatiles

Proving the aperiodicity of the einstein tiles is required if one wishes for tangible material applications. The general procedure here is to construct 4 distinct *metatiles*, from which the entire lattice is recursively constructed [2], [4], [3]. Figure 6 attached in Appendix A demonstrates each tile's respective inflation rule. Evaluating every possible neighbouring scheme has generalized these results for any tiling of the family, thus proving their aperiodicity [2].

III. STATEMENT OF ORIGINALITY

I hereby declare to be the sole author of this paper. The discovery of infinite aperiodic monotiles concludes a problem long thought to be unsolvable. Due to it's novelty, literature on this new form of quasi-crystalline lattice is limited. I strive to deepen our understanding of the new possibilities brought by this configuration. Any outsourced material presented in this paper has been properly credited through citations to the best of my knowledge. I would also like to thank Justin Schirmann for answering some of my questions, whose work inspired my own.

IV. ANALYSIS

The turtle's quasicrystal lattice is characterized by distinct spectral properties and fractal-adjacent features. Its aperiodic tiling was conveniently modeled using a tight binding vertex hamiltonian (1). We set the hopping energy $t = 1$ such that particles could hop to neighbouring sites with equal probability [3].

$$H_{Hat} = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + H.c \tag{1}$$

Here, the fermion annihilation and creation operators $(c^\dagger, c)$ iterate over all neighbouring pairs i, j. From this equation, I implemented a numerically equivalent tight binding replica using Kwant for Python 3.11.10 [5]. The code (See Appendix A) was derived from Schirmann *et al.* [6] and repurposed for the Turtle. I used the H8 inflation rules to construct the lattice from AppendixB Fig. 7. This is an equivalent, but more elegant, substitution scheme to those used in the proof (see II C). By observation, this 2D structure is reminiscent of a fractal. In fact, the Turtle's corresponding band structure in figure 3 consequently displays a fractal density of states (DOS), which is common for most quasi-crystals. Included in Fig. 3 is also the spectral function of 2nd inflation Turtle tiles, in juxtaposition with the Hat's own spectral analysis (from [3]).

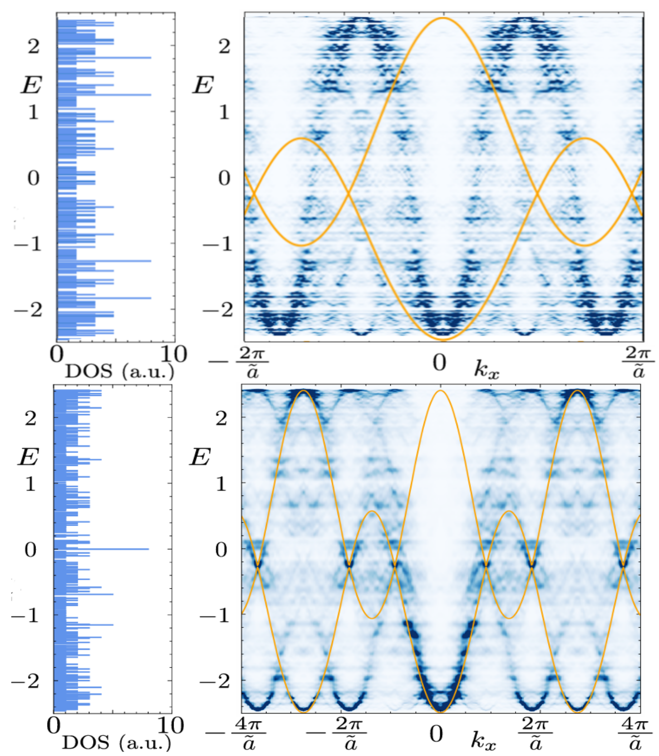
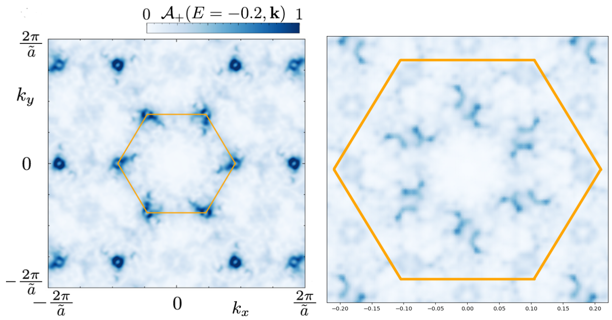


FIG. 3: Density of states and spectral functions of two aperiodic monotile lattices. **Top**: Turtle tiling spectral function with mismatch to graphene approximant (orange) over 1 brillouin zone. **Bottom**: Hat tiling over 2 brillouin zones displaying graphene like spectral diagram.

FIG. 4: K-space spectrum over 2D aperiodic monotile lattice. **Left**: Hat tiling with dark blue dirac points in a hexagonal shape. **Right**: Turtle tiling with rotational phase difference. Orange hexagon is plausibly wrong.



The investigation of infinite Turtle tiling also produced a plot of its 2D momentum space. Figure 4 presents a Turtle versus Hat comparison of their 2-dimensional spectral properties. All spectral data was calculated using the appropriate spectral formula 2:

$$A(E, \mathbf{k}) = \langle \mathbf{k} | \, \delta H_{Hat} - E \, | \mathbf{k} \rangle \, , \tag{2}$$

where $\mathbf{k}$ is the momentum vector for the required axis and E is on site energy [3]. I also provide an approximation to graphene's dispersion relation represented as an orange curve in the plots. Thus, a second nearest neighbour setup, equation 3, was used as an estimator of graphene like-properties.

$$E_{\pm}(\mathbf{k}) = \pm t_1 \sqrt{3 + f(\mathbf{k})} - t_2 f(\mathbf{k}) + \epsilon_0 \tag{3}$$

$$\text{where} \quad f(\mathbf{k}) = 2cos(\sqrt{3}k_x) + 4cos(\frac{\sqrt{3}k_x}{2})cos(\frac{\sqrt{3}k_y}{2})$$

In this case, we use parameters $(a_g, t_1, t_2, \epsilon_0) = (\frac{2a}{\sqrt{3}}, 0.82, -0.025, -0.2)$ where a_g is the graphene lattice constant, t_1 and t_2 are hopping constants and ϵ_0 is on-site energy offset. The values were taken from [3], tuned to match the Dirac nodelike features on the graphs. For sake of brevity, I shall focus on the spectral features in this paper, but propagation modes were similarly collected.

V. DISCUSSION

The lack of spectral correlation with the graphene approximant suggests that the Turtle based tiling does **not** exhibit graphene-like properties. Indeed, while the Hat's DOS features a peak at the 0 energy, the Turtles lack this feature. The absence of Dirac cones in fig. 3(a) furthermore enforces this difference in properties. Thus, the massless fermions responsible for graphene's exotic behaviour cannot exist in the investigated configuration. This is surprising, as the turtle tile is simply the inverse parametrization of the hat: $Tile(a = 1, b = \sqrt{3}) \xrightarrow{\text{Invert}} Tile(b, a)$. This means that an underlying hexagonal sublattice is less prominent in the Turtle tiling, whereas "≈ 53% of Hat vertices are captured by a [corresponding] sublattice" [3].

Nonetheless, we can draw some interesting conclusions from the k-space analysis of figure 5(b), where a somewhat complementary structure arises. Even though the 14-sided Turtle polykite was established to be minimally related to its honeycomb sublattice, hexagon outlines are still recovered in its 2D momentum spectrum. Moreover, there seems to be a phase shift of ≈ 30 with respect to the clearly defined Dirac points of the Hat lattice. In fact, spectral weight is mostly concentrated in between Dirac sites of the inverse tiling. This may point to increased connectivity between tiles, instead of topological insulation like Dirac points. Returning to the density of states distribution, Turtle tilings appear characteristically disordered. This structure, or lack thereof, suggests a fractal DOS with many Van Hove singularities. Such singularities indicate sharp kinks in band structure and enhance electric correlation near said peaks. Here, fig. 3(a) exhibits extreme variations at higher absolute energies, which could promote unconventional states of matter such as superconductivity.

VI. CONCLUSION

Although not graphene-like, the properties of the Turtle tiling remain promising. The prospect of quasi-lattice superconductivity is rather convincing, since aperiodicity is the same mechanism through which moire pattern materials generate their exotic properties [7]. Nonetheless, there seems to be a glaring issue with the generated graphene approximants (for the Turtle tiles only), which seem to be out of phase or unsuitable for the presented datasets. It may be fruitful to revisit the parameters given in [3], since they were carefully selected for the hats and are possibly incompatible with turtle tiling. Moreover, deeper analysis could be conducted on larger simulations, but cluster computing will be necessary due to the greater computational demand [8]. Other configurations, such as purposefully hexagonal assemblies in fig. 5, promise enticing motivations to continue research on the set of aperiodic monotiles. In essence and spirit, these early discoveries pave the way for an entirely new branch of condensed matter, one which harnesses chaos at a molecular scale.

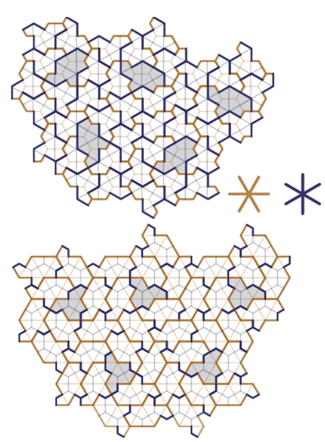


FIG. 5: Underlying hexagonal lattice of hat/turtle tiling combinations. Notice the 30° tilt between top (hat dominated) and bottom (turtle dominated) reappearing in this system.

VII. APPENDIX

Appendix A: Metatiles

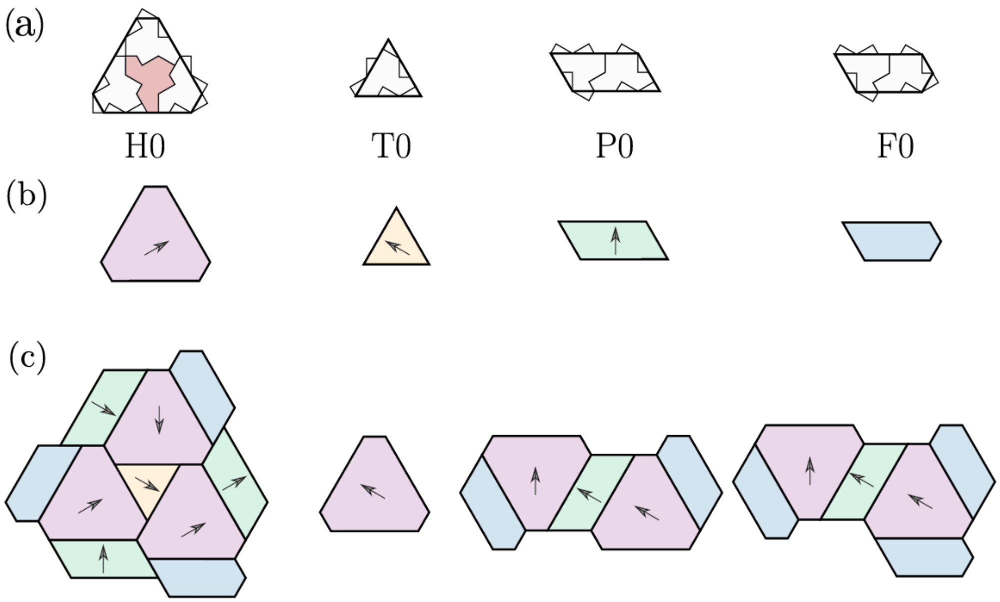


FIG. 6: "Inflation rules **(a)** The four initial metatiles (from left to right) $H0$, $T0$, $P0$ and $F0$ with $H0 = 4$ $T0 = 1$ $P0 = 2$ and $F0 = 2$ hat tiles, respectively. **(b)** We assign to each of the metatiles an orientation. **(c)** In ation rules, at each step of the process, the metatiles are combined respecting the orientation constraints. Finaly, we replace the metatiles by the corresponding patches of hats." [3]

Appendix B: H8 inflation rules and substitution sequence

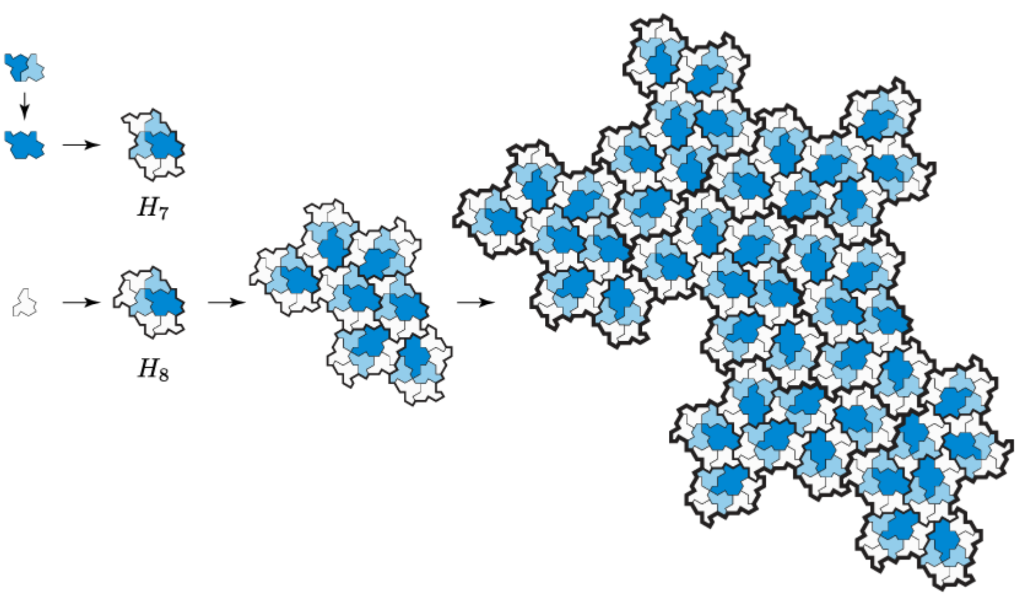


FIG. 7: H8 inflation rule, forming a fractal shape from an initial single Hat monotile. Similar procedures can be followed for other tiles in the set.

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[2] D. Smith, J. S. Myers, C. S. Kaplan, and C. Goodman-Strauss, An aperiodic monotile, Combinatorial Theory **4**, 10.5070/c64163843 (2024).
[3] J. Schirmann, S. Franca, F. Flicker, and A. G. Grushin, Physical properties of an aperiodic monotile with graphene-like features, chirality, and zero modes, Phys. Rev. Lett. **132**, 086402 (2024).
[4] D. Smith, J. S. Myers, C. S. Kaplan, and C. Goodman-Strauss, A chiral aperiodic monotile, Combinatorial Theory **4**, 10.5070/c64264241 (2024).
[5] C. W. Groth, M. Wimmer, A. R. Akhmerov, X. Waintal, Kwant: a software package for quantum transport.
[6] F. F. A. G. J. Schirmann, S. Franca, Code: Physical properties of the hat aperiodic monotile: Graphene-like features, chirality and zero-modes.
[7] P. Peng, Y. Peng, A. Shi, X. Yi, Y. Wei, and J. Liu, Aperiodic-quasiperiodic-periodic properties and topological transitions in twisted nested moiré patterns (2024), arXiv:2401.15849 [cond-mat.mes-hall].
[8] As of now, I have been waiting for ≥ 72 hours for a 4 expansion k-space diagram, but it has yet to come. This is part of the reason for my late submission, but I have already committed too far to give up now. This is an example of the gambler's fallacy. Hopefully, I will one day update this paper with proper graphs.