Complexities for High-Temperature Two-Handed Tile Self-Assembly*

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Abstract. Tile self-assembly is a formal model of computation capturing DNA-based nanoscale systems. Here we consider the popular *two-handed tile self-assembly model* or *2HAM*. Each 2HAM system includes a *temperature* parameter, which determines the threshold of bonding strength required for two assemblies to attach. Unlike most prior study, we consider general temperatures not limited to small, constant values. We obtain two results. First, we prove that the computational complexity of determining whether a given tile system uniquely assembles a given assembly is coNP-complete, confirming a conjecture of Cannon et al. (2013). Second, we prove that larger temperature values decrease the minimum number of tile types needed to assemble some shapes. In particular, for any temperature $\tau \in \{3, \dots\}$, we give a class of shapes of size n such that the ratio of the minimum number of tiles needed to assemble these shapes at temperature τ and any temperature less than τ is $\Omega(n^{1/(2\tau+2)})$.

1 Introduction

This work considers problems in a variation of *DNA tile self-assembly*, an approach for precise control of nanoscale structures that uses DNA base-pair interactions between four-sided DNA molecules first introduced by Seeman [23] and formalized by Winfree [27] as the mathematical *abstract Tile Assembly Model* or *aTAM*.

The wide range of complex and useful behaviors of the aTAM has since been established, including the model's ability to execute any algorithm [27] and assemble desired shapes using few tile types [2, 20, 25]. Since then, dozens of tile assembly models sharing traits with the aTAM have been studied, even giving rise to a structural complexity theory for tile assembly models [28].

Two-handed assembly. One of the most popular models of tile self-assembly is the *two-handed tile assembly model (2HAM)* [1, 4, 11, 19], also referred to the *hierarchical* [5, 9] or *polyomino* [15] model. The 2HAM differs from the original aTAM in its lack of a "seed": in the aTAM, assembly is limited to single-tile

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addition to a growing seed assembly, while in the 2HAM, assembly may occur by attachment of *any* two assemblies via bonds of sufficient strength. The difficulty of experimentally enforcing seeded assembly [21] motivates the study of the 2HAM.

Temperature. A recurring question in many model variations, including the 2HAM, is the importance of *temperature*: the threshold of bonding strength needed for attachment between assemblies. A long-standing open problem in tile assembly concerns the capabilities of systems at the lowest temperature, where one bond suffices for attachment [12, 16–18]. Dynamically varied temperature has also been studied as a mechanism for guiding assembly [14, 26].

In the aTAM, systems at higher temperatures exhibit a greater range of *dynamics*: behaviors that occur during the assembly process [6], and these additional behaviors can be used to reduce the *tile complexity* of some shapes: the number of tile types needed to assemble the shape [24]. On the other hand, if scaling (replacement of each tile by a square block of tiles) is permitted, then these additional dynamics (and corresponding reductions in tile complexity) can be recreated or *simulated* by lower temperature systems [10]. In contrast, higher temperature 2HAM systems exhibit additional dynamics that cannot be simulated by lower temperature 2HAM systems [8].

Our results. This work considers whether the additional dynamics in higher temperature 2HAM systems confer additional capabilities. We prove two results, one complexity theoretic and the other combinatorial, that give positive evidence.

The first result (Section 3) affirms a conjecture from 2013 [4] regarding the complexity of *verifying* that a system yields a unique specified terminal assembly. The proof critically uses high-temperature dynamics to demonstrate that such verification is coNP-hard.

The second result (Section 4) proves that for some shapes, higher temperatures yield more efficient assembly. Specifically, the ratio between the tile complexities of some shapes at temperature τ and any lower temperature is polynomial in the shape size. Seki and Ukuno [24] achieved a similar result in the aTAM, but for only a constant additive gap in tile complexity.

2 Definitions

Here we give a presentation of the two-handed tile assembly model (2HAM) and associated definitions used throughout the paper.

2.1 Tiles and assemblies

Tiles. A tile is an axis-aligned unit square centered at a point in $\mathbb{Z}^2$, where each edge is labeled by a *glue* selected from a glue set Π. A *strength function* $\mathrm{str} : \Pi \rightarrow \mathbb{N}$ denotes the *strength* of each glue. Two tiles that are equal up to translation have the same *type*.

Assemblies. A *positioned shape* is any subset of $\mathbb{Z}^2$. A *positioned assembly* is a set of tiles at unique coordinates in $\mathbb{Z}^2$, and the positioned shape of a positioned assembly A is the set of coordinates of those tiles.

For a given positioned assembly Υ, define the *bond graph* G_Υ to be the weighted grid graph in which each tile of Υ is a vertex and the weight of an edge between tiles is the strength of the matching coincident glues or 0.[1] A positioned assembly C is said to be *τ-stable* for positive integer τ provided the bond graph G_C has minimum edge cut at least τ.

For a positioned assembly A and integer vector $\boldsymbol{v} = (v_1, v_2)$, let $A_{\boldsymbol{v}}$ denote the assembly obtained by translating each tile in A by vector $\boldsymbol{v}$. An *assembly* is a set of all translations $A_{\boldsymbol{v}}$ of a positioned assembly A. A *shape* is the set of all integer translations for some subset of $\mathbb{Z}^2$, and the shape of an assembly A is the shape consisting of the set of all the positioned shapes of all positioned assemblies in A. The *size* of either an assembly or shape X, denoted as $|X|$, refers to the number of elements of any positioned element of X.

Combinable Assemblies. Informally, two assemblies are *τ-combinable* provided they may attach to form a τ-stable assembly. Formally, two assemblies A and B are *τ-combinable* into an assembly C provided there exists $A' \in A$ and $B' \in B$ such that $A' \bigcup B'$ is a τ-stable element of C.

2.2 Two-handed tile assembly model (2HAM)

A *two-handed tile assembly system (2HAM system)* is an ordered pair (T, τ) where T is a set of single tile assemblies, called the *tile set*, and $\tau \in \mathbb{N}$ is the *temperature*. Assembly proceeds by repeated combination of assembly pairs to form new τ-stable assemblies, starting with single-tile assemblies. The *producible assemblies* are those constructed in this way. Formally:

Definition 1 (2HAM producibility). *For a given 2HAM system $\Gamma = (T, \tau)$, the set of* producible assemblies *of Γ, denoted $\mathtt{PROD}_\Gamma$, is defined recursively:*

- *(Base) $T \subseteq \mathtt{PROD}_\Gamma$*
- *(Recursion) For any $A, B \in \mathtt{PROD}_\Gamma$ such that A and B are τ-combinable into C, then $C \in \mathtt{PROD}_\Gamma$.*

For a system $\Gamma = (T, \tau)$, we say $A \rightarrow_1^\Gamma B$ for assemblies A and B if A is τ-combinable with some producible assembly to form B, or if $A = B$. Intuitively this means that A may grow into assembly B through one or fewer combination reactions. We define the relation $\rightarrow^\Gamma$ to be the transitive closure of $\rightarrow_1^\Gamma$, i.e., $A \rightarrow^\Gamma B$ means that A may grow into B threw a sequence of combination reactions.

[1] Note that only matching glues have positive strength. The more general model of "flexible glues" where non-matching glue pairs may also have positive strength has been considered [7].

Definition 2 (Terminal assemblies). *A producible assembly A of a 2HAM system $\Gamma = (T, \tau)$ is* terminal *provided A is not τ-combinable with any producible assembly of Γ.*

Definition 3 (Unique assembly). *A 2HAM system* uniquely assembles *an assembly A if for all $B \in \mathtt{PROD}_\Gamma$, $B \rightarrow^\Gamma A$.*

3 Unique Assembly Verification in the 2HAM is coNP-Complete

Definition 4 (Unique assembly verification (UAV) problem). *Given a 2HAM system Γ and assembly A, does Γ uniquely assemble A?*

Adleman et al. [3] proved that the UAV problem in the aTAM is in P. Cannon et al. [4] first considered the UAV problem in the 2HAM. They proved that the problem is in coNP and conjectured that the problem is coNP-hard, suggested by their proof of the same result for an extension of the model to three dimensions (with cubic tiles). Here we confirm their conjecture, using high temperature to overcome previous planarity "barriers".

Theorem 1. *The UAV problem is* coNP*-complete.*

The reduction is from a problem involving *grid graphs*: graphs whose vertices are a subset of $\mathbb{Z}^2$ and two vertices are connected by an (undirected) edge if they have distance 1. Itai, Papadimitriou, and Szwarcfiter [13] proved that the following problem is NP-hard:

Definition 5 (Hamiltonian cycle problem in grid graphs). *Given a grid graph G, does G contain a Hamiltonian cycle?*

We reduce from the complement of this problem.

Lemma 1. *The UAV problem in the 2HAM is* coNP*-hard.*

Proof. Consider a grid graph $G = (V, E)$. From G we construct a tile system Γ_G and an assembly A_G such that Γ_G uniquely assembles A_G if an only if G has no Hamiltonian cycle. Without loss of generality, assume the leftmost and rightmost vertices of G have x-values 0 and n, and the bottommost and topmost vertices have y-values 0 and m, respectively. Construct a tile set T_G from G as described in Figure 1 to yield the system $\Gamma_G = (T_G, \tau = |V|)$.

The system Γ_G has a terminal assembly A_G consisting of a $2(n+1) \times 2(m+1)$ block of blue tiles connected to a $2(n-1) \times 2(m-1)$ block of red tiles, as shown in Figure 2. We also claim that this is the unique terminal assembly of Γ_G if and only if G has no Hamiltonian cycle.

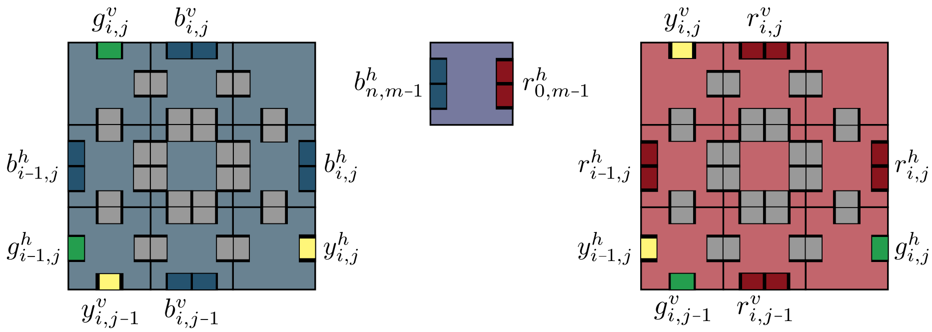


Fig. 1. This tileset consists of a collection of 3×3 blocks and a single connector tile. The center tile of each 3×3 block has bond strength of τ with its four neighbors. Each corner tile bonds to its horizontal and vertical neighbors with $\lceil \tau/2 \rceil$, $\lfloor \tau/2 \rfloor$ strength, respectively. A blue block is constructed for every location in $\{0, \ldots, n\} \times \{0, \ldots, m\}$, and a red block is constructed for locations in $\{1, \ldots, n-1\} \times \{1, \ldots, m-1\}$. Red and blue glues have strength τ, while green and yellow glues have strength 1 or 0 as determined by the grid graph: $g^h_{i,j}$ and $y^h_{i,j}$ have strength 1 if (i, j) and $(i, j-1)$ are vertices in G and strength 0 otherwise. The glues $g^v_{i,j}$ and $y^v_{i,j}$ have strength 1 when (i, j) and $(i-1, j)$ are vertices in G and strength 0 otherwise.

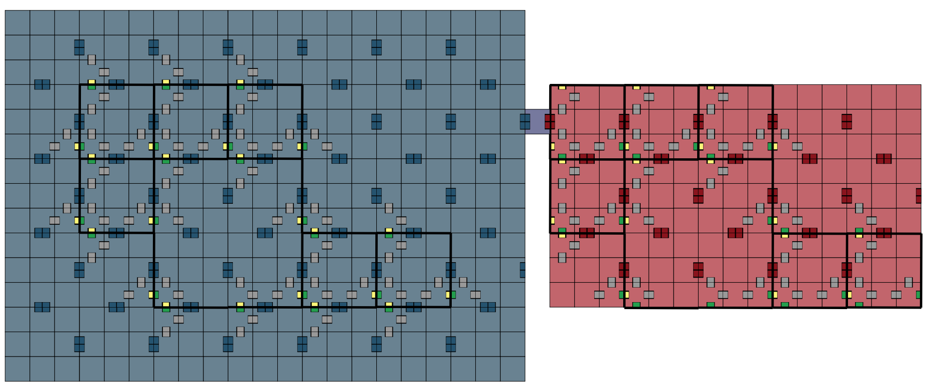


Fig. 2. For a given grid graph, the following assembly is the unique terminal assembly if and only if no Hamiltonian cycle exists.

Correctness: G has cycle $\Rightarrow$ No unique terminal assembly. Suppose G has a Hamiltonian cycle. Then there exists a producible assembly C_{inner} of red 3×3 blocks corresponding to the interior of the cycle. By design, C_{inner} has exactly $\tau = |V|$ yellow and green glues exposed. Similarly, there exists a producible assembly C_{outer} of blue 3×3 blocks corresponding to the exterior of the cycle with $\tau = |V|$ yellow and green glues in the same relative locations as those of C_{inner}. At temperature τ, C_{inner} and C_{outer} attach to form a large assembly that is *not* a subassembly of the previously described terminal assembly. See Figure 3 for such a pair combinable C_{inner} and C_{outer} and the grid graph they correspond to.

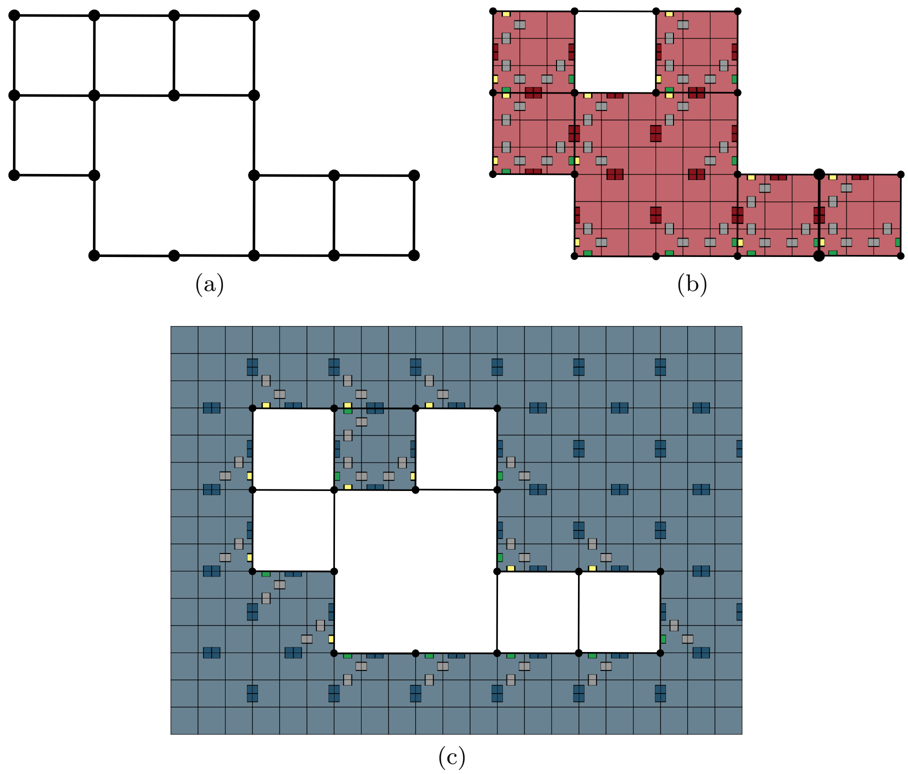


Fig. 3. (a) The input graph for the example reduction. If a Hamiltonian cycle exists, then the producible assemblies consisting of C_{outer} (c), the exterior of the cycle, and C_{inner} (b), the interior of the cycle, are combinable with exactly τ strength.

Correctness: No unique terminal assembly $\Rightarrow$ G has cycle. Now suppose that $\Gamma_G = (T_G, \tau = |V|)$ does not have a unique assembly, ie, there exists some producible assembly X that cannot assemble further into A_G (equivalently, is not a subassembly of A_G. The existence of X implies that there exists some producible assembly R, consisting of red blocks, that is attachable to a producible assembly of blue blocks by way of τ or more green and yellow glues. We first use R to construct a second "cleaned-up" producible assembly R' that is also attachable to a producible assembly of blue blocks. We then show that R' implies a Hamiltonian cycle determined by its shape.

Consider modifying the assembly R in the following way. First, if R contains the center tile for any 3×3 block of red tiles, add all missing tiles of the corresponding block. Second, for all other blocks, remove all tiles of this block from R. Call the resulting assembly of completed 3×3 blocks R'.

The assembly R' has the following properties. First, R' is producible. In particular, the removal of tiles from R as specified cannot disconnect the assembly. Second, R' may attach to a producible blue assembly by way of yellow and green glues summing to at least τ. This is the case because:

- No tile removed from R to yield R' is a corner tile of a block, since the presence of any corner tile of a block in a producible assembly implies that the assembly also contains the center tile of the block (and so R' contains all tiles from such a block if R contained any corner tile of the block).
- Any exposed green or yellow glue of R used to attach to a blue assembly remains an exposed glue in R', as any such glue is adjacent to a 3×3 block containing a blue (not red) center tile and so cannot be "covered" by the addition of tiles to R to create R'.

We now use R', an assembly that is producible and combinable with a blue assembly through yellow and green glues, to generate a Hamiltonian cycle in G. Consider the polyomino consisting of the collection of faces of G corresponding to each 3×3 block in R'. Starting at some arbitrary corner of this polyomino, walk its perimeter to generate a sequence of distinct points $p_0, \ldots p_{r-1}$. Each consecutive pair are adjacent in G, but points may or may not be in V.

For each consecutive pair $p_i, p_{(i+1) \bmod r} \in V$, the assembly R' exposes exactly 1 green or yellow glue on the side of the corresponding 3×3 block. On the other hand, for any consecutive pair with either point not in V, no green or yellow glues are exposed. Then since no location repeats and the total number of green and yellow glues must sum to at least τ (for attachment to a blue assembly), the sequence must be a length-V permutation of V where consecutive points are adjacent (and thus share an edge), implying that this permutation is a Hamiltonian cycle of G. □

4 Tile Complexity Gaps between Temperatures

The *tile complexity* of a shape S at temperature τ is the minimum number of tile types in a 2HAM system at temperature τ that uniquely assembles S. The *tile complexity gap* of a shape S between two temperatures τ_1 and τ_2 is the ratio of the minimum number of tile types in 2HAM systems at temperatures τ_1 and τ_2 that uniquely assemble S. Here we give, for any distinct pair of temperatures, an infinite family of shapes with large tile complexity gap at these temperatures.

We start by describing the construction for the special case of $\tau_1 = 2$ and $\tau_2 = 3$, shown in Figure 5. The shapes each consist of a base rectangle and all gadgets of the form shown in Figure 4 for some integer $m \geq 3$.

The gadget has three horizontal *sections* with m locations where the vertical bar connects with the base. At most m tiles are used for the left and right vertical column ($2m$ for the center column), and the height difference between any two of the three horizontal sections is at most $2m - 1$. There are m^6 different gadgets, since each section has m^2 possible column locations.

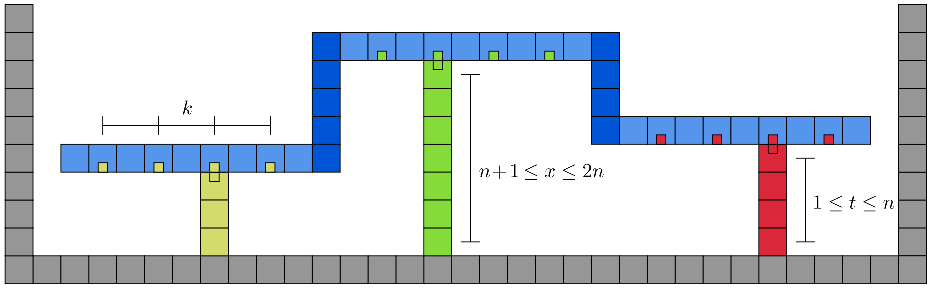


Fig. 4. A single gadget on the shape with m possible glue locations and m possible heights for each vertical bar. Note the spacing between horizontal glues ensures that the "hat" can not attach to the shape shifted because of the walls.

Theorem 2. *There exists a shape of size* n *with a tile complexity gap of* $\Omega((\frac{n}{\log n})^{1/7})$ *between* $\tau = 2$ *and* $\tau = 3$.

Proof. Since there are $\Theta(m^6)$ possible gadgets, and each gadget is $\Theta(m)$ tiles in width, the width of the shape is $\Theta(m^7)$ tiles. The base rectangle of the shape is a $\Theta(\log m) \times \Theta(m^7)$ rectangle requiring $\Theta(\log m)$ tile types. Thus, the shape contains $\Theta(m^7 \log m)$ total tiles.

The remainder of the proof is dedicated to proving that (1) the shape can be assembled at $\tau = 3$ using $O(m)$ tile types, and (2) requires $\Omega(m^2)$ tile types at $\tau = 2$. Thus the tile complexity gap is $\Omega(m)$. Since the size of S is $n = \Theta(m^7 \log m)$, $\Omega(m) = \Omega((\frac{n}{\log n})^{1/7})$.

The tile complexity at $\tau = 3$ *is* $O(m)$. All hat assembly can be assembled using the same $O(m)$ tile types at $\tau = 3$ as follows. Each of the three horizontal sections is built deterministically with m strength-1 glues exposed on the south side. The two vertical columns connecting the sections are assembled nondeterministically and may have any length from 2 to $2m$. This means every possible configuration is built ($4m^2$ hats). The three columns are seeded from the base and expose a strength-1 glue matching their respective section.

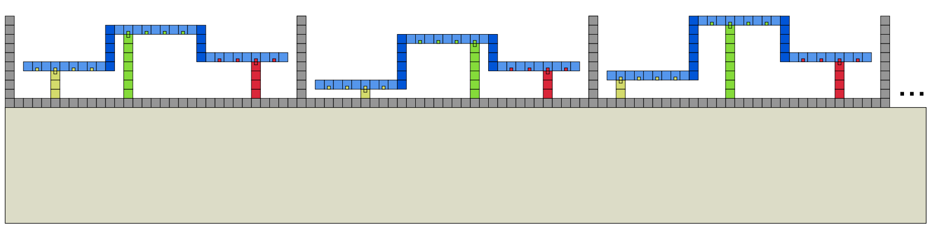


Fig. 5. The terminal assembly shape which consists of a rectangle used to seed all possible gadgets to attach to the top.

The hat can only attach if all three glues can match (columns and hat sections). The tiles for constructing the hat piece are shown in Figure 6. Note the spacing tiles in between each horizontal glue tile to ensure that the hat attaches without shifting left or right (because of the enclosing walls). Such gadgets can be assembled from $3(2m+1)$ tile types for the horizontal sections, and $2(4m-2)$ tile types for the vertical connecting strips. The columns from the base use $4m$ tiles. Since we use these same tiles for every gadget, the tile complexity is $\Theta(m)$.

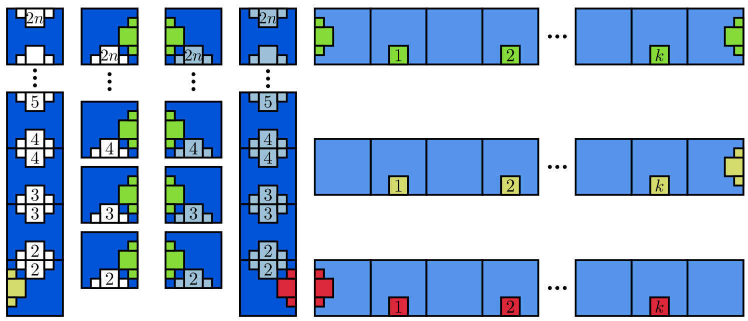


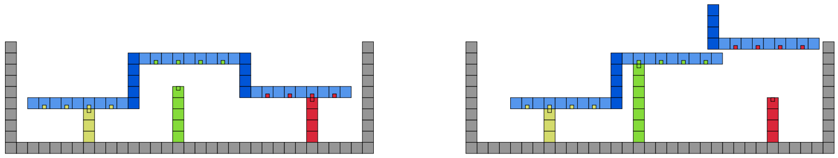
Fig. 6. Building the "hat" for the gadget nondeterministically. The single blocks represent a strength 1 bond and the three blocks a strength-3 bond.

The tile complexity at $\tau = 2$ is $\Omega(m^2)$. Assembling the hat using few tiles at $\tau = 2$ is difficult because only 2 of the 3 columns can ever be necessary for attachment. Since the hat is built before attaching to the three columns, the situation in Figure 7(a) may occur, or similar situations with one of the other two columns not attached. Since hat attaches in multiple parts, then the situation in Figure 7(b) may occur, or a similar situation with some parts translated. Thus the same tile set cannot be used for the hats in all gadgets.

Thus each section must be assembled with only one south glue placed in the correct tile where the column attaches. Then m versions of that gadget are built (for each column attachment location) so that the section with glue g_i, where $1 \leq i \leq m$, exposed can attach whenever glue g_i is open on one of the columns. In order for the section piece to not attach shifted (Figure 7(b)), the column must expose a corresponding glue for that horizontal position. This means for each horizontal position, we need m distinct deterministic tiles so that we can expose the correct g_i glue at the top of the column to attach the correct section without it being shifted. Thus, $\Omega(m^2)$ tile types are required. □

Theorem 3. *For any $\tau_1, \tau_2 \in \{2, 3, \dots\}$ with $\tau_1 < \tau_2$, there exists a shape of size n with tile complexity gap $\Omega(n^{1/(2\tau_2+2)})$ between τ_1 and τ_2.*

Proof. This follows from a similar analysis as the proof of Theorem 2. Since there are τ_2 sections of the hat piece, then there are $\Theta(m^{2\tau_2})$ gadgets, each of width



(a) (b)

Fig. 7. (a) Strength-1 glues at $\tau = 2$ cannot be used, otherwise the hat may attach to the wrong gadget. (b) The hat can not be attached in separate pieces if the sections are the same for each gadget, since it may also attach shifted, and thus the walls prevent the rest of the hat from attaching.

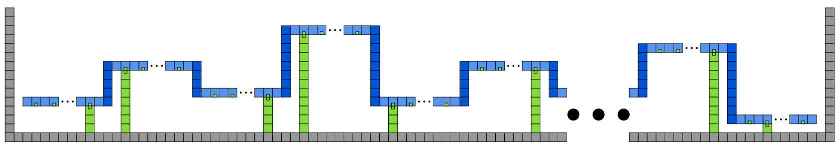


Fig. 8. Generalizing the shape for any τ by utilizing τ hats with τ glues per section.

$\Theta(\tau_2 m)$. So the width of the shape is $\Theta(\tau_2 m^{2\tau_2+1})$, and the size of the shape is $n = \Theta(m^{1/(2\tau_2+1)} \log \tau_2 m)$. Following the same argument as given in the proof of Theorem 2, $\Omega(m^2)$ tile types are needed to assemble the gadget correctly for any $\tau_1 < \tau_2$. ◻

5 Conclusion

There are a number of interesting directions to extend this work. First, while we have shown the UAV problem is coNP-complete, our reduction requires temperature to scale linearly in the assembly size. Since many systems of interest have small, and even constant temperature, we ask: does coNP-hardness hold for constant, or even logarithmic temperatures? When the model is extended to 3D, the answer is "Yes" for temperature $\tau = 2$ [4].

Our coNP-completeness result also pairs well with other recent results on verification problems in two-handed models of verification. For instance, that the *unique shape verification* or *USV problem* is $\mathsf{coNP}^{\mathsf{NP}}$-complete [22]. Similarly, in the more powerful *staged assembly model*, the UAV and USV problems are $\mathsf{coNP}^{\mathsf{NP}}$-hard and in PSPACE [22]. In this case, $\mathsf{coNP}^{\mathsf{NP}}$-hardness is known to hold even for $\tau = 2$ and constant stages and bins (additional complexity measures in the staged model), but characterizing the complexity as a function of the number of stages remains open.

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