

Turning Machines

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Abstract

Molecular robotics is challenging, so it seems best to keep it simple. We consider an abstract molecular robotics model based on simple folding instructions that execute asynchronously. Turning Machines are a simple 1D to 2D folding model, also easily generalisable to 2D to 3D folding. A Turning Machine starts out as a line of connected monomers in the discrete plane, each with an associated turning number. A monomer turns relative to its neighbours, executing a unit-distance translation that drags other monomers along with it, and through collective motion the initial set of monomers eventually folds into a programmed shape. We fully characterise the ability of Turning Machines to execute line rotations, and to do so efficiently: computing an almost-full line rotation of $5\pi/3$ radians is possible, yet a full 2π rotation is impossible. We show that such line-rotations represent a fundamental primitive in the model, by using them to efficiently and asynchronously fold arbitrarily large zig-zag-rastered squares and y -monotone shapes.

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1 Introduction

The challenge of building molecular robots has many moving parts, as the saying goes. These include molecular parts that move relative to each other; units needing some sort of memory state; the ability to transition between states; and perhaps even the ability to use computation to drive robotic movements. Here we consider a simple robotic model of reconfiguration called Turning Machines.



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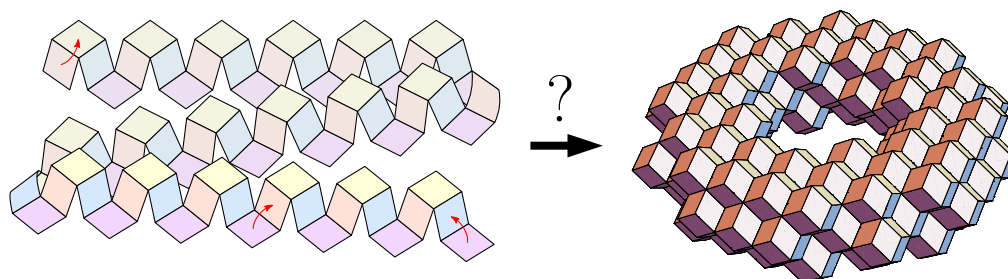
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■ **Figure 1** Turning Machine motivation: what shapes can be made by autonomously folding structures using simple local turning rules that effect non-local movement? Finding suitable abstract models and characterising their ability helps us to step back and create a vision of where we can go.

The main ethos behind our work is the notion of having a reconfigurable structure where component monomers actuate their position relative to their neighbours and governed by *simple* actuation rules. Volume exclusion applies (two monomers can not occupy the same position in space), almost for free we get massive parallelism and asynchronicity, and the complexity of allowable state changes is small: start with a natural number and decrement step-by-step to zero. The Turning Machine model embodies these concepts.

On the one hand, there are a number of senses in which molecular systems are *better* suited to robotic-style reconfiguration than macro-scale robotic systems: there is no gravity nor friction fighting against components' actuation, and should we know how to exploit them, randomness, freely diffusing fuel (robots need not carry all their fuel) and large numbers of components are all readily available as resources. On the other hand, building nanoscale components presents a number of challenges including implementing computational controllers at the nanoscale, as well as designing systems that self-assemble and interact in a regime where we can not easily send in human mechanics to diagnose and fix problems.

1.1 Turning machines

Monomers are the atomic components of a Turning machine and are arranged in a connected chain on the triangular/hexagonal grid, with each monomer along the chain pointing at the next. In an initial instance, the chain of monomers are sitting on the x -axis all pointing to the east. Each monomer has an initial integer turning number $s \in \mathbb{Z}$, the monomer's ultimate goal is to set that number to 0: if s is positive, the monomer tries to simultaneously decrement s and turn anti/counter-clockwise¹ by an angle of $\pi/3$, if s is negative, it tries to increment and turn clockwise by $\pi/3$.² If $s = 0$ the monomer has reached its target orientation and does not turn again. Figures 2 and 3 give the idea, and Section 2 gives a full definition.

A key point is that although a monomer actuates by rotating the direction in which it points, when it does so it “drags” (translates) all monomers that come after it in the chain in the same way the rotation motion of an arm (around a shoulder) appears to translate a flag through the air, or the way a cam in an combustion engine converts rotational shaft motion to translational piston motion.

¹ We define counter-clockwise to be anticlockwise and use these terms interchangeably.

² Having the monomer turning angle be confined to the range $(0, \pi/2]$ seems to capture a range of interesting and important blocking behaviours that would otherwise be missed by the model. Having the angle be $\pi/3$, which leads us to the choice of triangular grid over the square grid, is a somewhat arbitrary choice in the model definition.

1.2 Turning machines: the main programming challenge

Programming the model simply requires annotating an east-pointing line of monomers with turning numbers; an incredibly simple programming syntax.

Locally, individual monomers exhibit a small rotation, but globally this effects a large translation, or dragging, of many monomers. Thus globally, the main challenge is how to effect global rotations – in other words how to use translation to simulate rotation. In particular, how to do this when lots of monomers are asynchronously moving and bumping into each other, potentially blocking each other from moving.

Blocking comes in two forms. *Temporary blocking* where one monomer is in the way of another, but eventually will get out of the way, and *permanent blocking* where all monomers block each other in a locked configuration that will never free itself. We say that a target structure is foldable if all possible system trajectories lead to that structure, i.e. permanent blocking does not occur. A foldable structure may exhibit temporary blocking on some trajectories, indeed most of the work for our positive results in this paper comes down to showing that for certain folding tasks any blockings that happen are merely temporary kinks in the chain that are eventually worked out. We measure the amount of blocking by considering the completion time: a foldable structure where temporarily blocked monomers can quickly become unblocked finishes faster than one where blocking takes a while to sort out. Our model of time assumes that the time to apply a turning rule to a given unblocked monomer is an exponential random variable with rate 1, and the system evolves as a continuous time Markov chain with the discrete events being rules applied asynchronously and in parallel.

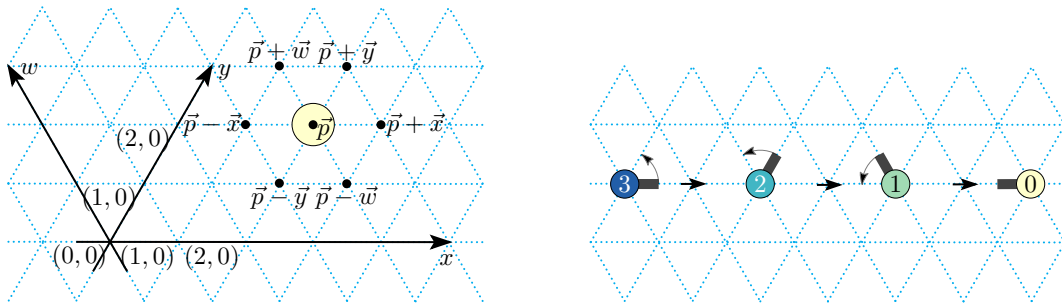
1.3 Results

We fully characterise the line rotation capability of the Turning Machine model, in two senses. First, we show that for each of the angles $\theta \in \{\pi/3, 2\pi/3, \pi, 4\pi/3, 5\pi/3\}$, and any number of monomers $n \in \mathbb{N}$ there is a Turning Machine with n monomers that starts on the x -axis and ends rotated by θ radians. We show this is the best one can do, that is, that rotation of $\theta \geq 2\pi$ is impossible (for any $n > 7$, there are always some trajectories that are permanently blocked). Second, line rotation is fast. Up to constant factors the speed is optimal, completing in expected time $O(\log n)$. This shows that despite the fact that line rotations in the range $\pi \leq \theta \leq 5\pi/3$ experience large number of blockings along their trajectories, these blockings are all temporary, and do not conspire to slow the system down by more than a constant factor on average.

To illustrate that line rotation results are indeed a fundamental primitive in the model, as an application, we show how to fold any $n \times n$ square, rastered in a zig-zag fashion (Theorem 17). More generally, this allows us to fold any shape from a wide class called y -monotone shapes (see Figure 9), all in optimal expected time $O(\log n)$.

1.4 Related and future work

Besides finding insights at the interface of computation and geometry, another ultimate aim of this kind of work is bridge the gap between what we can imagine in theory and what we can engineer in the lab [19]. Biological systems actuated at the molecular scale provide inspiration: in the gastrulation phase of embryonic development of the model organism *Drosophila melanogaster*, large-scale rearrangements of the embryo are effected by thousands of (nanoscale) molecular motors working together to rapidly push and pull the embryo into a target shape [9, 17].



■ **Figure 2** Turning machine model. Left: Triangular grid conventions. A configuration showing a single monomer on the triangular grid, along with axes x , y and w . Right: A monomer in state 3 pointing to the east undergoes three turning rule applications finishing in state 0 and no more rules are applicable. Locally, the monomer effects a rotation motion, subsequent figures show the induced global translational, or dragging, motion.

Our Turning Machine model is a restriction of the nubot model [20], a molecular robotic model with many features including self-assembly capabilities, random agitation (jiggling) of monomers, the ability to execute cellular automata style rules, and floppy/rigid molecular bonds. The parallel computing capabilities [4], and construction using random agitation and self-assembly [3] have been studied. Dabby and Chen consider related (experimental and theoretical) systems that use an insertion primitive to quickly grow long (possibly floppy) linear structures [8], later tightly characterised by Hescott, Malchik and Winslow [15, 14] in terms of number of monomer types and time. Hou and Chen [16] show that the nubot model can display exponential growth without needing to exploit state changes. Chin, Tsai and Chen [6] look at both minimising numbers of state changes and number of ‘2D layers’ to assembly 1D structures. There are a number related autonomous self-folding models, both 1D to 2D [5] and 2D to 3D [7], and reconfigurable robotic/programmable matter systems, e.g. [1, 2, 10, 11, 12, 18].

There are several avenues for future work. In this paper, we study model instances with natural number states, leading to anti-clockwise rotation motion (that is, anti-clockwise translation about the origin). Does the combination of clockwise and anti-clockwise turning rules increase the expressivity of the model? Using a variant [20, 3] of the model with random agitation of monomers would side-step our main negative result about the impossibility of full 2π line rotation by allowing reversible movement out of blocked configurations. Indeed, the analysis of such systems would provide intellectual fruit by mixing probability, geometry and computation. As indicated in Figure 1, it is straightforward to generalise the model to (say) 2D trees folding into 3D shapes, this provides an interesting avenue for exploration. In all of these cases fully characterising the class of shapes that can be folded, and characterising the time to fold such classes of structures, provides a number of questions whose answers would expand our understanding of the capabilities of simple reconfigurable robotic systems.

2 Turning machine model definition

In this section we define the Turning Machine model. Formally speaking, the model is a restriction of the Nubot model [20], for simplicity we instead use a custom formalism.

Grid. Positions are pairs in \mathbb{Z}^2 defined on a two-dimensional triangular grid using x and y axes as shown in Figure 2. For convenience, we define a third axis, w , centred on the origin and running through the point $(x, y) = (-1, 1)$. We let $\pm\vec{x}$, $\pm\vec{y}$, $\pm\vec{w}$ denote the unit vectors along the x , y and w axes.

Monomer, configuration, trajectory. A monomer is a pair $m = (s(m), \text{pos}(m))$ where $s(m) \in \mathbb{Z}$ is a state and $\text{pos}(m_i) \in \mathbb{Z}^2$ is a position. A *configuration*, of length $n \in \mathbb{N}$, is a tuple of monomers $c = (m_0, m_1, \dots, m_{n-1})$ whose positions $\sigma(c) = \text{pos}(m_0), \text{pos}(m_1), \dots, \text{pos}(m_{n-1})$ define a length $n - 1$ simple directed path (or non-self-intersecting chain) in \mathbb{Z}^2 (on the triangular grid) and where $\text{pos}(m_0) = (0, 0)$.³

A configuration is a tuple of $n \in \mathbb{N}$ monomers $(m_0, m_1, \dots, m_{n-1})$. A *final configuration* has all monomers in state 0. A pair of configurations (c_i, c_{i+1}) is said to be a *step* if c_i yields c_{i+1} via a single *rule application* (defined below) which we write as $c_i \rightarrow c_{i+1}$. A trajectory, of length k , is a sequence of configurations c_0, c_1, \dots, c_{k-1} where, for each $i \in \{0, 1, \dots, k - 2\}$ the pair (c_i, c_{i+1}) is a step $c_i \rightarrow c_{i+1}$. A Turning machine *initial configuration* c_0 is said to *compute the target configuration* c_t if all trajectories that start at c_0 lead to c_t , and is said to compute its target configuration if it reaches the configuration with all monomers in state 0. A *Turning machine* instance is an initial configuration. For a monomer m_i , we let $s_0(m_i)$ denote its state in the initial configuration.

Turning rule: state decrement. Let $S_{\text{init}} \subsetneq \mathbb{Z}$ be the set of states that appear in the initial configuration.⁴ Let $s_{\min} = \min(S_{\text{init}} \cup \{0\})$ and $s_{\max} = \max(S_{\text{init}} \cup \{0\})$, and let $S = \{s_{\min}, s_{\min} + 1, \dots, s_{\max}\}$ be the called the Turning machine *state set*. The *turning rules* of a turning machine are defined by a function r such that for all states $s \in (S \setminus \{0\})$:

$$r(s) = \begin{cases} s - 1 & \text{if } s > 0, \\ s + 1 & \text{if } s < 0. \end{cases} \quad (1)$$

Let \mathcal{C} be the set of all configurations. The turning rule $R : \mathcal{C} \times \mathbb{Z} \rightarrow \mathcal{C}$ is a function and $R(c, i)$ is said to be *applicable* to monomer m_i in configuration c if $s(m_i) \neq 0$ and the rule is not blocked (defined below). If the rule is applicable, we write $R(c, i) = c'$ and say that $R(c, i)$ yields the new configuration c' , and we say that (c, c') is a step.

Turning rule: blocking. For $i \in \{0, 1, \dots, n - 1\}$, we define the head and tail of monomer m_i as $\text{head}(m_i) = m_{i+1}, m_{i+2}, \dots, m_{n-1}$ and $\text{tail}(m_i) = m_0, m_1, \dots, m_i$.

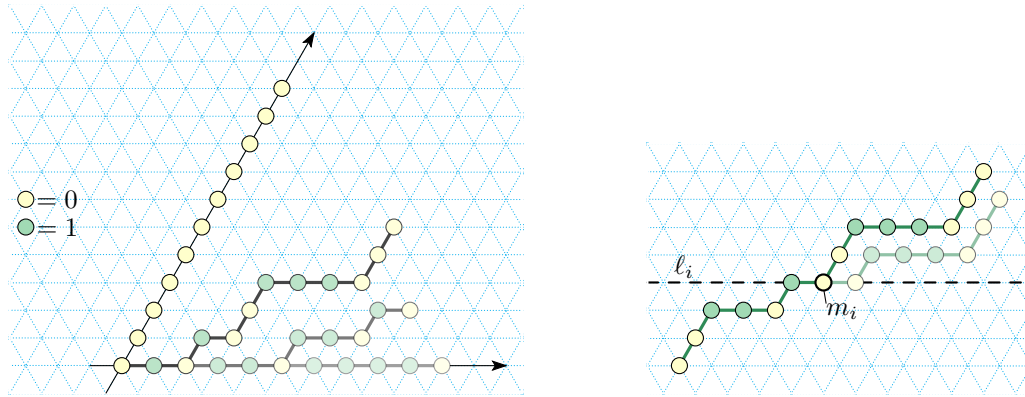
Consider the following tuple of unit vectors: $\vec{d} = (\vec{x}, \vec{y}, \vec{w}, -\vec{x}, -\vec{y}, -\vec{w})$, and let \vec{d}_k denote the k th element of that tuple. Let $\vec{d}_i = \text{pos}(m_{i+1}) - \text{pos}(m_i)$, i.e. the unit vector from monomer m_i to m_{i+1} , and then let $i' = (i + 2) \bmod 6$. For a vector $\vec{v} \in \mathbb{Z}^2$ we write $m_i + \vec{v}$ to mean the monomer m_i translated by \vec{v} . Define⁵ $\text{head}^{\rightarrow}(m_i) = m_{i+1} + \vec{d}_{i'}, m_{i+2} + \vec{d}_{i'}, \dots, m_{n-1} + \vec{d}_{i'}$. If the set of positions of $\text{tail}(m_i)$ has a non-empty intersection with the set of positions of $\text{head}^{\rightarrow}(m_i)$ we say that the rule is blocked, and the rule is not applicable. If the rule is not blocked, it is applicable and the resulting next configuration is $c' = \text{tail}(m_i), \text{head}^{\rightarrow}(m_i) = m_0, m_1, \dots, m_i, m_{i+1} + \vec{d}_{i'}, m_{i+2} + \vec{d}_{i'}, \dots, m_{n-1} + \vec{d}_{i'}$.

A configuration c is said to be *permanently blocked* if (a) not all states are 0, and (b) none of the monomers in c has an applicable rule. A monomer m within a configuration c is said to be *temporarily blocked* if (a) m is not in state 0, and (b) there is no rule applicable to m , and (c) there is a trajectory starting at c that reaches a configuration c' where there is a rule applicable to m .

³ In the language of [20], one can imagine that for all $i \in \{0, 1, \dots, n - 2\}$, there is a rigid bond between monomer m_i and monomer m_{i+1} , and otherwise there are no bonds.

⁴ Throughout this paper, only natural number states are used. However, for generality, symmetry and potential future work, we intentionally define the model to have integer states.

⁵ Another way to state this is that when a monomer m_i moves, $\text{head}(m_i)$ translates in the direction corresponding to the current direction of m_i rotated by the angle $2\pi/3$.



■ **Figure 3** Left: The Turning Machine L_n^1 that rotates a line of $n = 11$ monomers by $\pi/3$; illustration for Lemma 5. Four configurations are shown. The initial configuration has all monomers in state 1 sitting on the x -axis, in the final configuration all are in state 0 and sitting on the $\pi/3$ line. Two intermediate configurations are shown, respectively after 2, and then after 5, turning rule applications. Right: A configuration of some Turning Machine from the class \mathcal{M}_{11}^3 with the chain running from bottom left to top right. Lemmas 5 and 6 uses the fact that $\text{tail}(m_i)$ sits on or below ℓ_i , $\text{head}(m_i)$ sits on or above ℓ_i , and $\text{head}^\rightarrow(m_i)$ sits strictly above ℓ_i .

Time. A Turning Machine evolves as a continuous time Markov process. The rate for each rule application is 1. If there are k applicable transitions for a configuration c_i (i.e. k is the sum of the number of rule applications that can be applied to all monomers in c_i), then the probability of any given transition being applied is $1/k$, and the time until the next transition is applied is an exponential random variable with rate k (i.e. the expected time is $1/k$). The probability of a trajectory is then the product of the probabilities of each of the transitions along the trajectory, and the expected time of a trajectory is the sum of the expected times of each transition in the trajectory. Thus, $\sum_{t \in \mathcal{T}} \Pr[t] \cdot \text{time}(t)$ is the expected time for the system to evolve from configuration c_i to configuration c_j , where \mathcal{T} is the set of all trajectories from c_i to c_j , and $\text{time}(t)$ is the expected time for trajectory t .

▶ **Example.** The proof of Lemma 5 in Appendix A, and Figure 3, illustrate these concepts.

3

 Classes of Turning Machines: line rotation and square

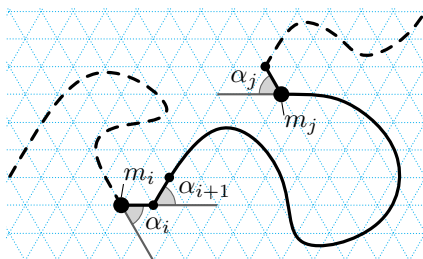
Every Turning Machine analysed in this paper starts with $n \in \mathbb{N}$ monomers, sitting on the x -axis, as formalised in the following definition.

▶ **Definition 1** ($\mathcal{M}_n^{\leq \sigma}$). Let $n, \sigma \in \mathbb{N}$. We let $\mathcal{M}_n^{\leq \sigma}$ denote the set of n -monomer Turning Machines with initial configuration $c_0 = m_0, m_1, \dots, m_{n-1}$ having all monomers positioned on the x -axis ($\text{pos}(m_i) = (i, 0) \in \mathbb{Z}^2$) and pointing to the east, and with initial states $s_0(m_i)$ bounded by σ , i.e. $s_0(m_i) \leq \sigma$ for all $0 \leq i \leq n-2$, and $s_0(m_{n-1}) = 0$.

We next define a sub class of $\mathcal{M}_n^{\leq \sigma}$ machines, called “line rotation” Turning Machines.

▶ **Definition 2** (Line rotation Turning Machine). Let $n \in \mathbb{N}$ and let L_n^σ be the Turning Machine with initial configuration of n monomers $c_0 = m_0, m_1, \dots, m_{n-1}$ all pointing to the east, positioned on the x -axis ($\text{pos}(m_i) = (i, 0) \in \mathbb{Z}^2$), and for $0 \leq i \leq n-2$ all monomers in the same state $s_0(m_i) = \sigma \in \mathbb{N}^+$ and $s_0(m_{n-1}) = 0$.

▶ **Remark 3.** The initial monomer state $\sigma \geq 0$ dictates that each monomer wishes to turn (have a rule applied) a total σ times, i.e. be rotated through an angle of $\sigma\pi/3$.



■ **Figure 4** Illustration of turn angle (Definition 7). The turn angles α_i and α_{i+1} are positive (and to the left), and α_j is negative (and to the right).

► **Remark 4 (Target configuration).** For intuition, if there was no notion of blocking in the Turning Machine model, that is, if the model permitted self-intersecting configurations (which it does not), then the final configuration c of the Turning Machine in Definition 2 is a straight line of monomers sitting along the ray that starts at the origin and is at an angle of $\sigma\frac{\pi}{3}$, i.e. at positions $(0, 0), (0, -1), \dots, (0, -(n-1))$ and all pointing to the west. We call c the desired *target configuration* of the line rotation Turning Machine L_n^σ . Also, if there was no notion of blocking: expected time to completion would be fast, $O(\log n)$ (by a generalisation of the analysis used in the proof of Lemma 5). However, a model with no blocking would be rather uninteresting.

Figure 3 (left) illustrates Lemma 5 and Appendix A contains its straightforward, yet instructive, proof.

► **Lemma 5.** *For each $n \in \mathbb{N}$, the line-rotating Turning Machine L_n^1 computes its target configuration, and does so in expected $O(\log n)$ time.*

Lemma 6 is illustrated in Figure 3 (right).

► **Lemma 6.** *Let $n \in \mathbb{N}$ and let $L_n^{\leq 3}$ be a Turning Machine in $\mathcal{M}_n^{\leq 3}$ (Definition 1). Let m_i for $0 \leq i \leq n-1$ be a monomer in some reachable configuration c of $L_n^{\leq 3}$. The monomers $\text{head}(m_i)$ are positioned on or above ℓ_i , and $\text{tail}(m_i)$ are positioned on or below ℓ_i .*

Proof. The claim follows from the fact that in any configuration of $L_n^{\leq 3}$, and for any $j \in \{0, 1, \dots, n-2\}$ the angle of the vector $\overrightarrow{\text{pos}(m_j)\text{pos}(m_{j+1})}$ (from monomer m_j to m_{j+1}) is either $0^\circ, 60^\circ, 120^\circ$, or 180° (and, in particular, is not strictly between 180° and 360°). ◀

4 Tools for reasoning about Turning machines

The notion of turn angle of a monomer is crucial to our analysis and is illustrated in Figure 4.

► **Definition 7 (Turn angle).** *Let c be the configuration of an n -monomer Turning Machine and let $0 \leq i < n-1$. The turn angle α_i at monomer m_i is the angle between $\overrightarrow{\text{pos}(m_{i-1})\text{pos}(m_i)}$ and $\overrightarrow{\text{pos}(m_i)\text{pos}(m_{i+1})}$, and it is the positive counterclockwise angle if the points $\text{pos}(m_{i-1}), \text{pos}(m_i), \text{pos}(m_{i+1})$ make a left turn⁶, and the negative clockwise angle otherwise.*

⁶ The notion of left or right turn along the three points $\text{pos}(m_{i-1}), \text{pos}(m_i), \text{pos}(m_{i+1})$ can be formalised by considering the line ℓ_i running through $\text{pos}(m_i)$, in the direction $\overrightarrow{\text{pos}(m_{i-1})\text{pos}(m_i)}$, noting that ℓ_i cuts the plane in two, and defining the left- and right-hand side of the plane with respect to the vector along ℓ_i .

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For a monomer m_i , the following definition gives a measure, $\Delta s(m_i)$, of how its state $s(m_i)$ has progressed since the initial configuration.

► **Definition 8.** Let c be a reachable configuration of an n -monomer Turning Machine. Define $\Delta s(m_i)$ to be the number of rule applications to (moves of) the monomer m_i from the initial configuration to c . That is, $\Delta s(m_i) = s_0(m_i) - s(m_i)$, where $s_0(m_i)$ is the initial state of m_i , and $s(m_i)$ is the state of m_i in configuration c .

► **Lemma 9** (Difference of State is ≤ 2). Let $n \in \mathbb{N}$, and let c be any reachable configuration of an n -monomer Turning Machine T_n with non-negative initial states, then

$$|\Delta s(m_i) - \Delta s(m_{i+1})| \leq 2,$$

for all $0 \leq i < n - 1$.

Proof. Let m_k^t , for $t \in \mathbb{N}$ and $k \in \{0, 1, \dots, n - 1\}$, denote the k^{th} monomer in the t^{th} configuration c_t . Initially, $\Delta s(m_j^0) = 0$ for all monomers m_j , and thus $|\Delta s(m_i^0) - \Delta s(m_{i+1}^0)| = 0$.

Observe, that $|\Delta s(m_i) - \Delta s(m_{i+1})| \neq 3$ because otherwise $\text{pos}(m_i) = \text{pos}(m_{i+2})$ making c a self-intersecting (non-simple) configuration, contradicting its definition.

By Equation (1), when a rule is applied to one of m_i^t or m_{i+1}^t its state decreases by 1 and its $\Delta s(\cdot)$ increases by 1. Then $|\Delta s(m_i^t) - \Delta s(m_{i+1}^t)| = |\Delta s(m_i^{t-1}) - \Delta s(m_{i+1}^{t-1})| \pm 1$. When a rule is applied to some other monomer m_k with $i \neq k \neq j$, then $|\Delta s(m_i^t) - \Delta s(m_{i+1}^t)| = |\Delta s(m_i^{t-1}) - \Delta s(m_{i+1}^{t-1})| \pm 0$. Thus, after each rule application the value of $|\Delta s(m_i) - \Delta s(m_{i+1})|$ changes by at most 1, and as it cannot be equal to 3, we have that $|\Delta s(m_i) - \Delta s(m_{i+1})| \leq 2$. ◀

We can now show the following lemma, which proves a relation between the states of any two monomers of a Turning Machine and the geometry of the current configuration.

► **Lemma 10.** Let c be any reachable configuration of an n -monomer Turning Machine T_n , whose initial configuration c_0 has all monomers pointing in the same direction, and let m_i and m_j be two monomers of c such that $i < j < n - 1$, then

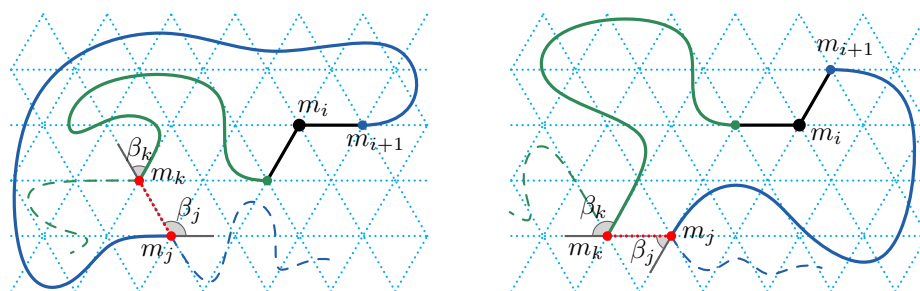
$$\Delta s(m_j) - \Delta s(m_i) = \frac{3}{\pi} \sum_{k=i+1}^j \alpha_k,$$

where α_k is the turn angle at monomer m_k .

Proof. For any intermediate configuration, the turn angle α_{i+1} between monomers m_i and m_{i+1} depends only on the number of moves each monomer has made. Initially, $\alpha_{i+1} = 0$, and it increases by $\pi/3$ each time monomer m_i moves, and decreases by $\pi/3$ every time monomer m_{i+1} moves. By Lemma 9, for two consecutive monomers m_i and m_{i+1} , in any configuration, $|\Delta s(m_i) - \Delta s(m_{i+1})| \leq 2$. Hence, for a pair of consecutive monomers m_i and m_{i+1} , the turn angle α_{i+1} is in the range $[-2\frac{\pi}{3}, 2\frac{\pi}{3}]$, and thus $\alpha_{i+1} = \Delta s(m_{i+1}) - \Delta s(m_i)$. Summing over all i gives the lemma conclusion. ◀

The following technical lemma is used extensively for our main results. Intuitively, it tells us that high-state monomers are not blocked.

► **Lemma 11.** Let $T_n \in \mathcal{M}_n^s$ be a Turning Machine with maximum state $s \leq 5$. In any reachable configuration c of T_n no monomer m_i with $\Delta s(m_i) \leq 1$ is blocked (neither temporarily blocked nor permanently blocked).



■ **Figure 5** Illustration for Lemma 11. Monomer m_i is shown in black, $\text{head}(m_i)$ is shown in blue and $\text{tail}(m_i)$ is shown as the green curve plus the black monomer m_i . Left: monomer m_i is in its initial state ($\Delta s(m_i) = 0$), and polygon P is traversed counter-clockwise. Right: monomer m_i has moved once ($\Delta s(m_i) = 1$), and polygon P is traversed clockwise.

Proof. Suppose, for the sake of contradiction, there is a blocked monomer m_i with $\Delta s(m_i) \leq 1$. Then there exist two monomers $m_j \in \text{head}(m_i)$ and $m_k \in \text{tail}(m_i)$ such that $\text{pos}(m_k) = \text{pos}'(m_j)$, where $\text{pos}'(m_j)$ is the position of m_j in $\text{head}^\rightarrow(m_i)$ (see Figure 5).

By definition of head and tail we know that $k \leq i < j$. Consider the closed chain $P = \text{pos}(m_k), \text{pos}(m_{k+1}), \dots, \text{pos}(m_{j-1}), \text{pos}(m_j), \text{pos}(m_k)$. Since configurations are simple, P defines a simple polygon. The turn angles of a simple polygon sum to 2π if the polygon is traversed anticlockwise (interior of P is on the left-hand side while traversing), or -2π if the polygon is traversed clockwise (interior of P is on the right-hand side). For P , this sum is defined as:

$$\alpha_P = \sum_{\ell=k+1}^{j-1} \alpha_\ell + \beta_j + \beta_k = \pm 2\pi,$$

where α_ℓ is the turn angle at monomer m_ℓ , and β_j and β_k are the turn angles of the polygon at vertices $\text{pos}(m_j)$ and $\text{pos}(m_k)$ respectively (see Figure 5). More precisely,

$$\begin{aligned} \alpha_\ell &= \angle(\overrightarrow{\text{pos}(m_\ell)} - \overrightarrow{\text{pos}(m_{\ell-1})}, \overrightarrow{\text{pos}(m_{\ell+1})} - \overrightarrow{\text{pos}(m_\ell)}), \\ \beta_j &= \angle(\overrightarrow{\text{pos}(m_j)} - \overrightarrow{\text{pos}(m_{j-1})}, \overrightarrow{\text{pos}(m_k)} - \overrightarrow{\text{pos}(m_j)}), \text{ and} \\ \beta_k &= \angle(\overrightarrow{\text{pos}(m_k)} - \overrightarrow{\text{pos}(m_j)}, \overrightarrow{\text{pos}(m_{k+1})} - \overrightarrow{\text{pos}(m_k)}). \end{aligned}$$

Furthermore, by Lemma 10,

$$\Delta s(m_{j-1}) - \Delta s(m_k) = \frac{3}{\pi} \sum_{\ell=k+1}^{j-1} \alpha_\ell.$$

Thus,

$$\Delta s(m_{j-1}) = \Delta s(m_k) + \frac{3}{\pi} \sum_{\ell=k+1}^{j-1} \alpha_\ell = \Delta s(m_k) + \frac{3}{\pi} (\pm 2\pi - \beta_j - \beta_k) = \Delta s(m_k) \pm 6 - \frac{3}{\pi} (\beta_j + \beta_k).$$

Observe that when a monomer m_i moves, its head translates in the direction corresponding to the current direction of m_i rotated by angle $2\pi/3$. Therefore, the state of m_k can be represented as a function of the state of m_i and the angle β_k , more precisely

$$\Delta s(m_k) = \Delta s(m_i) + 2 + \frac{3}{\pi} \beta_k.$$

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(See Figure 5 for an example.) Therefore, by the previous two equalities

$$\Delta s(m_{j-1}) = \Delta s(m_i) + 2 \pm 6 - \frac{3}{\pi}\beta_j.$$

Recall, that the angle $\beta_j \in [-2\pi/3, 2\pi/3]$, that $0 \leq \Delta s(m_i) \leq 1$ by the assumption of the lemma, and that $\Delta s(m_{j-1}) \leq s$. If the polygon defined by P is traversed counter-clockwise, then

$$\Delta s(m_{j-1}) = \Delta s(m_i) + 8 - \frac{3}{\pi}\beta_j \geq 0 + 8 - 2 = 6,$$

which implies that $s(m_{j-1})$ is out of the range of valid states, as m_{j-1} must have moved more times as its initial state. Else, if the polygon P is traversed clockwise, then

$$\Delta s(m_{j-1}) = \Delta s(m_i) - 4 - \frac{3}{\pi}\beta_j \leq 1 - 4 + 2 = -1,$$

which again implies that $s(m_{j-1})$ is out of the range of valid states, as m_{j-1} must have moved in the wrong direction. In either case we contradict that the state $s(m_{j-1})$ is in the range of valid states, and, therefore, the monomer m_i is not blocked. ◀

► **Lemma 12.** *Let L_n^s be a line-rotating Turning Machine with $s \leq 5$. Let c be a reachable configuration of L_n^s where each monomer m_i in c has $s_c(m_i) < s$. Then the line-rotating Turning Machine L_n^{s-1} has a reachable configuration c' such that for every m_i , $s_{c'}(m_i) = s_c(m_i)$ and the geometry (chain of positions) of c is equal to that of the rotation of c' by $\pi/3$ around the origin.*

Proof. Consider the sequence ρ_c rule applications (moves) that brings the initial configuration of L_n^s to configuration c . We claim that ρ_c can be converted into another sequence $\rho_{c'}$, of the same length, in which the first $n - 1$ moves are by monomers in state s .

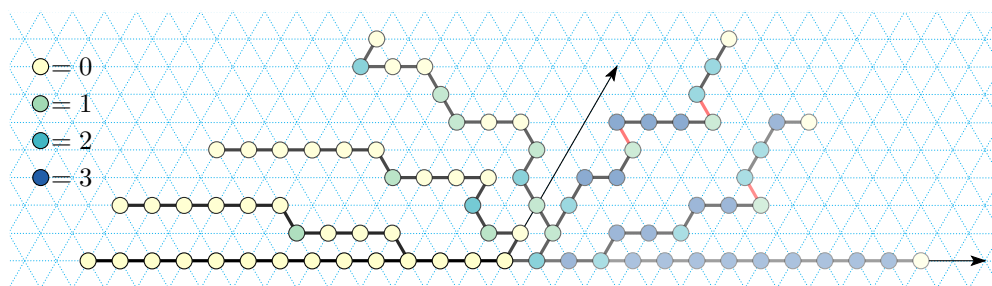
First, we claim: for any two consecutive moves, where the second move is applied to a monomer in state s , swapping the two moves results in a valid sequence of moves transforming the Turning Machine into the same configuration. Let the first move be applied to monomer m_i which transitions from state s' to $s' - 1$, and the second move be applied to monomer m_j which transitions from state s to $s - 1$. Suppose for the sake of contradiction that swapping the moves results in at least one of the monomers m_i or m_j being blocked. We begin by attempting to apply the move to monomer m_j , but, by Lemma 11, that move is not blocked. Then we attempt to apply a move to monomer m_i , but that is not blocked either since the coordinates of all monomers before and after swapping the two moves are exactly the same; i.e. the resulting configuration is a valid (non-self-intersecting) configuration in both cases. Hence neither monomer is blocked.

Thus, the original sequence of moves resulting in configuration c , can be converted into another sequence where the first $n - 1$ moves are applied to monomers in state s . Then, after the first $n - 1$ moves the configuration of L_n^s is equivalent to the initial configuration of L_n^s but rotated by $\pi/3$ and with all monomers in state $s - 1$. Hence equivalent to the initial configuration of L_n^{s-1} rotated by $\pi/3$.

Applying the remaining moves to L_n^{s-1} will transform it into configuration c' . ◀

5 Line rotation to $5\pi/3$

In this section we show that for $1 \leq s \leq 5$ the line-rotation Turning Machine L_n^s computes its target configuration of a $s\pi/3$ rotated line (Theorem 13), and does so in expected time $O(\log n)$ (Theorem 14). In addition to those results for any state $s \leq 5$, in Appendix A we



► **Figure 6** Example trajectory of the Turning Machine L_n^3 that rotates a line of east-pointing monomers by an angle of π . Illustration for Theorem 14 with $s = 3$ (and for Lemma 20 and Theorem 21 in Appendix A). Seven configurations are shown, the initial configuration has all monomers in state 3 (blue), final in state 0 (yellow). Darker shading indicates later in time. A red bond (edge) indicates a blocked monomer. The proof of Lemma 20 shows that only monomers in state 1 are ever blocked and only when they are adjacent to a monomer in state 3, and that all such blockings are temporary – if we wait long enough they become unblocked.

include stand-alone proofs for each of $s = 1$, $s = 3$, and $s = 4$ which showcase a variety of geometric techniques for analysing Turning Machine movement, but are not needed to prove our main results. Also, the cases of $s = 1$ and $s = 3$ are illustrated in Figures 3 and 6.

► **Theorem 13.** *For each $n \in \mathbb{N}$ and $1 \leq s \leq 5$, the line-rotation Turning Machine L_n^s computes its target configuration.*

Proof. We prove by induction on $1 \leq s \leq 5$ that any reachable configuration c of L_n^s is not permanently blocked.

Base case $s = 1$. In any configuration reachable by L_n^1 , monomers have either state $s = 1$ or 0. Monomers in state $s = 1$ cannot be permanently blocked by Lemma 11. Thus, any non-final configuration is not permanently blocked.

Assume for $s - 1$ the claim is true, i.e. it holds for L_n^{s-1} . We will prove that for s it is also true, i.e. it holds for L_n^s . Suppose, for the sake of contradiction, there is a permanently blocked configuration c of L_n^s for some $n \in \mathbb{N}$ and $s \leq 5$. If there is no monomer in c in state s , then by Lemma 12 there exists a corresponding configuration c' in L_n^{s-1} with monomers $m'_0, m'_1, \dots, m'_{n-1}$, such that, for any monomer m_i in c with state $s_i < s$ the corresponding monomer m'_i in c' has the same state s_i . Configurations c and c' form chains equal up to rotation by angle $\pi/3$. Configuration c' is not blocked by the induction hypothesis, thus configuration c cannot be blocked either.

On the other hand, if there is a monomer m_i in configuration c in state s , then by Lemma 11 it is unblocked, and configuration c , again, is not blocked.

Hence the induction hypothesis holds for s , and L_n^s does not have a reachable permanently blocked configuration. ◀

► **Theorem 14.** *For each $n \in \mathbb{N}$ and $1 \leq s \leq 5$, the line-rotation Turning Machine L_n^s computes its target configuration in expected $O(\log n)$ time.*

Proof. By Theorem 13, L_n^s computes its target configuration. For the time analysis we use a proof by induction on $u \in \{0, 1, \dots, s\}$, in decreasing order.

The induction hypothesis is that for a reachable configuration c_u of L_n^s with maximum state value u (there may be states $< u$ in the configuration), the expected time to reach a configuration c_{u-1} with maximum state $u - 1$ is $O(\log n)$.

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For the base case we let $u = s$ and assume c is such that all monomers are in state u . Hence c is an initial configuration and hence, by definition, is reachable. By Lemma 11, monomers in state s are never blocked and hence we claim that the first configuration with maximum state $u - 1$ appears after expected time $O(\log n)$. To see this claim, note that for each monomer m_i in state $s(m_i) = u$ the rule application that sends m_i to state $u - 1$ occurs at rate 1, independently of the states and positions of the other monomers (by Lemma 11, there is no blocking of a monomer in state $u = s$). Since there are n monomers in state u , the expected time for all n to transition to $u - 1$ is [13]:

$$\sum_{k=1}^n \frac{1}{k} = O(\log n). \quad (2)$$

We assume the inductive hypothesis is true for $0 < u + 1 \leq s$, and we will prove it holds for u . Thus, there exists a reachable configuration c_u where the maximum state value is $u \leq s$, which is reachable from c_{u+1} in expected $O(\log n)$ time. Let there be $n' \leq n$ monomers in state u in c_u . By Lemma 12, there is a line-rotating Turning Machine L_n^u that has a reachable configuration c'_u such that for every m_i in c_u , $s_{c'_u}(m_i) = s_{c_u}(m_i)$ and the positioning of c_u is equal to the rotation of c'_u by $\pi/3$ around the origin. By Lemma 11 monomers in state u in L_n^u are never blocked, hence monomers in state u in c_u are not blocked either. Setting $n = n'$ in Equation (2), and noting that $O(\log n') = O(\log n)$, proves the inductive hypothesis for u .

Since we need to apply the inductive argument at most $s \leq 5$ times, by linearity of expectation, the expected finishing time for the s processes is their sum, $5 \cdot O(\log n) = O(\log n)$. ◀

6 Line rotation to 2π is impossible

► **Theorem 15.** *For all $n \in \mathbb{N}, n \geq 7$, the line-rotating Turning Machine L_n^6 does not compute its target configuration. In other words, there is a permanently blocked reachable configuration.*

Proof. Figure 7, looking only at blue monomers and edges, shows a valid trajectory of L_7^6 , then ends in a permanently blocked configuration, hence the lemma holds for $n = 7$.

Let $n > 7$, and in Figure 7 let the red line segment denote a straight line ℓ_{n-7} of $n - 7$ monomers co-linear with the red line segment. By inspection, it can be verified that (a) in all 25 configurations the line ℓ does not intersect any blue monomer, and moreover (b) the transitions from configurations 1 through 14, configurations 17 through 23, and configuration 24 to 25 are all valid, meaning that the length $n - 7$ line ℓ_{n-7} does not block the transition. The transitions for configurations 14 through 17 are valid by Theorem 13 (with $s = 3$) and the fact that the last blue monomer (the origin of ℓ_{n-7}) is strictly above all other blue monomers (hence the 180° rotation of ℓ_{n-7} proceeds without permanent blocking by blue monomers). The transition for configuration 23 to 24 is valid by applying Lemma 5 (or Theorem 13, with $s = 1$) reflected through a horizontal line that runs through the last blue monomer, and the fact that the last blue monomer (the origin of ℓ_{n-7}) is strictly below all other blue monomers (hence the 60° rotation of ℓ_{n-7} proceeds without permanent blocking). Thus all transitions are valid and the permanently blocked configuration is reachable, giving the lemma statement. ◀

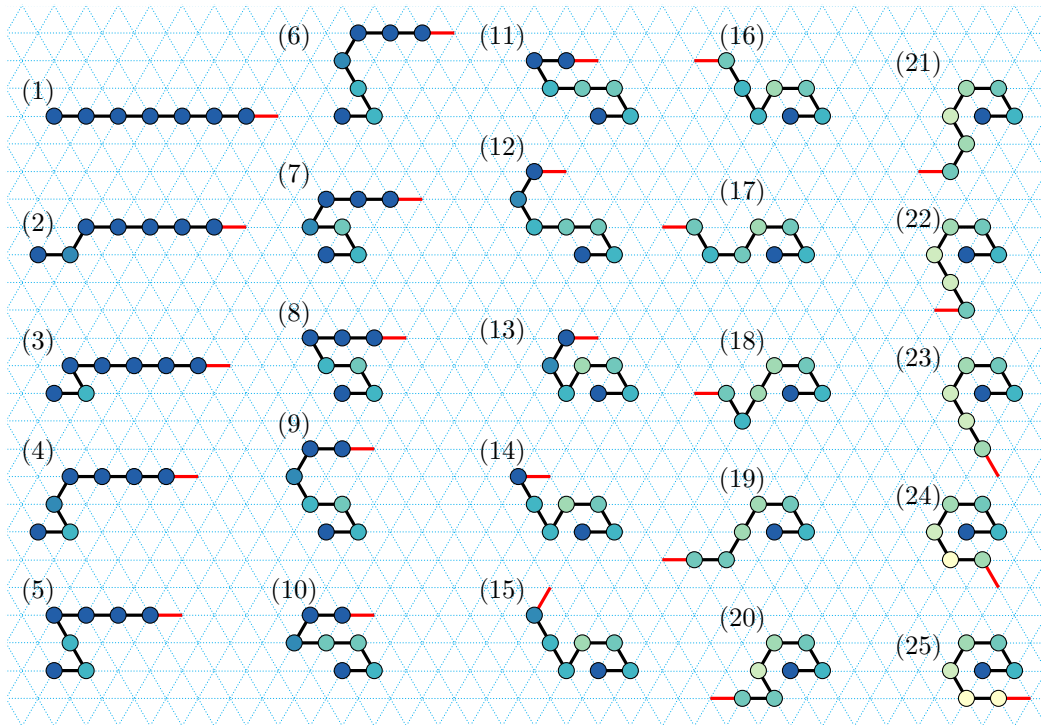


Figure 7 Impossibility of 360° line rotation, by showing that for all $n \in \mathbb{N}$, the line-rotation Turning Machine L_n^6 has a reachable but permanently blocked configuration. Looking at the evolution of the first seven monomers (i.e. ignore the rotation of the red line segment) we see one trajectory of the Turning machine that exhibits permanent blocking in the final (bottom-right) configuration, which has respective states 6,4,3,2,1,0,0. We imagine the red line segment as representing an arbitrary long sequence of monomers running collinear with it, and transitions 14–16, 22–23, and 24–25, each representing the (many step) rotation of the red line by consecutive angles of 60°. These rotations of the red line can proceed by two applications of Theorem 13 (first with $s = 3$, then with $s = 1$) and the fact that the first monomer of the red line is strictly above, or below, the first seven monomers. Hence the final, permanently blocked, configuration is reachable no matter what length the red line is.

7 Folding zig-zag squares and y -monotone shapes

As a demonstration of our techniques, in this section we show how to build two shapes with Turning Machines: an $n \times n$ square, and any y -monotone shape.

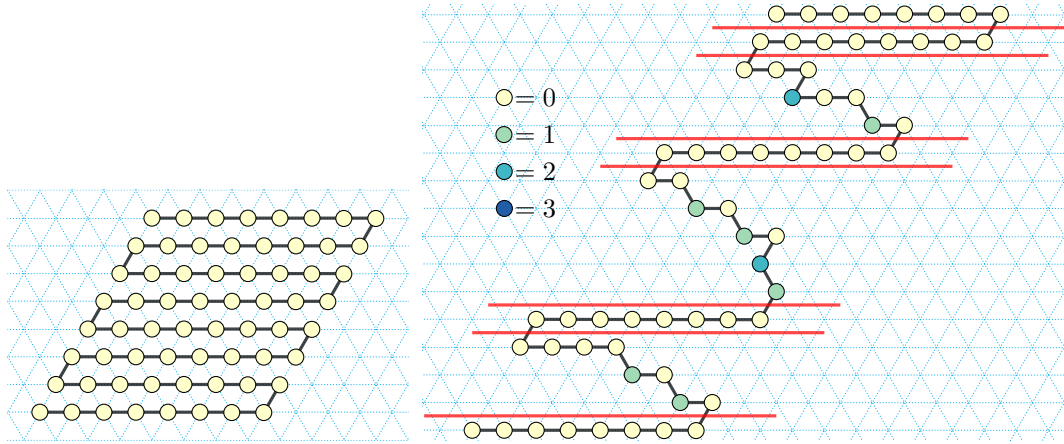
We first define a specific curve which fills a square row by row in a zig-zag fashion. An example is shown in Figure 8 (left).

► **Definition 16** ($n \times n$ zig-zag square). For any $n \in \mathbb{N}$, an $n \times n$ zig-zag square is the length n^2 configuration such that the position of monomer m_i is given by the following expression:

$$\text{pos}(m_i) = \begin{cases} (i \% n, \lfloor \frac{i}{n} \rfloor), & \text{if } i \% (2n) < n, \\ (n - 1 - i \% n, \lfloor \frac{i}{n} \rfloor), & \text{if } i \% (2n) \geq n, \end{cases}$$

where $i \% n$ denotes the remainder of i divided by n .

We now show that the zig-zag square can be built by a Turning Machine.



■ **Figure 8** Left: A target $n \times n$ zig-zag square, for $n = 8$. Right: an intermediate configuration c after all 1-monomers have moved (for $0 \leq k \leq 3$, a k -monomer begins in state k). The horizontal lines (in red) subdivide the T_n^{zz} into independent subchains equivalent to n separate line-rotating Turning Machines L_n^3 .

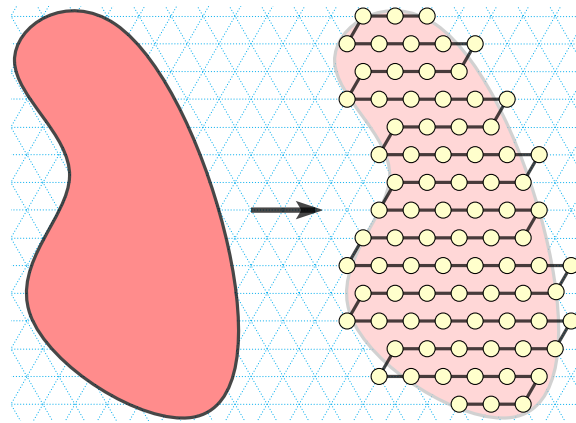
► **Theorem 17.** For any $n \in \mathbb{N}$, let T_n^{zz} be an n^2 -monomer Turning Machine with initial configuration having all monomers positioned on the x -axis ($\text{pos}(m_i) = (i, 0) \in \mathbb{Z}^2$) and pointing to the east, with initial state sequence

$$S = \begin{cases} (0^{n-1}13^{n-1}1)^{\frac{n}{2}-1}0^{n-1}13^{n-1}0, & \text{if } n \text{ is even,} \\ (0^{n-1}13^{n-1}1)^{(n-1)/2}0^n, & \text{if } n \text{ is odd.} \end{cases}$$

Then, T_n^{zz} computes the $n \times n$ zig-zag square (Definition 16) in expected time $O(\log n)$.

Proof. For notation, we let k -monomers be the monomers whose initial state is k . Thus, the Turning Machine consists of sequences of 0- and 3-monomers, separated by single 1-monomers. Observe that all 1-monomers are never blocked. Thus, after expected $O(\log n)$ time they all move to their final orientation along the y -axis. Consider such a configuration c , in which all 1-monomers are in state 0. The remaining rules can only be applied to 3-monomers. Consider a set of horizontal lines passing through the midpoint of the unit-length line-segment that spans from the position $\text{pos}(m_i)$ of each 1-monomer m_i to $\text{pos}(m_{i+1})$. These lines separate consecutive sequences of 0-monomers and sequences of 3-monomers from one another in the \mathbb{R}^2 plane. This implies, that after the two adjacent 1- monomers have moved, the full segment M of 3-monomers in between them moves independently of the rest of the configuration. We claim that the evolution of these processes is modelled by the computation of a line-rotating Turning Machine L_n^3 . Before its left-bordering 1-monomer has moved, the segment M of 3-monomers acts as a length n instance of L_{n+1}^3 , with an additional 1-monomer, its first monomer, that simply has not moved yet. Since we know that monomer is first released after $O(\log n)$ time, this does not (asymptotically) change the expected time bound for the L_{n+1}^3 machine.

By Theorem 14, each of the sequences of 3-monomers will evolve into their target configuration in $O(\log n)$ expected time independent of one another, which would naively give an overall expected time of $O(\log^2 n)$ time. However, by Lemma 11 we know that no 3-monomer that is in state 3 or state 2, and no 1-monomer, is ever blocked. Hence, we can



■ **Figure 9** A y -monotone shape in \mathbb{R}^2 approximated with a zig-zag chain on the triangular grid.

analyse all n^2 monomers as one system, noting that all such monomers complete in time $O(\log n)$, at which point we have a reachable configuration that has all 3-monomers in either state 0 and 1 (all others in state 0) which in turn finishes in $O(\log n)$ expected time.⁷ ◀

► **Definition 18** (y -monotone shape). *A set $A \subset \mathbb{R}^2$ is y -monotone, if any horizontal line h intersects S along one continuous segment of h .*

Similarly to the construction of the zig-zag square presented above, we can build an approximation of any y -monotone shape A by discretizing it and filling the resulting shape row by row in a zig-zag manner (refer to Figure 9). The resulting state sequence of the Turning Machine T_n^{zz} consists of intervals of 0-monomers and 3-monomers of various lengths separated by single 1-monomers.

We conclude with the following theorem statement. In it we assume that the state sequence S is such that the final configuration approximates some given y -monotone shape A . The proof is the same as that for Theorem 17 (but using a variety of horizontal segment lengths n).

► **Theorem 19.** *Let $T_n^{y\text{-mon}}$ be a Turning Machine with initial configuration having all monomers positioned on the x -axis ($\text{pos}(m_i) = (i, 0) \in \mathbb{Z}^2$) and pointing to the east, with initial state sequence S consisting of intervals of 0- and 3-monomers separated by single 1-monomers. Then $T_n^{y\text{-mon}}$ computes its target configuration in $O(\log n)$ expected time.*

References

- 1 Greg Aloupis, Sébastien Collette, Mirela Damian, Erik D Demaine, Robin Flatland, Stefan Langerman, Joseph O'Rourke, Suneeta Ramaswami, Vera Sacristán, and Stefanie Wuhler. Linear reconfiguration of cube-style modular robots. *Computational Geometry*, 42(6-7):652–663, 2009.
- 2 Greg Aloupis, Sébastien Collette, Erik D. Demaine, Stefan Langerman, Vera Sacristán, and Stefanie Wuhler. Reconfiguration of cube-style modular robots using $O(\log n)$ parallel moves. In *International Symposium on Algorithms and Computation*, pages 342–353. Springer, 2008.

⁷ This is similar to the technique used in the proof of Theorem 14.

- 3 Ho-Lin Chen, David Doty, Dhiraj Holden, Chris Thachuk, Damien Woods, and Chun-Tao Yang. Fast algorithmic self-assembly of simple shapes using random agitation. In *DNA20: The 20th International Conference on DNA Computing and Molecular Programming*, volume 8727 of *LNCS*, pages 20–36, Kyoto, Japan, September 2014. Springer. Full version: [arXiv:1409.4828](#).
- 4 Moya Chen, Doris Xin, and Damien Woods. Parallel computation using active self-assembly. *Natural Computing*, 14(2):225–250, 2014. arXiv version: [arXiv:1405.0527](#).
- 5 Kenneth C. Cheung, Erik D. Demaine, Jonathan R. Bachrach, and Saul Griffith. Programmable assembly with universally foldable strings (moteins). *IEEE Transactions on Robotics*, 27(4):718–729, 2011.
- 6 Yen-Ru Chin, Jui-Ting Tsai, and Ho-Lin Chen. A minimal requirement for self-assembly of lines in polylogarithmic time. *Natural Computing*, 17(4):743–757, 2018.
- 7 Robert Connelly, Erik D. Demaine, Martin L. Demaine, Sándor P. Fekete, Stefan Langerman, Joseph S.B. Mitchell, Ares Ribó, and Günter Rote. Locked and unlocked chains of planar shapes. *Discrete & Computational Geometry*, 44(2):439–462, 2010.
- 8 Nadine Dabby and Ho-Lin Chen. Active self-assembly of simple units using an insertion primitive. In *SODA: The 24th Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 1526–1536, January 2012.
- 9 Rachel E. Dawes-Hoang, Kush M. Parmar, Audrey E. Christiansen, Chris B. Phelps, Andrea H. Brand, and Eric F. Wieschaus. Folded gastrulation, cell shape change and the control of myosin localization. *Development*, 132(18):4165–4178, 2005.
- 10 Erik D. Demaine, Jacob Hendricks, Meagan Olsen, Matthew J. Patitz, Trent A. Rogers, Nicolas Schabanel, Shinnosuke Seki, and Hadley Thomas. Know when to fold'em: self-assembly of shapes by folding in oritadami. In *DNA: International Conference on DNA Computing and Molecular Programming*, pages 19–36. Springer, 2018.
- 11 Cody Geary, Pierre-Étienne Meunier, Nicolas Schabanel, and Shinnosuke Seki. Programming biomolecules that fold greedily during transcription. In *MFCS: The 41st International Symposium on Mathematical Foundations of Computer Science*. Schloss Dagstuhl-Leibniz-Zentrum fuer Informatik, 2016.
- 12 Robert Gmyr, Kristian Hinnenthal, Irina Kostitsyna, Fabian Kuhn, Dorian Rudolph, Christian Scheideler, and Thim Strothmann. Forming tile shapes with simple robots. *Natural Computing*, pages 1–16, 2019.
- 13 Ronald L. Graham, Donald E. Knuth, and Oren Patashnik. *Concrete mathematics*, 1989.
- 14 Benjamin Hescott, Caleb Malchik, and Andrew Winslow. Tight bounds for active self-assembly using an insertion primitive. *Algorithmica*, 77:537–554, 2017.
- 15 Benjamin Hescott, Caleb Malchik, and Andrew Winslow. Non-determinism reduces construction time in active self-assembly using an insertion primitive. In *COCOON: The 24th International Computing and Combinatorics Conference*, pages 626–637. Springer, 2018.
- 16 Chun-Ying Hou and Ho-Lin Chen. An exponentially growing nubot system without state changes. In *International Conference on Unconventional Computation and Natural Computation*, pages 122–135. Springer, 2019.
- 17 Adam C Martin, Matthias Kaschube, and Eric F Wieschaus. Pulsed contractions of an actin–myosin network drive apical constriction. *Nature*, 457(7228):495–499, 2008.
- 18 Othon Michail, George Skretas, and Paul G. Spirakis. On the transformation capability of feasible mechanisms for programmable matter. *Journal of Computer and System Sciences*, 102:18–39, 2019.
- 19 Hamid Ramezani and Hendrik Dietz. Building machines with DNA molecules. *Nature Reviews Genetics*, pages 1–22, 2019.
- 20 Damien Woods, Ho-Lin Chen, Scott Goodfriend, Nadine Dabby, Erik Winfree, and Peng Yin. Active self-assembly of algorithmic shapes and patterns in polylogarithmic time. In *ITCS: The 4th conference on Innovations in Theoretical Computer Science*, pages 353–354. ACM, 2013. Full version: [arXiv:1301.2626](#) [cs.DS].

A Line rotation by $\pi/3$, π and $4\pi/3$

In this appendix we present proofs that line-rotating Turning Machine for respective angles of $\pi/3$, π and $4\pi/3$ terminates in expected time $O(\log n)$. These claims are superseded by the results in the main paper, but we include the proofs as they give a number of techniques to analyse the Turning Machine model.

A.1 Line rotation by $\pi/3$: L_n^1

The following proof of line rotation by $\pi/3$ radians is intended to be a simple example worked out in detail. Let L_n^1 be the Turning Machine defined in Definition 2 with $\sigma = 1$, as illustrated in Figure 3 (left).

► **Lemma 5.** *For each $n \in \mathbb{N}$, the line-rotating Turning Machine L_n^1 computes its target configuration, and does so in expected $O(\log n)$ time.*

Proof. The initial configuration (Figure 3, left) of L_n^1 is a line of $n-1$ monomers in state 1 with an additional final monomer in state 0, i.e. at time 0 the n states are $s(m_0)s(m_1) \cdots s(m_{n-1}) = 1^{n-1}0$. Since monomer states only change by decrementing from 1 to 0, any configuration on any trajectory of L_n^1 has its (composite) state of the form $\{0, 1\}^{n-1}0$. Consider a configuration c in a trajectory of evolution of L_n^1 , and the corresponding state⁸ $x \in \{0, 1\}^{n-1}0$. Let m_i^c denote the i th monomer of L_n^1 in configuration c . For any $i \in \{0, 1, \dots, n-2\}$ such that $s(m_i^c) = 1$, consider the unique configuration c' where $c \rightarrow c'$ and $s(m_i^{c'}) = 0$ (and, by definition of next configuration step, $j \neq i$ implies $s(m_j^{c'}) = s(m_j^c)$).

We claim that $\text{tail}(m_i^c)$ does not share any positions with $\text{head}^{\rightarrow}(m_i^c)$, in other words, that c' is a non-self-intersecting configuration. To show this, consider a horizontal line ℓ_i through monomer m_i^c and observe that in c' (and in c), the monomers $\text{tail}(m_i^c) = m_0^c, m_1^c, \dots, m_i^c$ lie on or below ℓ_i (because the path $\text{pos}(m_0^c), \text{pos}(m_1^c), \dots, \text{pos}(m_i^c)$ is connected and consists of unit length segments each at an angle of either 0° or 60° clockwise relative to the x -axis), but the monomers $\text{head}^{\rightarrow}(m_i^c) = m_{i+1}^{c'}, m_{i+2}^{c'}, \dots, m_{n-1}^{c'}$ lie strictly above ℓ_i (because $\text{pos}(m_{i+1}^{c'})$ is strictly higher than $\text{pos}(m_i^c)$, and because the path $\text{pos}(m_{i+1}^{c'}), \text{pos}(m_{i+2}^{c'}), \dots, \text{pos}(m_{n-1}^{c'})$ is connected and consists of unit length segments each at an angle of 0° or 60° to the x -axis). Hence there are no blocked configurations reachable by L_n^1 (neither permanent nor temporary blocking).

At each reachable configuration c , starting from the initial configuration, we can choose i independently from the set of non-zero states. The expected time for the first rule application is $1/(n-1)$ since it is the expected time of the minimum of $n-1$ independent exponential random variables each with rate 1. The next is $1/(n-2)$, and so on. By linearity of expectation, the expected value of the total time T is $E[T] = \sum_{k=1}^{n-1} \frac{1}{k} = O(\log n)$, where the sum is the $(n-1)$ th partial sum of the harmonic series, known to have a $O(\log n)$ bound. Hence L_n^1 completes in expected $O(\log n)$ time. ◀

A.2 Line rotation by π : L_n^3

Next, we analyse line rotation of π radians.

► **Lemma 20.** *Let L_n^3 be a line-rotating Turning machine, then:*

- (i) *any reachable configuration of L_n^3 has no more than $2n/3$ blocked monomers, and*
- (ii) *there exists a configuration of L_n^3 that has exactly $2n/3$ blocked monomers.*

⁸ In fact any $x \in \{0, 1\}^{n-1}0$ is the state of a reachable configuration, but we don't need to prove that.

Proof. Consider any reachable configuration c of L_n^3 , and let monomer m_i be blocked in c . By Lemma 11, monomers in state 2 and 3 are never blocked. By definition, monomers in state 0 are not blocked. Thus if m_i is blocked it is in state 1, i.e. $s(m_i) = 1$. We claim that in this case either $s(m_{i-1}) = 3$ or $s(m_{i+1}) = 3$ (or both). Consider the following two cases for $s(m_{i+1})$:

1. If $s(m_{i+1}) \in \{1, 2\}$, then by Lemma 6 all monomers of $\text{head}^\rightarrow(m_i)$, except its first monomer m'_{i+1} , lie strictly above ℓ_i , and since $\text{tail}(m_i)$ lies on or below ℓ_i , we get that $\text{tail}(m_i)$ does not intersect $\text{head}^\rightarrow(m_i)$, except possibly at $\text{pos}(m'_{i+1})$. Whether $\text{pos}(m'_{i+1})$ intersects $\text{tail}(m_i)$ depends on the state of m_{i-1} :
 - (a) If $s(m_{i-1}) \in \{1, 2\}$, then all monomers of $\text{tail}(m_i)$ lie strictly below ℓ_i (except its first monomer m_i which is not at position $\text{pos}(m'_{i+1})$), hence $\text{pos}(m'_{i+1})$ cannot intersect $\text{tail}(m_i)$. Then m_i cannot be blocked.
 - (b) If $s(m_{i-1}) = 0$, then m'_{i+1} does not intersect $\text{tail}(m_i)$: Indeed, $\text{pos}(m_{i-1}) = \text{pos}(m_i) + \vec{x} = \text{pos}(m'_{i+1}) + 2\vec{x} \neq \text{pos}(m'_{i+1})$. Furthermore, let $m_j, m_{j+1}, \dots, m_{i-1}$ be the longest consecutive subsequence of monomers in state 0 preceding monomer m_i . Then $\text{pos}(m_j), \text{pos}(m_{j+1}), \dots, \text{pos}(m_{i+1})$ are all strictly to the west of $\text{pos}(m_i)$. If $j-1 \geq 0$, the non-zero-state⁹ monomer m_{j-1} enforces that the monomers m_0, m_1, \dots, m_{j-1} lie strictly below ℓ_i . Thus m_i is not blocked.

Therefore, monomer m_{i-1} can only be in state 3.

2. If $s(m_{i+1}) = 0$: Both $\text{head}^\rightarrow(m_i)$ and $\text{tail}(m_i)$ have monomers on ℓ_i , but we claim the positions of $\text{head}^\rightarrow(m_i)$ do not intersect those of $\text{tail}(m_i)$. If $s(m_{i-1}) \in \{1, 2\}$, then all monomers of $\text{tail}(m_i)$ except m_i lie strictly below ℓ_i , and thus $\text{head}^\rightarrow(m_i)$ does not intersect $\text{tail}(m_i)$ (and recall that $\text{head}^\rightarrow(m_i)$ does not intersect $\text{pos}(m_i)$ because configurations are simple). If $s(m_{i-1}) = 0$ then the monomers $M = \{m_{i-1}, m_i, m'_{i+1}\}$ lie along ℓ_i (pointing west). Note that a prefix of M is a suffix of $\text{tail}(m_i)$ and a (disjoint) suffix of M is a prefix of $\text{head}^\rightarrow(m_i)$. Hence, in order for $\text{tail}(m_i)$ to intersect $\text{head}^\rightarrow(m_i)$, one or both must depart from ℓ_i , but, by Lemma 6, $\text{tail}(m_i)$ can only do so by having monomers strictly below ℓ_i , and $\text{head}^\rightarrow(m_i)$ can only do so by having monomers strictly above ℓ_i . Thus, monomer m_{i-1} can only be in state 3.

Therefore, if m_i is blocked, then either m_{i-1} or m_{i+1} is in state 3, and thus is unblocked. Hence, there cannot be three monomers in a row which are blocked, resulting in Conclusion (i) of the lemma.

For Conclusion (ii), consider a line-rotating Turning Machine L_n^3 with $n = 3k$ for some k . The configuration c with state sequence $S = (131)^{k-1}130$ has exactly $2n/3$ blocked monomers, as every monomer in state 1 is either blocked by a preceding monomer in state 3, or by a following monomer in state 3. ◀

► **Theorem 21** (Rotate a line by π). *For each $n \in \mathbb{N}$, the line-rotating Turning Machine L_n^3 computes its target configuration, and does so in expected time $O(\log n)$.*

Proof. By Lemma 20, no configuration has a permanently blocked monomer, hence every trajectory of L_n^3 ends in the target configuration.

At the initial step, the rate of rule applications is $n - 1$ (there are $n - 1$ monomers in state 3). Over time, for successive configurations along a trajectory, the rate of rule applications may decrease for two reasons: (a) some monomers may be temporary blocked, and (b) after a monomer transitions to state 0 no more rules are applicable to it. We reason about both:

⁹ Which must be in state 1 or 2, since 3 would give a self-intersection along the configuration.

(a) Lemma 20(ii) shows that a configuration with state sequence $s = (131)^{n/3-1}130$ has $2n/3$ blocked monomers, and Lemma 20(i) states that no configuration has more than $2n/3$ blocked monomers for n divisible by 3. Using that fact, and in order to simplify the proof, we shall analyse a new, possibly slower, system where for any configuration c that has $n' \leq n$ monomers in state $\neq 0$, we “artificially” block $2n'/3$ monomers.¹⁰ Since this assumption merely serves to slow the system, it is sufficient to give an upper bound on the expected time to finish.

(b) A second “slowdown” assumption will be applied during the analysis and is justified as follows. Intuitively, the number of monomers transitioning to state 0 increases with time, and since monomers in state 0 have no applicable rules, this causes a *decrease* in the rate of rule applications. Consider a hypothetical continuous-time Markov system M , with $3n$ steps with rate decreasing by 1 every third step, that is, with successive rates $n, n, n, n-1, n-1, n-1, n-2, \dots, 2, 1, 1, 1$. By linearity of expectation, the expected value of the finishing time T is the sum of the expected times $E[t_i]$ for each of the individual steps $i \in \{1, 2, \dots, 3n\}$:

$$E[T] = \sum_{i=1}^{3n} E[t_i] = \sum_{m=1}^n 3 \cdot \frac{1}{m} = 3 \sum_{m=1}^n \frac{1}{m} = 3H_n \leq 3(\ln(n) + 1) = O(\log n), \quad (3)$$

where H_n is the n^{th} partial sum of the harmonic series $\sum_{m=1}^{\infty} \frac{1}{m}$ with $H_n \leq \ln(n) + 1$ (see [13]). Since, in L_n^3 , it requires at least 3 steps to send a monomer from state 3 (the initial state) to state 0, no trajectory sends monomers to state 0 at a faster rate than a (hypothetical) trajectory where a transition to state 0 appears at every third configuration (step). Hence, if there were no blocking whatsoever, then the expected time for L_n^3 would be no larger than $3H_n$ (given by Equation (3)).

Taking the blocking “slowdown assumption” in (a) into account, if the rate at step i is r_i , then the slowed down rate is $\frac{1}{3}r_i$ giving an expected time of

$$E[T] = \sum_{i=1}^{3n} E[t_i] = \sum_{m=1}^n 3 \cdot \frac{1}{3} \cdot \frac{1}{m} = 9 \sum_{m=1}^n \frac{1}{m} = 9H_n \leq 9(\ln(n) + 1) = O(\log n). \quad (4)$$

Since our two assumptions merely serve to define a new system that is necessarily slower than L_n^3 , we get the claimed expected time upper bound of $O(\log n)$ for L_n^3 . ◀

A.3 Line rotation by $4\pi/3$: L_n^4

► **Lemma 22.** *Let m_i be a blocked monomer in some reachable configuration c of a line rotation Turning Machine L_n^s with $n \in \mathbb{N}$ and $1 \leq s \leq 4$, and let $m_j \in \text{head}(m_i)$ and $m_k \in \text{tail}(m_i)$ be a pair of monomers which block the movement of m_i , then in the subchain of L_n^s from m_k to m_{j-1} the number of unblocked monomers is at least half the number of blocked monomers.*

Proof. Similarly to the proof of Lemma 11, consider the closed chain $P = \text{pos}(m_k), \dots, \text{pos}(m_j), \text{pos}(m_k)$. Let $x(m_i)$ denote the x -coordinate of the position of monomer m_i , and $y(m_i)$ denote the y -coordinate of the position of monomer m_i . Note, that for any ℓ ,

¹⁰The monomers are not necessarily geometrically blocked, we are merely stopping any rule from being applied to them. No configuration in a trajectory of L_n^3 witnesses a larger slowdown due to blocking than the slowdown we have imposed on the configurations of T_n' .

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- if $s(m_\ell) = s$, then $x(m_{\ell+1}) = x(m_\ell) + 1$ and $y(m_{\ell+1}) = y(m_\ell)$,
- if $s(m_\ell) = s - 1$, then $x(m_{\ell+1}) = x(m_\ell)$ and $y(m_{\ell+1}) = y(m_\ell) + 1$,
- if $s(m_\ell) = s - 2$, then $x(m_{\ell+1}) = x(m_\ell) - 1$ and $y(m_{\ell+1}) = y(m_\ell) + 1$,
- if $s(m_\ell) = s - 3$, then $x(m_{\ell+1}) = x(m_\ell) - 1$ and $y(m_{\ell+1}) = y(m_\ell)$,
- if $s(m_\ell) = s - 4$, then $x(m_{\ell+1}) = x(m_\ell)$ and $y(m_{\ell+1}) = y(m_\ell) - 1$.

Let $x(m_k) - x(m_j) = \varepsilon_x$ and $y(m_k) - y(m_j) = \varepsilon_y$, with $\varepsilon_x, \varepsilon_y \in \{-1, 0, 1\}$. The total change in x -coordinate and the total change in y -coordinate, when traversing P , is zero, that is,

$$\begin{aligned} \sum_{\ell=k}^{j-1} (x(\ell+1) - x(\ell)) + \varepsilon_x &= 0, \\ \sum_{\ell=k}^{j-1} (y(\ell+1) - y(\ell)) + \varepsilon_y &= 0. \end{aligned} \tag{5}$$

Considering the first part of Equation (5), and taking into account that the x -coordinate increases only when traversing monomers in state s , and the x -coordinate decreases only when traversing monomers in state $s - 2$ or $s - 3$, we get $\#(s) + \varepsilon_x = \#(s - 2) + \#(s - 3)$, where $\#(u)$ denotes the number of monomers with state u in the subchain from m_k to m_{j-1} . Observe, by Lemma 11, monomers in states s and $s - 1$ cannot be blocked, and since $s \leq 4$, only the monomers in states $s - 2$ or $s - 3$ can be blocked. This implies, that within the subchain from m_k to m_{j-1} , the number of blocked monomers is at most within an additive factor 1 from the number of unblocked monomers.

Suppose, for a given subchain from m_k to m_{j-1} , the number of monomers in state s is strictly positive (that is, $\#(s) \geq 1$). Then, $\#(s) \geq \frac{1}{2}(\#(s - 2) + \#(s - 3))$, that is, in the subchain, the number of unblocked monomers is at least half the number of blocked monomers.

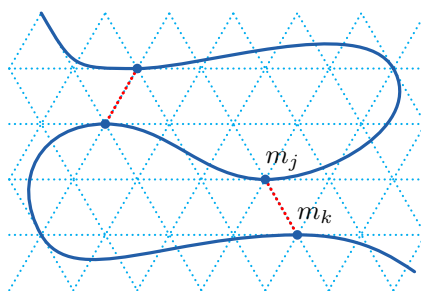
Now suppose that the number of monomers in state s in the subchain is zero (that is, $\#(s) = 0$). As the blocked monomer m_i has state either $s - 2$ or $s - 3$, the x -coordinate decreases by 1 when traversing it. The x -coordinate only increases when traversing monomers in state s . Therefore, if there are no monomers in state s , ε_x has to be 1, and, besides the blocked monomer m_i , the subchain from m_k to m_{j-1} consists only of monomers in states $s - 4$ and $s - 1$.

Furthermore, as $\varepsilon_x = 1$, we have that $pos(m_k) = pos(m_j) - \vec{w}$ (that is, m_i is in state $s - 3$). We claim that there is at least one monomer in state $s - 1$ in the subchain from m_k to m_{j-1} . Indeed, consider the second part of Equation|5. Traversing the edge between monomers m_k and m_j changes the y -coordinate by $\varepsilon_y = y(m_j) - y(m_k) = y(-\vec{w}) = -1$. Thus there has to be at least one monomer traversing which increases the y -coordinate. This can only be a monomer in state $s - 1$. Thus, in the subchain from m_k to m_{j-1} , there is one blocked monomer m_i and at least one unblocked monomer in state $s - 1$, and the total number of unblocked monomers is at least the number of blocked monomers. ◀

► **Theorem 23.** *For each $n \in \mathbb{N}$ and $1 \leq s \leq 4$, the line rotation Turning Machine L_n^s computes its target configuration in $O(\log n)$ steps.*

Proof. By Theorem 13 the Turning Machine L_n^s computes its target configuration. That it computes the target configuration in $O(\log n)$ steps follows from the claim that in any intermediate configuration c , the number of blocked monomers is not greater than $3n/4$.

To prove this claim, consider a reachable configuration c of L_n^s , and consider all blocked monomers $B = \{m_i : m_i \text{ is blocked}\}$. Let $e_{j,k}$ be the edge connecting the positions of two monomers m_j and m_k which block the movement of some monomer $m_i \in B$ (note, that m_i



■ **Figure 10** Subdivision D' of the plane consists of chain L_s^n (shown in blue), and all edges (shown in red), connecting pairs of monomers blocking the movement of some monomer, such that these edges are incident to the outer face of D' .

can be blocked by more than one pair of monomers). Let $E = \{e_{j,k}\}$ be the set of all such edges for all pairs m_j and m_k which block some monomer in L_s^n . Observe, that no two edges in E cross each other, as they are unit segments in the triangular graph, and for the same reason no edge in E crosses the chain L_s^n . Let the chain L_s^n together with the set of edges E partition the plain into plane subdivision D (refer to Figure 10). The bounded faces of D are formed of subchains of L_s^n and edges from E . Now, remove the edges of E from D which are not incident to the outer face, resulting in a plane subdivision D' . In it, every bounded face is formed by a single subchain of L_s^n and a single edge from E .

Observe, that all monomers of L_s^n which are blocked are incident to at least one bounded face. Otherwise, there would be two monomers m_j and m_k blocking the move with the edge $e_{j,k}$ not in E , thus contradicting the definition of E .

For each bounded face f_i in D' , by Lemma 22, we have $\#_i(\text{unblocked}) \geq \frac{1}{2}\#_i(\text{blocked})$, where $\#_i(\text{unblocked})$ denotes the number of unblocked monomers incident to the face f_i , and $\#_i(\text{blocked})$ denotes the number of blocked monomers incident to the face f_i .

Note, that each unblocked monomer can be incident to at most two bounded faces of D' , and recall that each blocked monomer is incident to at least one bounded face of D' . Then,

$$\#(\text{unblocked}) \geq \frac{1}{2} \sum_{f_i \in D'} \#_i(\text{unblocked}) \geq \frac{1}{2} \left(\frac{1}{2} \sum_{f_i \in D'} \#_i(\text{blocked}) \right) \geq \frac{1}{4} \#(\text{blocked}),$$

where the sums are over the bounded faces of D' , and $\#(\text{unblocked})$ denotes the total number of unblocked monomers in L_s^n , and $\#(\text{blocked})$ denotes the total number of blocked monomers in L_s^n .

Since there is a constant fraction of unblocked monomers in any configuration, the total expected time it takes L_n^s to compute its target configuration is $O(\log n)$. ◀