On Flat-State Connectivity of Chains with Fixed Acute Angles*

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Abstract

We prove that two classes of fixed-angle, open chains with acute angles are "flat-state connected." A chain is *flat-state connected* if it can be reconfigured between any two of its planar realizations without self-crossing. In a companion paper (under preparation) [ADD+], several fixed-angle linkages will be proved flat-state connected or disconnected. In particular, all orthogonal or obtuse-angle open chains are flat-state connected. But it remains open whether this holds for acute-angle open chains. In this paper, we prove that two classes of such chains are indeed flat-state connected: those with equal acute angles, and those with equal edge lengths and angles in $(60°, 90°]$. We claim, but do not prove, an extension of the latter result to the range $[45°, 90°]$ without length restriction.

1 Introduction

The focus of this paper is *fixed-angle* polygonal chains, those which maintain a fixed angle between each pair of incident edges, in addition to fixed edge lengths. These chains are natural models of protein backbones, and consequently are of considerable interest in polymer physics. Here we continue the study [ADD+], but specialized to open chains. A *fixed-angle chain* is determined by its fixed sequence of edge lengths and angles between adjacent edges. A *realization* C of a chain is specified by the position of its $n+1$ vertices: $v_0, v_1, \ldots, v_n$. A *flat state* of a chain is an embedding of it into a plane without self-intersection. The question we seek to answer is this: Is there a motion that reconfigures a chain between any two of its flat states? The motion passes through nonflat configurations in $\mathbb{R}^3$ intermediate between the two flat states, and should avoid self-crossing and maintain the fixed lengths and angles throughout. If a chain satisfies this property, we say it is *flat-state connected*. As mentioned in the abstract, it is known that all orthogonal or obtuse-angle open chains are flat-state connected, but the question is unresolved for acute-angle chains. We prove this for two classes of such chains. In both cases, the proof proceeds by reconfiguring the chains into a canonical form. Once we know any flat state can reach this canonical form, we know two flat states are connected via this form.

The motions that maintain fixed angles are called *dihedral motions*, terminology borrowed from biochemistry, because they can be "factored" into *edge spins* [ST00], each about an interior edge e_i that alters the "dihedral angle" between the planes determined by e_i and the adjacent edges e_{i-1} and e_{i+1}.

2 Equal Acute Angles

Let $C = (v_0, v_1, \ldots, v_n)$ be an open chain with links or edges $e_i = (v_{i-1}, v_i)$, $i = 1, \ldots, n$; thus the vector along the ith link is $v_i - v_{i-1}$. Let the fixed angle between each two consecutive edges be 2α, with $\alpha \leq 45°$. The canonical form of the chain is the zig-zag embedding in which each e_{i-1} and e_{i+1} lie on opposite sides of e_i. This embedding is monotone, and clearly avoids self-intersection. We will show that if C is embedded in the xy-plane, we can reconfigure it via dihedral motions into its canonical form in a plane P parallel to the z-axis; we call all such planes *vertical.*

One algorithm in [ADD+] for orthogonal and obtuse open chains is similar but simpler. Each link is picked up one at a time into P, which rotates to accomodate the picking up but remains at all times vertical. That algorithm is simple because it is easy to keep the chain in the positive $z > 0$ halfspace at all times, thus avoiding collision with the portion not yet lifted. For acute-angled chains, this is no longer so straightforward. Nevertheless, the overall design of our algorithm is the same, with two differences. Let C be the portion of the chain in the xy-plane, and C' the portion already lifted into P. First, the canonical form in P is at all times tilted so that any line containing an edge of C' makes an angle α with the xy-plane. Second, the lifting move is less straightforward.

After iteration i of the algorithm, the following invariants have been established:

- $C = (e_{i+1}, \ldots, e_n)$ remains unmoved in the xy-plane.

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- $C' = (e_1, \ldots, e_i)$ is canonically embedded in P.
- P is vertical.
- C' lies in the $z > 0$ half space, except for its endpoint v_i.
- Each edge e_i of C' makes an angle of α with the xy-plane.

We choose to illustrate the algorithm for orthogonal chains, $2\alpha = 90°$ (for which, as mentioned, there is a simpler algorithm). The issues are the same, and it is perhaps easier to understand the lifting move in this case. Fig. 1 illustrates the invariant situation for an orthogonal chain after step i. Step $i + 1$ lifts edge e_{i+1}

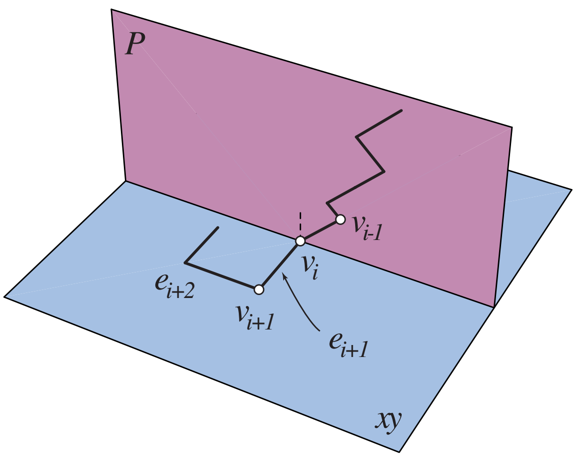

Figure 1: After step i. Note that each edge in P forms an angle of $\alpha = 45°$ with the xy-plane.

to a plane P', as illustrated in Fig. 2. It is clear that

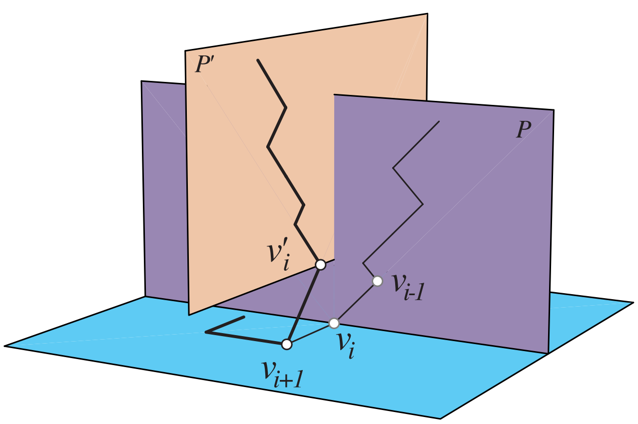

Figure 2: After step $i + 1$.

all the invariants have been reestablished. The only difficult part is showing that the lifting of e_{i+1} and the twisting of P to P', can be accomplished by dihedral motions, i.e., without altering the fixed angles at the joints.

The rotation of v_i about e_{i+2} to v'_i (see Fig. 2) clearly maintains the fixed angle 2α at v_{i+1}: we simply rotate e_{i+1} along the cone of angle 2α, whose axis is e_{i+2} and apex v_{i+1}. This cone, which will play a role below, represents all the positions of e_{i+1} that maintain the fixed angle at v_{i+1}. For the illustrated case, $2\alpha = 90°$, this cone is in fact a disk perpendicular to e_{i+2}. This rotation is continued until e_{i+1} forms the angle α with the xy-plane. The chain C' from e_1 to e_{i-1} moves rigidly in $\mathbb{R}^3$, so its angles remain fixed. It only remains to argue that the moves can be made in such a way that the angles at v_{i-1} and v_i remain fixed, and that at all times the edges of C' make an angle α with the xy-plane.

Consider this last requirement. We spin P about a vertical line L through v_i. To accomplish this, we spin $e_i = (v_{i-1}, v_i)$ about this vertical line, keeping its angle with the vertical fixed at $\pi/2 - \alpha$, and therefore its angle with the xy-plane fixed at α. This has e_i moving on a cone V whose axis is L and whose apex is v_i. See Fig. 3. In order to maintain an angle of 2α at v_i, e_i must simultaneously move on another cone W, this of angle 2α, centered on e_{i+1} with apex v_i. Therefore, e_i should lie along the line of intersection of these two cones, both of whose apex is v_i. When it does, the plane P is determined, and the angle at v_{i-1} is retained at 2α, as illustrated in Fig. 3. It only remains to argue

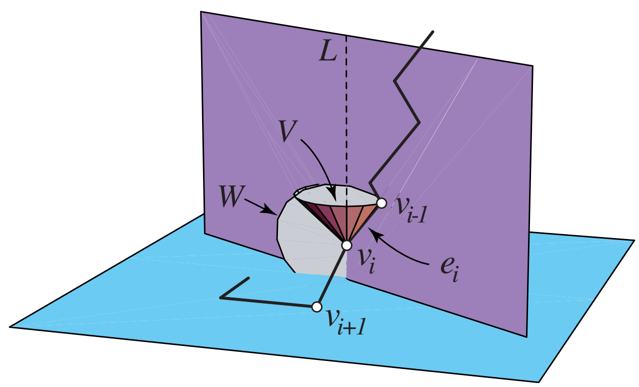

Figure 3: Intermediate between steps i and $i+1$. Edge e_i moves on two cones, one, V, of angle $\pi/2 - \alpha = 45°$, and one, W, of angle $2\alpha = 90°$.

that the two cones V and W indeed intersect.

The movement of V is easy to understand: it merely translates in $\mathbb{R}^3$, attached to its apex v_i. W, however, rotates in space as its axis e_{i+1} rotates. Let B be interval of angles that rays in W make with the line L. B starts at $[\pi/2 - 2\alpha, \pi/2 + 2\alpha]$ when e_{i+1} is in the xy-plane ($[0°, 180°]$ in Fig. 1), and ends at $[\pi/2 - \alpha, \pi/2 + 3\alpha]$ when e_{i+1} forms an angle of α with the xy-plane ($[45°, 225°]$ in Fig. 2). Throughout, $|B|$ spans 4α, the angle of W about e_{i+1}. In between the smallest angle β of B changes monotonically, because e_{i+1} is lifting its angle with the xy-plane monotonically as it rotates about e_{i+2}. Therefore, throughout the lifting move, $\beta \in [\pi/2 - 2\alpha, \pi/2 - \alpha]$. Recalling that the angle of V with respect to L is $\pi/2 - \alpha$, we see that at all times $V \cap W \neq \emptyset$; the two cones become tangent at the end of the motion. Therefore, a motion that keeps the angle at v_i fixed while maintaining the invariants is possible. We have proved

Theorem 2.1 *Any two flat states of an open chain with fixed, equal angles $0 < 2\alpha \leq 90°$ are connected by a dihedral motion.*

3 Unit-Length Chains with Angles in $(60°, 90°]$

In this section we prove that unit-length chains with angles in the range $(60°, 90°]$ are flat-state connected. Our algorithm may also be used for linkages with nonacute angles.

Let the angles of a chain $C = (v_0, v_1, \ldots, v_n)$ be $\alpha_1, \alpha_2, \ldots, \alpha_{n-1}$, as shown in Fig. 4.

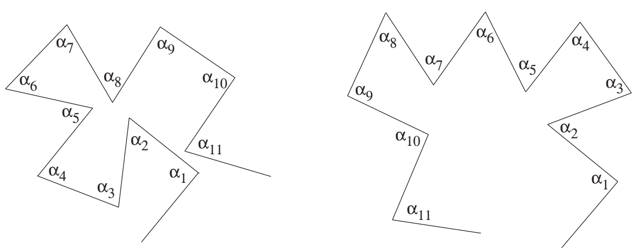

Figure 4: Two flat states of a unit-length chain with nonobtuse angles greater than 60°.

3.1 The Canonical Configuration

We say that an angle α_i is a *left (right) turn* if v_{i+1} is to the left (right) of $\overrightarrow{v_{i-1}v_i}$; we abbreviate the turns as L and R when convenient. The canonical configuration is again embedded in a vertical plane, orthogonal to the chain C in the xy-plane. But, unlike in the previous section, the turns do not necessarily alternate left-right.

Let e_1 be placed horizontally. There are two choices for placing any given edge e_i with angle α_i. Our choice for placing edge e_i with a left or right turn will be based on the *height* (z-coordinate) of the new endpoint (v_i) of this intermediate chain. We choose to place each new edge so that the new endpoint is at a maximum height—a greedy approach. Fig. 5 shows how we would build the canonical configuration of the linkage in Fig. 4, with the height of each vertex v_i labeled z_i.

Lemma 3.1 *In the canonical configuration of a chain, the height of even vertices increases monotonically, and similarly for odd vertices.*

Proof: Omitted in this version. The restriction of the angle to $(60°, 90°]$ is crucial here. $\square$

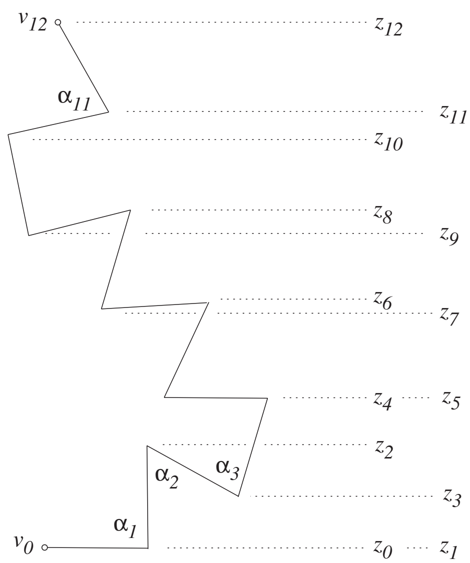

Figure 5: A canonical configuration in the vertical plane P.

We see from Lemma 3.1 that whenever $z_{k-1} > z_k$ and α_{k-1} is a left (right) turn, then α_k must be a right (left) turn. Furthermore $z_{k+1} > z_{k-1}$.

We wish to prove that a linkage in canonical form must be non-self-intersecting. We use the following facts:

1. Three consecutive edges cannot self-intersect.
2. Five consecutive edges with the turn sequence (L, R, R, L) cannot self-intersect.
3. Four consecutive edges cannot self-intersect unless all turns are L or all R.

These facts lead to a proof of the following lemma, whose proof is omitted.

Lemma 3.2 *A chain in canonical form must be non-self-intersecting.*

Note that the canonical form is unique if none of its edges point directly upward. If an edge points upward, the subchain above it may be placed in two positions that satisfy the canonical criteria. In order to create a unique canonical configuration we may choose to form right turns after vertical edges. Even if we do not have such a rule, it is clear that different versions of the canonical form are flat-state connected.

3.2 Reconfiguring to Canonical Form

C lies in the xy-plane. We now describe how to reconfigure it into its canonical form in the vertical plane. We begin by lifting e_1 so that it projects vertically onto e_2. Now suppose that we have part of the chain C still in

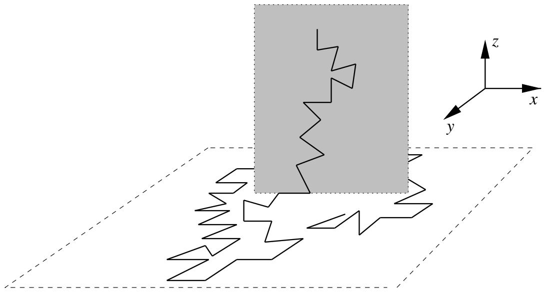

Figure 6: A chain partially in canonical form.

the original configuration, and part of it, C', embedded in the vertical plane P in canonical form, as in Fig. 6.

We want to move C' into a position above the next edge e_{i+1} of C, as illustrated in Fig. 7. The edge e_i common to both planes will be lifted so that C' will project down to the line through the next horizontal edge e_{i+1}.

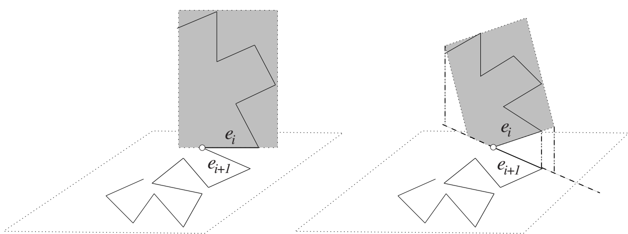

Figure 7: Lifting edge e_i into canonical form.

We perform two simultaneous dihedral motions during this operation. Edges that are already in canonical configuration remain coplanar (in a vertical plane) throughout these motions. We rotate e_i about e_{i+1}, on the cone of angle α_i with axis e_{i+1}, and at the same time we rotate the canonical plane accordingly, so that it always projects vertically through e_i. We call these two dihedral motions *primary*.

During these motions, we wish to maintain the properties of the canonical chain. We need to intervene only if an edge e_k points directly upward during the primary motion. At this instant, the chain C_k above e_k may be placed arbitrarily in either of two possible positions in the canonical plane. If the overall motion were to continue as is, e_k and the edge above it will no longer satisfy the greedy property. Thus we rotate C_k about e_k and proceed with the primary motion, until another edge becomes vertical or e_i reaches its target position above e_{i+1}.

It is best to visualize this idea from a view direction perpendicular to the canonical plane. From this viewpoint, the canonical chain appears to be rotating continuously in its plane. Fig. 8 shows a canonical chain rotating counterclockwise in its plane. Dashed edges show the alternative position of each edge. We see that as the chain rotates, edges maintain their greedy positions until an edge e_k becomes vertical. If the chain continues to rotate, the property will no longer hold for the edge above e_k. Performing a dihedral rotation of C_k about e_k resolves this problem for e_k.

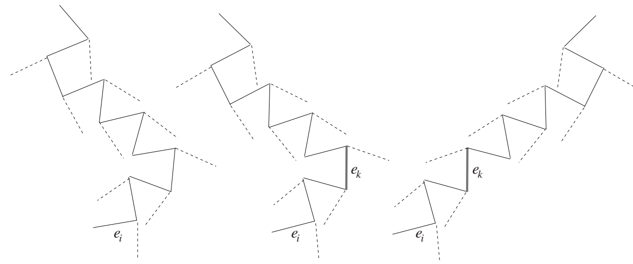

Figure 8: When e_k becomes vertical, the chain above rotates to maintain the canonical height property.

Unfortunately, an edge e can become vertical many times throughout the life of this algorithm; we have an example that forces it to make an exponential number of dihedral rotations. Although this does not affect the main claim of connectivity for $(60°, 90°]$-chains, it does detract from the method.

In search of alternatives, we found (too late for inclusion in this abstract) a new algorithm that establishes flat-state connectivity for any chain with angles α_i such that $\alpha_i \leq a_{i-1} + \alpha_{i+1}$ (the first and last angle can have any value). In particular, this relationship is satisfied for angles in the range $[45°, 90°]$. Not only is this angle range wider, but the restriction to unit-length is no longer needed.

4 Open Problem

The main open problem is to prove or disprove that every open chain with acute angles is flat-state connected. A step towards this would be resolving the question for unit-length acute-angled chains.

References

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