Classifying Three-Fold Symmetric Hexagons

by

Amanda Kimbrell Gantt

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INTRODUCTION

An *octahedron* is a polyhedron with six vertices, twelve edges, and eight triangular faces. Since a hexagon has six vertices and six edges, it is possible to embed a hexagon within an octahedron in many different ways. Suppose we determine the lengths of all six edges of the hexagon and the measure of the angle between each of the two edges incident on each vertex. In the octahedron, the length of the third side of the triangular face containing two edges of the hexagon will then be determined. Hence all the lengths of all twelve edges of the octahedron will be determined. Bricard [**2**] studied octahedra where all twelve edges had specified lengths. In general one might expect any such octahedron to be rigid, but Bricard found that when the lengths of the twelve edges had certain types of symmetry the octahedron could be flexible. This means that it is possible for hexagons to be flexible. This has long been known to be the case for an equilateral hexagon where all the angles are $\cos^{-1}(-\frac{1}{3})$, since the molecule cyclohexane has that structure; in organic chemistry the flexible family of shapes of cyclohexane is known as the twist/boat family [**6**]. Dr. Dix [**6**] continued Bricard's research by finding explicit solutions for flexible

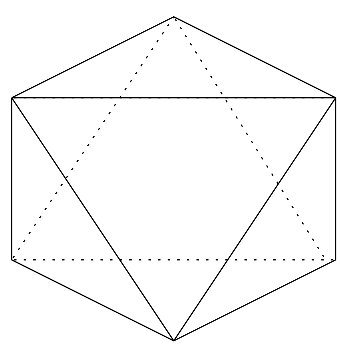

FIGURE 1. An Octahedron

and rigid hexagons when the six lengths and six angles have a two-fold symmetry as one cycles around the hexagon. An interesting feature of the family of two fold symmetric hexagons was that none of them were knotted. Hexagons are the polyhedra with the fewest number of sides which could possibly be knotted [**7**]. We do not know if an explicit formula for knotted hexagons has ever been published. In Dix [**6**], it was conjectured that such formulas could be obtained for hexagons whose six lengths and six angles have three-fold symmetry as one cycles around the hexagon. We will henceforth refer to such hexagons as $three - fold\ symmetric$.

Using the same methodology as used on the two fold symmetric case in [**6**], we will study in this thesis how to classify three-fold symmetric hexagons. We will gain a full understanding of a three-fold symmetric hexagon under the assumptions that all six angles are equal. When all six angles are equal, we give a sufficient condition on the lengths and angles for the existence of a knotted hexagon and conjecture that it is also necessary. Even when all the angles are not equal, if the two independent lengths and the two independent angles are specified, we can enumerate all possible shapes the hexagon can assume (excluding certain cases where certain triples of vertices are collinear).

CHAPTER 1

PREVIOUS RESEARCH

Our tool for studying the shape of a three-fold symmetric hexagon in three dimensional space is the Z-System. The Z-System was created to specify the three dimensional shape of a molecule. In this thesis, we are studying the special case of hexagons. This gives us a general idea of how Z-Systems can be used in a simpler case.

In the next four sections, we will develop this general theory of Z-Systems which will be demonstrated by the study of our hexagons. From the last section, we will learn how to build hexagons with three-fold symmetry from its bonds, angles, and wedges.

1.1. Z-SYSTEM

The concept of a Z-System [**6**] starts with an arbitrary graph G. For example, we could take G to be the graph associated to a molecule: the atoms would be the vertices and the covalent bonds would be the edges. In this paper, we are identifying G as a hexagonal cycle, or a closed path with six vertices.

An unoriented Z-System builds on G by specifying three tree graphs named τ_1, τ_2, and τ_3. Recall that a tree is a connected acyclic graph. This means that any two vertices are connected in the graph by some path and the graph contains no cycle (as a subgraph). The tree τ_1 is chosen to be a spanning tree in G. This tells us that τ_1 is a tree subgraph of G containing all the vertices of G. The line graph $L(\tau_1)$ of τ_1 is a graph where each edge of τ_1 is an vertex of $L(\tau_1)$. Also, any two distinct edges of τ_1 constitute an edge of $L(\tau_1)$ if and only if the corresponding edges of τ_1 share a common vertex in τ_1 [**3**]. Next we choose τ_2 to be a spanning tree in the line graph $L(\tau_1)$ of τ_1. Finally, we can choose τ_3 to be a spanning tree in $L(\tau_2)$ of τ_2. The vertices of our spanning tree τ_1 will be called *atoms*. In

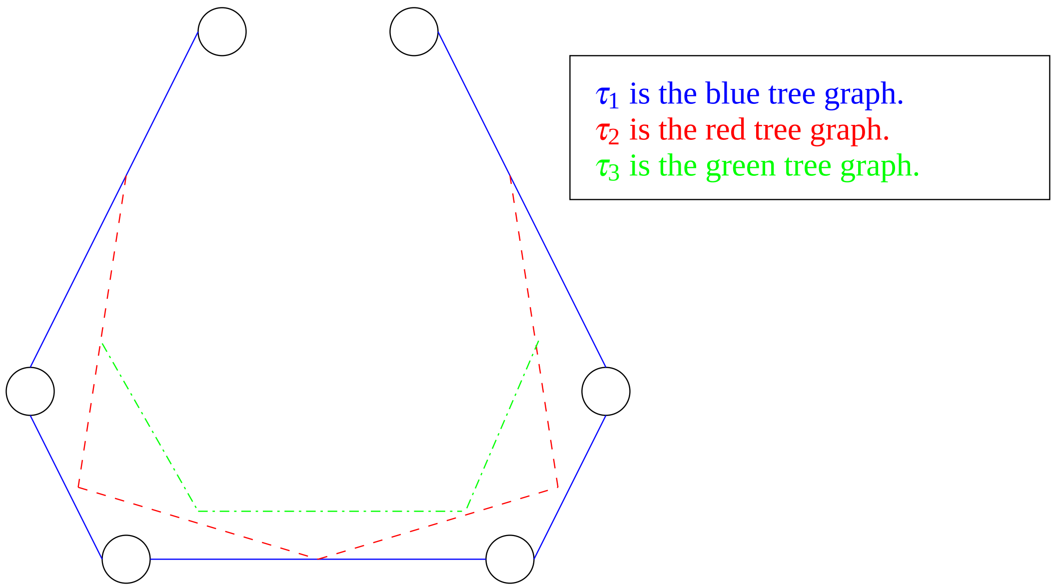

FIGURE 2. An unoriented Z-System built on G

our three-fold symmetric hexagon G, there exists only six atoms. The edges connecting those atoms in τ_1 will be referred to as *bonds*. Since τ_2 has vertices that are edges of τ_1, we will also refer to the vertices of τ_2 as bonds. The edges of τ_2 will be named *angles*. Since τ_3 is a subgraph of $L(\tau_2)$, τ_3 vertices are the same as the edges of τ_2, therefore they are also called angles. Finally, we can name the edges of τ_3 *wedges*.

The purpose of the unoriented Z-System (τ_1, τ_2, τ_3) is to provide an index set for the coordinates necessary to determine a specific three dimensional shape of the graph G. We can label each edge β of τ_1 by a length ℓ_β. This $\ell_\beta > 0$ is the distance between the two associated vertices in three dimensional space. The edges α of τ_2 will have the label of θ_α where $\theta_\alpha \in (0, 180^\circ)$ is the measure of the angle between the two line segments of the bonds. We label each edge ω of τ_3 with a pair $(d^*_\omega, \phi_\omega)$ where d^*_ω is an oriented tetrahedron (explained below) associated with ω, and ϕ_ω is the wedge angle that satisfies $-180^\circ < \phi_\omega \leq 180^\circ$. The wedge angle is the signed angle between two half-planes sharing the same boundary line. The interpretation of the sign of ϕ_ω is determined by our value of d^*_ω which is explained further in the next section.

1.2. WEDGES

As we saw above, a wedge ω is an unordered pair of angles $\{\alpha, \alpha'\}$ which share a common bond β. This wedge is labeled by a pair (d^*, ϕ). Each angle is an unordered pair $\{b, b'\}$ of bonds which share a common atom and corresponds to a set of three atoms, the *triangle* associated to that angle. In this section, we will discuss (d^*, ϕ) in more detail.

The wedge ω determines a *tetrahedron* d, which is a four element set of atoms determined as follows. The tetrahedron is the union of the two triangles that correspond with the two angles. Let $d = \{A_0, A_1, A_2, A_3\}$ be the tetrahedron of the wedge $[\alpha, \alpha']$ with triangle one $\{A_0, A_1, A_2\}$ being the vertices correlating to angle α and triangle two $\{A_1, A_2, A_3\}$ being the vertices correlating to angle α'. The common bond is $\{A_1, A_2\}$.

An orientation of d is an equivalence class of orderings of the four element set d. Two orderings are deemed equivalent if one can be obtained from the other via an even permutation. There are two possible orientations of the set d. To find these two orientations, it must be noted that there are 24 permutations of the set d, which creates two disjoint subclasses consisting of 12 permutations each. These permutations are:

$$\begin{array}{ccc}
(A_0, A_1, A_2, A_3) & \longrightarrow_{\swarrow} & (A_1, A_0, A_2, A_3) \\
(A_1, A_0, A_3, A_2) & \longrightarrow_{\swarrow} & (A_0, A_1, A_3, A_2) \\
(A_0, A_3, A_1, A_2) & \longrightarrow_{\swarrow} & (A_2, A_3, A_1, A_0) \\
(A_2, A_1, A_3, A_0) & \longrightarrow_{\swarrow} & (A_2, A_1, A_0, A_3) \\
(A_1, A_2, A_0, A_3) & \longrightarrow_{\swarrow} & (A_1, A_2, A_3, A_0) \\
(A_0, A_2, A_3, A_1) & \longrightarrow_{\swarrow} & (A_0, A_3, A_2, A_1) \\
(A_1, A_3, A_2, A_0) & \longrightarrow_{\swarrow} & (A_3, A_1, A_2, A_0) \\
(A_3, A_1, A_0, A_2) & \longrightarrow_{\swarrow} & (A_3, A_0, A_1, A_2) \\
(A_3, A_0, A_2, A_1) & \longrightarrow_{\swarrow} & (A_3, A_2, A_0, A_1) \\
(A_3, A_2, A_1, A_0) & \longrightarrow_{\swarrow} & (A_0, A_2, A_1, A_3) \\
(A_2, A_0, A_1, A_3) & \longrightarrow_{\swarrow} & (A_2, A_0, A_3, A_1) \\
(A_2, A_3, A_0, A_1) & \longrightarrow_{\swarrow} & (A_1, A_3, A_0, A_2)
\end{array}.$$

These two columns represent the two distinct orientations; furthermore each arrow representing a transposition. $[A_0, A_1, A_2, A_3]$ will denote the orientation containing the permutation (A_0, A_1, A_2, A_3). Therefore, the two possible orientations of d are $[A_0, A_1, A_2, A_3]$ and $[A_1, A_0, A_2, A_3]$.

Suppose $\{A_1, A_2\} = \beta$ is the common bond of wedge ω. Let us investigate the similarities and differences of these two columns of permutations by taking (A_0, A_1, A_2, A_3) and

(A_3, A_2, A_1, A_0) from the first column of permutations and (A_3, A_1, A_2, A_0) and (A_0, A_2, A_1, A_3) from the second column. These four permutations are the only ones that contain A_1 and A_2 in the middle columns. We can see from our figure 3 that the same spatial configuration can be described in terms of all four permutations, but they require two distinct values of ϕ to do so.

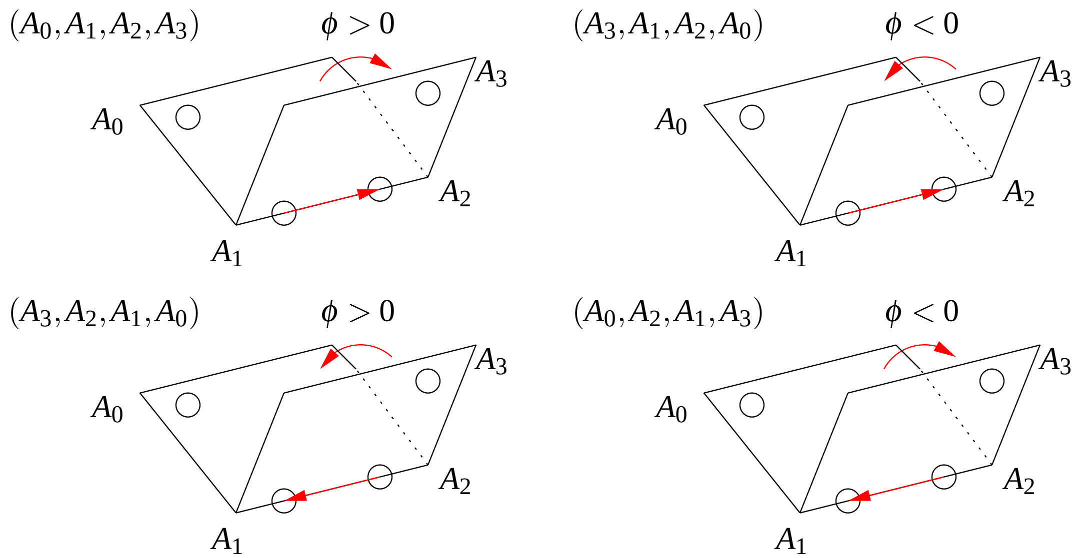

FIGURE 3. Permutations of Wedges

The sign of the angle between the two half planes is defined by the orientation of the axis of rotation (using the right hand rule) as well as the definition of which half plane start and ends the rotation. The first three atoms in a permutation determine which half plane starts the rotation, and the last three atoms determine which half plane ends the rotation. We can observe from the example in our figure how the orientation effects the value of ϕ. Permutations from column one correspond to values of ϕ that are greater than zero, and permutations from column two correspond to values of ϕ that are less than zero. Within each orientation there are two permutations which interpret the wedge angle ϕ, but both correspond to the same spatial configuration. If we change the orientation, we must also change the sign of ϕ.

There are two different types of wedges: *dihedrals* and *impropers*. Let A be the shared atom of the two bonds that correspond to angle α, and let A' be the shared atom of the two

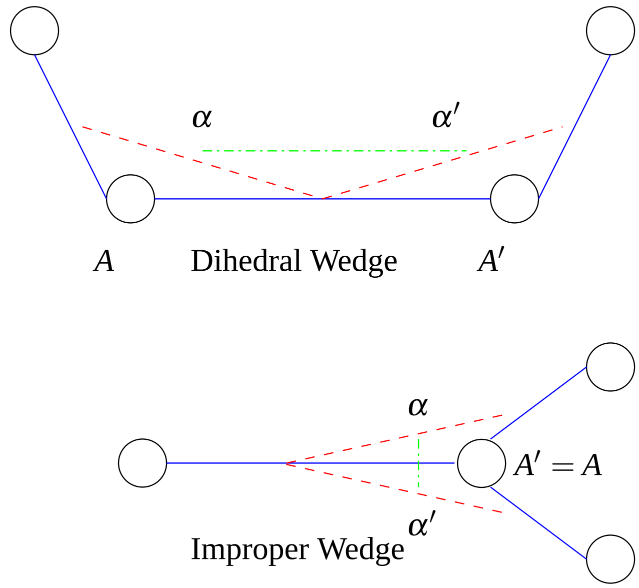

FIGURE 4. A Dihedral Wedge and an Improper Wedge

bonds that corresponds to angle α'. The wedge determined by the unordered pair of angles $\{\alpha, \alpha'\}$ is called *dihedral* if $A \neq A'$ and *improper* if $A = A'$ (see figure 3). In our hexagon graph G, all of the unordered pairs of angles which share a common bond are dihedral.

For a dihedral wedge, there is only two possible ways that the atoms can be be ordered beginning at one end of the chain of bonds and ending at the other. These two orderings are in the same equivalence class. Therefore, we know that every dihedral wedge can be assigned a canonical orientation, and we will always use this canonical orientation.

Learning about the structure of our wedge angles has shown us that we must investigate ϕ on $(-180°, 180°]$. When we are searching for ϕ values that create a three-fold symmetric hexagon, we must study the full range to find all possible solutions.

1.3. Sites and Poses

Let $\Gamma = (\tau_1, \tau_2, \tau_3)$ be an unoriented Z-System for a graph G where the $\mathscr{N}$ is the set of all vertices of G. We can denote a *site* by $r = (A_0, A_1, A_2)$ of Γ. This *site* is an ordered triple of distinct vertices from $\mathscr{N}$ with $\{A_0, A_1\}$ determining a vertex of τ_2 (i.e. a bond), and $\{A_0, A_1, A_2\}$ is the triangle corresponding to a vertex of τ_3 (i.e. an angle). In this arrangement, the angle has a common vertex at either A_0 or A_1.

Let each vertex $A \in \mathscr{N}$ be assigned a position $\mathbf{R}_A \in \mathbb{R}^3$ so that the graph G becomes embedded in three dimensional space. We can define a *pose* as a Cartesian coordinate system that is determined by our site r and by the embedding. This Cartesian coordinate system will have its origin at $\mathbf{R}_{A_0}$. The x-axis will be parallel to $\mathbf{R}_{A_1} - \mathbf{R}_{A_0}$, and the y-axis will be in the half-plane that is bounded by the x-axis and containing the point $\mathbf{R}_{A_2}$. In this Cartesian coordinate system, the direction of the z-axis is then determined by the right-hand rule. A pose is specified by means of a 3×4 matrix $(\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$. In this matrix, the position vector $\mathbf{e}_0 = \mathbf{R}_{A_0}$ is the origin, $\mathbf{e}_1$ is a unit vector that determines the x-axis, and $\mathbf{e}_2$ is a unit vector that determines the y-axis. The unit vector $\mathbf{e}_3$ is the direction of the z-axis. Therefore,

$$
\begin{aligned}
\mathbf{e}_0 &= \mathbf{R}_{A_0} \\
\mathbf{e}_1 &= \frac{\mathbf{R}_{A_1} - \mathbf{R}_{A_0}}{||\mathbf{R}_{A_1} - \mathbf{R}_{A_0}||} \\
\mathbf{e}_2 &= \frac{(\mathbf{1} - \mathbf{e}_1\mathbf{e}_1^T)(\mathbf{R}_{A_2} - \mathbf{R}_{A_0})}{||(\mathbf{1} - \mathbf{e}_1\mathbf{e}_1^T)(\mathbf{R}_{A_2} - \mathbf{R}_{A_0})||} \\
\mathbf{e}_3 &= \mathbf{e}_1 \times \mathbf{e}_2
\end{aligned}
$$

In the third formula, $\mathbf{1}$ denotes the (3×3) identity matrix, and $\mathbf{e}_1^T$ is the (1×3) row vector created from the transpose of column vector $\mathbf{e}_1$. The site r then determines from the embedding the Cartesian coordinate system (or the *pose*) denoted by $E_r(\mathbf{R}) = (\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$. To make $E_r(\mathbf{R})$ well-defined, the singular embeddings $\mathbf{R} : \mathscr{N} \to \mathbb{R}$ must be excluded, i.e. those where the denominators in the formulas for $\mathbf{e}_1$ and $\mathbf{e}_2$ are zero.

In our pose $(\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ where $\mathbf{e}_0 \in \mathbb{R}^3$, $X = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ is a right-handed orthonormal basis of $\mathbb{R}^3$. This X is contained in $SO(3)$;and its determinant is $+1$. Also, the inverse of X is its transpose. If $\mathbf{x}$ is a point in space, it can be described by the coordinate vector $\mathbf{c} = \begin{pmatrix} x & y & z \end{pmatrix}^T$ in the pose E, i.e.

$$
\mathbf{x} = \mathbf{e}_0 + \mathbf{e}_1 x + \mathbf{e}_2 y + \mathbf{e}_3 z = (\mathbf{e}_0, X) \begin{pmatrix} 1 \\ \mathbf{c} \end{pmatrix}.
$$

If $E = (\mathbf{e}_0, X)$ and $E' = (\mathbf{e}'_0, X')$ are any two poses, then there is a unique (4×4) matrix $M = \begin{pmatrix} 1 & (0,0,0) \\ \mathbf{b} & A \end{pmatrix}$, whose first row is $(1,0,0,0)$, such that $E' = EM$. This can be seen as follows:

$$(\mathbf{e}'_0, X') = (\mathbf{e}_0, X) \begin{pmatrix} 1 & (0,0,0) \\ \mathbf{b} & A \end{pmatrix} = (\mathbf{e}_0 + X\mathbf{b}, XA)$$

where $A = X^{-1}X'$ and $\mathbf{b} = X^{-1}(\mathbf{e}'_0 - \mathbf{e}_0)$. The matrix M is a *coordinate transformation matrix*. This matrix can transform one coordinate vector $\mathbf{c}$ into another coordinate vector $\mathbf{c}'$ with the respect to these poses by $\mathbf{x} = E \begin{pmatrix} 1 \\ \mathbf{c} \end{pmatrix} = E' \begin{pmatrix} 1 \\ \mathbf{c}' \end{pmatrix} = EM \begin{pmatrix} 1 \\ \mathbf{c}' \end{pmatrix}$. Therefore,

$$\begin{pmatrix} 1 \\ \mathbf{c} \end{pmatrix} = \begin{pmatrix} 1 & (0,0,0) \\ \mathbf{b} & A \end{pmatrix} \begin{pmatrix} 1 \\ \mathbf{c}' \end{pmatrix} \qquad \text{i.e. } \mathbf{c} = \mathbf{b} + A\mathbf{c}'.$$

Let r and r' be two sites belonging to the Z-system Γ, and let $\mathbf{R}$ be a three dimensional embedding of the graph G. Let M be the coordinate transformation matrix where $E_{r'}(\mathbf{R}) = E_r(\mathbf{R})M$; then M can be computed in terms of the numerical labels of Γ as will now be described. From Lemma 3.2 of [**6**], we know that there exists a sequence of distinct sites $r = r_0, r_1, \ldots, r_m = r'$ that belong to Γ. Every successive pair (r_{j-1}, r_j) for $1 \le j \le m$ is one of the following three types:

a. r_j can be obtained from r_{j-1} by exchanging the first two atoms.

b. r_j can be obtained from r_{j-1} by exchanging the last two atoms.

c. $r_{j-1} = (A_0, A_1, A)$ and $r_j = (A_0, A_1, A')$, where there is a wedge of Γ connecting the angles corresponding to $\{A_0, A_1, A\}$ and $\{A_0, A_1, A'\}$.

By the Theorem in section 3.3 of [**6**], for each $1 \le j \le m$:

1. If we can obtain r_j from r_{j-1} by exchanging the first two vertices named A_0 and A_1, then let $\{A_0, A_1\}$ be the bond of Γ with its length $\ell > 0$. Thus

$E_{r_j}(\mathbf{R}) = E_{r_{j-1}}(\mathbf{R})T_1(\ell)$, where:

$$T_1(\ell) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \ell & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

2. If we can obtain r_j from r_{j-1} by exchanging the last two vertices named A_1 and A_2, then $\{A_0, A_1, A_2\}$ corresponds to an angle of Γ with its label $\theta > 0$. Thus, $E_{r_j}(\mathbf{R}) = E_{r_{j-1}}(\mathbf{R})T_2(\theta)$, where:

$$T_2(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & \sin\theta & 0 \\ 0 & \sin\theta & -\cos\theta & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

3. If $r_{j-1} = (A_0, A_1, A)$ and $r_j = (A_0, A_1, A')$ where there is a wedge of Γ connecting the angles corresponding to $\{A_0, A_1, A\}$ and $\{A_0, A_1, A'\}$, and the wedge is labeled by $(\pm[A, A_0, A_1, A'], \phi)$. Then $E_{r_j}(\mathbf{R}) = E_{r_{j-1}}(\mathbf{R})T_3(\pm\phi)$, where:

$$T_3(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos\phi & -\sin\phi \\ 0 & 0 & \sin\phi & \cos\phi \end{pmatrix}.$$

From this information, the coordinate transformation matrix M can be calculated as a product of the above matrices. When $E_{r'}(\mathbf{R}) = E_r(\mathbf{R})M$, we can solve for the value of M:

$$\begin{aligned} E_{r'}(\mathbf{R}) =& E_{r_m}(\mathbf{R}) = E_{r_{m-1}}(\mathbf{R})T^{(m-1)} = E_{r_{m-2}}(\mathbf{R})T^{(m-2)}T^{(m-1)} = \ldots \\ =& E_{r_0}(\mathbf{R})T^{(0)}T^{(1)}\ldots T^{(m-1)} = E_r(\mathbf{R})M. \end{aligned}$$

Therefore, $M = T^{(0)}T^{(1)}\ldots T^{(m-1)}$.

1.4. Bridging Algorithm

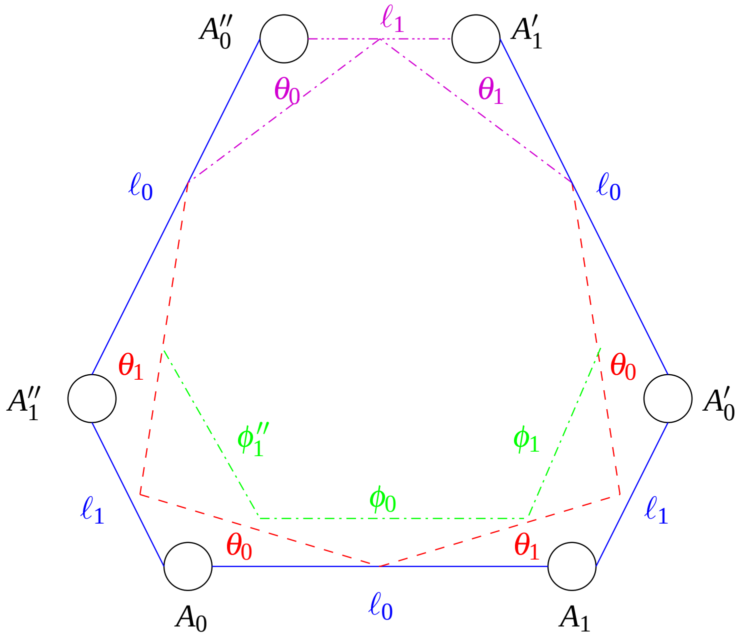

Figure 5. Labeled Hexagon

In this section, we will describe the Bridging Algorithm from [**6**] that has been transposed into the language needed to describe our hexagon. The problem we must solve is as follows; if we are given values ℓ_0, ℓ_1, θ_0, and θ_1, then we must find ϕ_0, ϕ_1, and ϕ_1'' such that:

a. $\|\mathbf{R}_{A_1'} - \mathbf{R}_{A_0''}\| = \ell_1$,

b. $(\mathbf{R}_{A_0'} - \mathbf{R}_{A_1'}) \cdot (\mathbf{R}_{A_0''} - \mathbf{R}_{A_1'}) = \ell_0 \ell_1 \cos\theta_1$,

c. $(\mathbf{R}_{A_1'} - \mathbf{R}_{A_0''}) \cdot (\mathbf{R}_{A_1''} - \mathbf{R}_{A_0''}) = \ell_0 \ell_1 \cos\theta_0$.

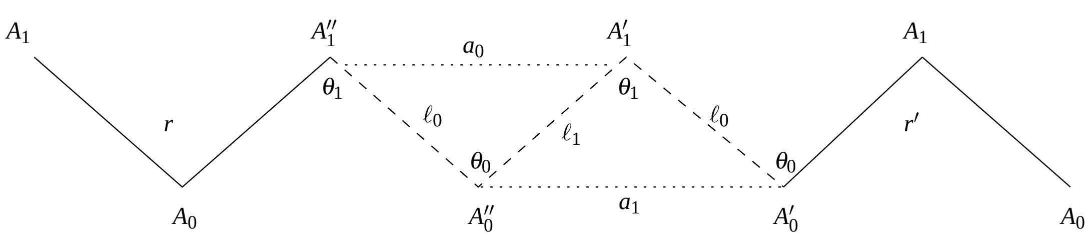

Figure 6. Bridging the Atoms

To accomplish this, we can use a more general Bridging Algorithm described in [**6**]. This more general bridging problem is as follows. In Appendix B we show how to define an embedding $\mathbf{R}(\phi_0)$ of the atoms A_1'', A_0, A_1 and A_0' in three dimensional space. Given sites $r = (A_1'', A_0, A_1)$ and $r' = (A_0', A_1, A_0)$ together with poses $E_r(\mathbf{R}(\phi_0))$ and $E_{r'}(\mathbf{R}(\phi_0))$ where $E_{r'}(\mathbf{R}(\phi_0)) = E_r(\mathbf{R}(\phi_0))M(\phi_0)$. We need to find the positions $\mathbf{R}_{A_0''}$ and $\mathbf{R}_{A_1'}$ such that conditions $\mathbf{a}, \mathbf{b}$, and $\mathbf{c}$, hold as well as:

d. $\|\mathbf{R}_{A_1''} - \mathbf{R}_{A_0''}\| = \ell_0$

e. $\|\mathbf{R}_{A_0'} - \mathbf{R}_{A_1'}\| = \ell_0$

f. $(\mathbf{R}_{A_0''} - \mathbf{R}_{A_1''}) \cdot (\mathbf{R}_{A_0} - \mathbf{R}_{A_1''}) = \ell_0 \ell_1 \cos\theta_1$

g. $(\mathbf{R}_{A_1'} - \mathbf{R}_{A_0'}) \cdot (\mathbf{R}_{A_1} - \mathbf{R}_{A_0'}) = \ell_0 \ell_1 \cos\theta_0$.

In [**6**] the solution of this more general bridging problem was broken down into three steps. First we find the first end point $\mathbf{R}_{A_0''}$ satisfying three conditions, and then we can find the second end point $\mathbf{R}_{A_1'}$ that satisfies three other conditions. During the last step, we will choose ϕ_0 so that a seventh condition holds. The following are the three steps of the Bridging Algorithm:

1. Find, as functions of ϕ_0 and $\sigma \in \{-1, 1\}$, the position $\mathbf{R}_{A_0''}$ of the vertex A_0'' relative to the configuration $\mathbf{R}(\phi_0)$ such that:

$$\|\mathbf{R}_{A_0''} - \mathbf{R}_{A_1''}(\phi_0)\| = \ell_0 \tag{1}$$

$$(\mathbf{R}_{A_0''} - \mathbf{R}_{A_1''}(\phi_0)) \cdot (\mathbf{R}_{A_0}(\phi_0) - \mathbf{R}_{A_1''}(\phi_0)) = \ell_0 \ell_1 \cos\theta_1, \tag{2}$$

$$\|\mathbf{R}_{A_0''} - \mathbf{R}_{A_0'}(\phi_0)\| = a_1, \tag{3}$$

$$\sigma \det \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{R}_{A_1''} & \mathbf{R}_{A_0} & \mathbf{R}_{A_0'} & \mathbf{R}_{A_0''} \end{pmatrix} \geq 0 \tag{4}$$

where $a_1^2 = \ell_1^2 + \ell_0^2 - 2\ell_0\ell_1 \cos\theta_1$.

2. Find, as functions of ϕ_0 and $\sigma' \in \{-1, 1\}$, the position $\mathbf{R}_{A_1'}$ of the vertex A_1' relative to the configuration $\mathbf{R}(\phi_0)$ such that:

$$\|\mathbf{R}_{A_1'} - \mathbf{R}_{A_0'}(\phi_0)\| = \ell_0, \tag{5}$$

$$(\mathbf{R}_{A_1'} - \mathbf{R}_{A_0'}(\phi_0)) \cdot (\mathbf{R}_{A_1}(\phi_0) - \mathbf{R}_{A_0'}(\phi_0))) = \ell_0 \ell_1 \cos\theta_0, \tag{6}$$

$$\|\mathbf{R}_{A_1'} - \mathbf{R}_{A_1''}(\phi_0)\| = a_0, \tag{7}$$

$$\sigma' \det \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{R}_{A_0'} & \mathbf{R}_{A_1} & \mathbf{R}_{A_1''} & \mathbf{R}_{A_1'} \end{pmatrix} \geq 0 \tag{8}$$

where $a_0^2 = \ell_1^2 + \ell_0^2 - 2\ell_0\ell_1 \cos\theta_0$.

3. For each pair $(\sigma, \sigma') \in \{-1, 1\}^2$, find ϕ_0 such that:

$$\|\mathbf{R}_{A_0''}(\phi_0, \sigma) - \mathbf{R}_{A_1'}(\phi_0, \sigma')\| = \ell_1.$$

In order to solve step one, we first need some notation. Let the known position of A_0' be:

$$\mathbf{R}_{A_0'}(\phi_0) = E_{r'}(\mathbf{R}(\phi_0)) \begin{pmatrix} 1 \\ \mathbf{0} \end{pmatrix} = E_r(\mathbf{R}(\phi_0)) M(\phi_0) \begin{pmatrix} 1 \\ \mathbf{0} \end{pmatrix} = E_r(\mathbf{R}(\phi_0)) \begin{pmatrix} 1 \\ \mathbf{x}_1'(\phi_0) \end{pmatrix},$$

where $\begin{pmatrix} 1 \\ \mathbf{x}_1'(\phi_0) \end{pmatrix} = M(\phi_0) \begin{pmatrix} 1 \\ \mathbf{0} \end{pmatrix}$ and $\mathbf{x}_1' = (x_1', y_1', z_1')^T$. Let the unknown position of A_0'' be: $\mathbf{R}_{A_0''} = E_r(\mathbf{R}(\phi_0)) \begin{pmatrix} 1 \\ \mathbf{x}_0 \end{pmatrix}$ where $\mathbf{x}_0 = (x_0, y_0, z_0)^T$. The following lemma solves the system of equations giving us the values of x_0, y_0 and z_0.

LEMMA 1.1. *If* $[y_1'(\phi_0)]^2 + [z_1'(\phi_0)]^2 > 0$ *then* $(1)-(4)$ *has at least one real solution* $\langle x_0, y_0, z_0 \rangle$ *if and only if*

$$\left| \ell_0^2 \sin\theta_1{}^2 + [y_1'(\phi_0)]^2 + [z_1'(\phi_0)]^2 + (\ell_0 \cos\theta_1 - x_1'(\phi_0))^2 - a_1^2 \right| \tag{9}$$

$$\leq 2\ell_0 \sin\theta_1 \sqrt{[y_1'(\phi_0)]^2 + [z_1'(\phi_0)]^2}.$$

If these conditions hold then all the solutions are of the form :

$$x_0 = \ell_0 \cos\theta_1 \tag{10}$$

$$\begin{aligned}\langle y_0, z_0\rangle =& \langle y_1'(\phi_0), z_1'(\phi_0)\rangle \frac{\ell_0 \sin\theta_1 \cos\alpha}{\sqrt{[y_1'(\phi_0)]^2+[z_1'(\phi_0)]^2}} \\ &+\sigma\langle -z_1'(\phi_0), y_1'(\phi_0)\rangle \frac{\ell_0 \sin\theta_1 \sin\alpha}{\sqrt{[y_1'(\phi_0)]^2+[z_1'(\phi_0)]^2}},\end{aligned} \tag{11}$$

$$\phi_1'' = -\gamma - \sigma\alpha \tag{12}$$

where $\sigma \in \{-1, 1\}$, $\alpha \in [0, 180^\circ]$ *is such that*

$$\cos\alpha = \frac{\ell_0^2 \sin^2\theta_1 + [y_1'(\phi_0)]^2 + [z_1'(\phi_0)]^2 + (\ell_0\cos\theta_1 - x_1'(\phi_0))^2 - a_1^2}{2\ell_0 \sin\theta_1 \sqrt{[y_1'(\phi_0)]^2+[z_1'(\phi_0)]^2}} \tag{13}$$

and

$$\gamma = arg(y_1'(\phi_0) + i z_1'(\phi_0)). \tag{14}$$

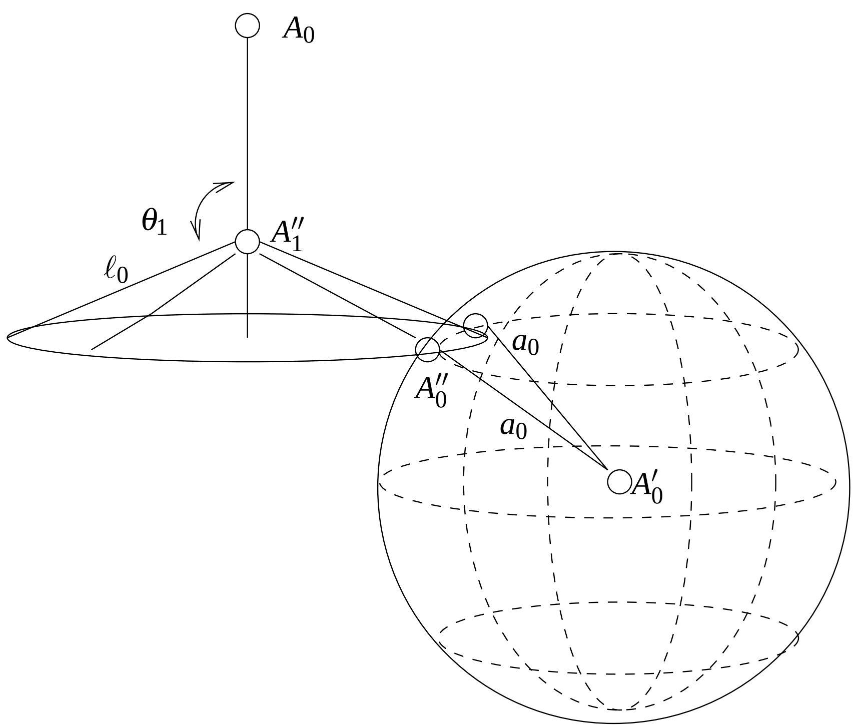

FIGURE 7. The Sphere and Cone of the Solutions of A_0''

PROOF. As seen in figure 6, we can find a sphere of radius a_1 centered at A'_0 of possible values of A''_0. There is a circle of values of A''_0 that has to satisfy the given angle and length from A''_1. We use the coordinate system given by pose $E_r(R(\phi_0))$ whose origin is at A''_1 and whose x-axis points from A''_1 to A_0. We can find the x coordinate of A''_0, i.e. $x_0 = \ell_0 \cos\theta_1$. Let us consider the plane of all points whose x coordinate is $\ell_0 \cos\theta_1$. This plane will contain two circles of possible values of A''_0, as shown in Figures 7 and 8. The first circle has the radius $\ell_0 \sin\theta_1$ and is centered at the origin. The second circle comes from the intersection of the plane $x = \ell_0 \cos\theta_1$ and the sphere mentioned above. This second circle has its center at $\langle y'_1(\phi_0), z'_1(\phi_0)\rangle$ and its radius ρ, where $a_1^2 = \rho^2 + [\mathbf{x}'_1(\phi_0) - \ell_0 \cos\theta_1]^2$. The intersection of these two circles produces the values of $\mathbf{x}_0(\phi_0, 1)$ and $\mathbf{x}_0(\phi_0, -1)$. As seen in figure 8, we can find the unit vector from the projection of A''_1 to the projection of A'_0. This vector is $\frac{\langle y'_1(\phi_0), z'_1(\phi_0)\rangle}{\sqrt{[y'_1(\phi_0)]^2 + [z'_1(\phi_0)]^2}}$. We can find the perpendicular unit vector in the counter clockwise direction to be $\frac{\langle -z'_1(\phi_0), y'_1(\phi_0)\rangle}{\sqrt{[y'_1(\phi_0)]^2 + [z'_1(\phi_0)]^2}}$. In figure 8, let $0 \le \alpha \le 180°$ denote the angle between the rays indicated. This angle α is found using the law of cosines. Therefore, $\rho^2 = \ell_0^2 \sin^2\theta_1 + [y'_1(\phi_0)]^2 + [z'_1(\phi_0)]^2 - 2\ell_0 \sin\theta_1 \cos\alpha \sqrt{[y'_1(\phi_0)]^2 + [z'_1(\phi_0)]^2}$. Solving for $\cos\alpha$ leads to (13). The inequality (9) assures us that the two circles actually intersect. We then denote σ as the sign of the triple product $(\mathbf{R}_{A_0} - \mathbf{R}_{A''_1}) \times (\mathbf{R}_{A'_0} - \mathbf{R}_{A''_1}) \cdot (\mathbf{R}_{A''_0} - \mathbf{R}_{A''_1})$. We can also obtain this triple product from the determinant of the three by three matrix,

$$\left((\mathbf{R}_{A_0} - \mathbf{R}_{A''_1}), (\mathbf{R}_{A'_0} - \mathbf{R}_{A''_1}), (\mathbf{R}_{A''_0} - \mathbf{R}_{A''_1}) \right).$$

We notice that the determinant of this matrix would be the same as the determinant of

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ \mathbf{R}_{A''_1} & (\mathbf{R}_{A_0} - \mathbf{R}_{A''_1}) & (\mathbf{R}_{A'_0} - \mathbf{R}_{A''_1}) & (\mathbf{R}_{A''_0} - \mathbf{R}_{A''_1}) \end{pmatrix}.$$

By simple column operations, we see:

$$\sigma = sign \ \det \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{R}_{A''_1} & \mathbf{R}_{A_0} & \mathbf{R}_{A'_0} & \mathbf{R}_{A''_0} \end{pmatrix}.$$

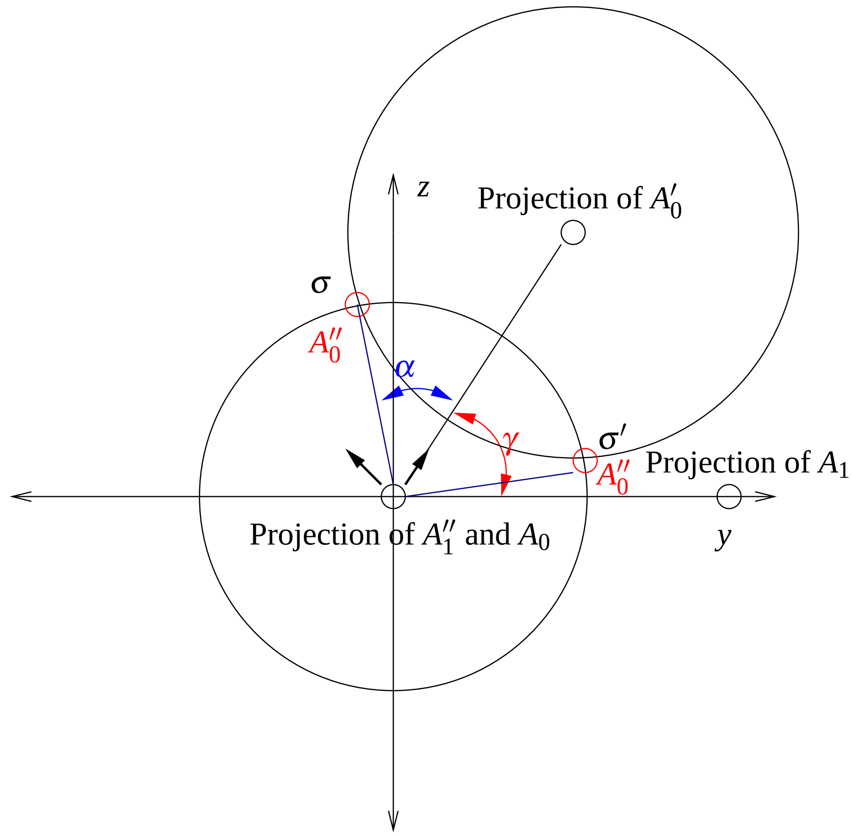

FIGURE 8. Intersection of Circles of Solutions of A_0''

We can use the two unit vectors and σ to determine the position of A_0''. The cross product $(\mathbf{R}_{A_0} - \mathbf{R}_{A_1''}) \times (\mathbf{R}_{A_0'} - \mathbf{R}_{A_1''})$ is parallel to the unit vector $\frac{\langle -z_1'(\phi_0), y_1'(\phi_0)\rangle}{\sqrt{[y_1'(\phi_0)]^2+[z_1'(\phi_0)]^2}}$, so

$$\begin{aligned}\langle y_0, z_0\rangle =& \ell_0 \sin\theta_1 \frac{\langle y_1'(\phi_0), z_1'(\phi_0)\rangle}{\sqrt{[y_1'(\phi_0)]^2+[z_1'(\phi_0)]^2}} \cos\alpha \\ &+ \sigma \ell_0 \sin\theta_1 \frac{\langle -z_1'(\phi_0), y_1'(\phi_0)\rangle}{\sqrt{[y_1'(\phi_0)]^2+[z_1'(\phi_0)]^2}} \sin\alpha\end{aligned}$$

This is clearly the same as (11). Next, we must study how to solve for the value of ϕ_1''. To find this wedge angle, we must learn its orientation. From figure 5, it is given that $d^* = [A_0'', A_1'', A_0, A_1]$. The axis of rotation is oriented from A_1'' to A_0, i.e. along the positive x axis. The initial half plane contains as a boundary the x-axis and contains the point A_0''. The final half-plane contains as a boundary x-axis and contains the point A_1. So $\phi_1'' = -\gamma - \sigma\alpha$ where is the angle indicated on Figure 8, i.e. $\gamma = \arg[y_1'(\phi_0) + iz_1'(\phi_0)]$, as in (14). □

This lemma defines the function $\mathbf{x}_0(\phi_0,\sigma)$ and completes the first step of the Bridging Algorithm. The lemma also defines the function $\phi_1''(\phi_0,\sigma)$.

In the next step, we must solve for $\mathbf{R}_{A_1'}$, which is our second end point. Before we state this lemma, we must identify some more notations. The known position A_1'' is

$$\mathbf{R}_{A_1''}(\phi_0) \;=\; E_r(\mathbf{R}(\phi_0))\begin{pmatrix}1\\ \mathbf{0}\end{pmatrix} \;=\; E_{r'}(\mathbf{R}(\phi_0))M(\phi_0)^{-1}\begin{pmatrix}1\\ \mathbf{0}\end{pmatrix} \;=\; E_{r'}(\mathbf{R}(\phi_0))\begin{pmatrix}1\\ \mathbf{x}_1(\phi_0)\end{pmatrix},$$

then $\begin{pmatrix}1\\ \mathbf{x}_1(\phi_0)\end{pmatrix} = M(\phi_0)^{-1}\begin{pmatrix}1\\ \mathbf{0}\end{pmatrix}$ and $\mathbf{x}_1 = (x_1,y_1,z_1)^T$.

We can now characterize our $M(\phi_0)$ in block formation where

$$M(\phi_0) = \begin{pmatrix}1 & \mathbf{0}^T\\ \mathbf{x}_1'(\phi_0) & A\end{pmatrix}$$

and where $A \in SO(3)$. Therefore, the $M(\phi_0)^{-1} = \begin{pmatrix}1 & \mathbf{0}^T\\ -A(\phi_0)^T\mathbf{x}_1'(\phi_0) & A(\phi_0)^T\end{pmatrix}$. This means that $\mathbf{x}_1(\phi_0) = -A(\phi_0)^T\mathbf{x}_1'(\phi_0)$. The unknown position of A_1 is $\mathbf{R}_{A_1'} = E_{r'}(\mathbf{R}(\phi_0))\begin{pmatrix}1\\ \mathbf{x}_0'\end{pmatrix}$ where $\mathbf{x}_0' = (x_0',y_0',z_0')^T$. The solutions of $\mathbf{x}_0'(\phi_0,\sigma')$ are obtained from a lemma similar to lemma 1.1.

LEMMA 1.2. *If* $[y_1(\phi_0)]^2+[z_1(\phi_0)]^2>0$ *then* $\langle x_0',y_0',z_0'\rangle$ *has at least one real solution if and only if*

$$\begin{aligned}&\left|\ell_0^2\sin^2\theta_0+[y_1(\phi_0)]^2+[z_1(\phi_0)]^2+(\ell_0\cos\theta_0-x_1(\phi_0))^2-a_0^2\right| \\ &\le 2\ell_0\sin\theta_0\sqrt{[y_1(\phi_0)]^2+[z_1(\phi_0)]^2}.\end{aligned} \tag{15}$$

If these conditions hold then all the solutions are of the form :

$$x_0' = \ell_0\cos\theta_0 \tag{16}$$

$$\begin{aligned}\langle y_0', z_0'\rangle =& \langle y_1(\phi_0), z_1(\phi_0)\rangle \frac{\ell_0 \sin\theta_0 \cos\alpha'}{\sqrt{[y_1(\phi_0)]^2+[z_1(\phi_0)]^2}} \\ &+\sigma'\langle -z_1(\phi_0), y_1(\phi_0)\rangle \frac{\ell_0 \sin\theta_0 \sin\alpha'}{\sqrt{[y_1(\phi_0)]^2+[z_1(\phi_0)]^2}},\end{aligned} \tag{17}$$

$$\phi_1 = -\gamma' - \sigma'\alpha' \tag{18}$$

where $\sigma' \in \{-1, 1\}$, $\alpha' \in [0, 180^\circ]$ *is such that*

$$\cos\alpha' = \frac{\ell_0^2 \sin^2\theta_0 + [y_1(\phi_0)]^2 + [z_1(\phi_0)]^2 + (\ell_0\cos\theta_0 - x_1(\phi_0))^2 - a_0^2}{2\ell_0 \sin\theta_0 \sqrt{[y_1(\phi_0)]^2+[z_1(\phi_0)]^2}} \tag{19}$$

and

$$\gamma' = arg(y_1(\phi_0) + iz_1(\phi_0)).$$

This lemma defines the function $\mathbf{x}_0'(\phi_0, \sigma')$ and completes the second step of the Bridging Algorithm. Lemma 1.2 also defines the function $\phi_1(\phi_0, \sigma')$. Note that we can obtain lemma 1.2 from lemma 1.1 by exchanging the primed and unprimed elements and exchanging θ_0 for θ_1.

In step one, we found $\mathbf{R}_{A_0''} = E_r(\mathbf{R}(\phi_0))\begin{pmatrix} 1 \\ \mathbf{x}_0(\phi_0, \sigma)\end{pmatrix}$, and in step two we found $\mathbf{R}_{A_1'} = E_{r'}(\mathbf{R}(\phi_0))\begin{pmatrix} 1 \\ \mathbf{x}_0'(\phi_0, \sigma')\end{pmatrix}$. In the third step, we must impose a distance constraint between these two points. To do this, we must first convert $\mathbf{R}_{A_1'}$ into the coordinate system at the site r, i.e. $E_r(\mathbf{R}(\phi_0))$.

$$\begin{aligned}\mathbf{R}_{A_1'}(\phi_0) = E_{r'}(\mathbf{R}(\phi_0))\begin{pmatrix} 1 \\ \mathbf{x}_0'(\phi_0, \sigma')\end{pmatrix} &= E_r(\mathbf{R}(\phi_0))M(\phi_0)\begin{pmatrix} 1 \\ \mathbf{x}_0'(\phi_0, \sigma')\end{pmatrix} \\ &= E_r(\mathbf{R}(\phi_0))\begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{x}_1'(\phi_0) & A\end{pmatrix}\begin{pmatrix} 1 \\ \mathbf{x}_0'(\phi_0, \sigma')\end{pmatrix} \\ &= E_r(\mathbf{R}(\phi_0))\begin{pmatrix} 1 \\ \mathbf{x}_1'(\phi_0) + A(\phi_0)\mathbf{x}_0'(\phi_0, \sigma')\end{pmatrix}.\end{aligned}$$

We must impose the distance constraint $\ell_1^2 = \|\mathbf{R}_{A_0''}(\phi_0,\sigma) - \mathbf{R}_{A_1'}(\phi_0,\sigma')\|^2$. Therefore, for each $(\sigma,\sigma') \in \{-1,1\}^2$, the equation to be solved for ϕ_0 becomes

$$\begin{aligned}
\ell_1^2 =&\|\mathbf{R}_{A_0''}(\phi_0,\sigma) - \mathbf{R}_{A_1'}(\phi_0,\sigma')\|^2 = \|\mathbf{x}_0(\phi_0,\sigma) - \mathbf{x}_1'(\phi_0) - A(\phi_0)\mathbf{x}_0'(\phi_0,\sigma')\|^2 \\
=&(\mathbf{x}_0 - \mathbf{x}_1' - A\mathbf{x}_0')^T(\mathbf{x}_0 - \mathbf{x}_1' - A\mathbf{x}_0') = \mathbf{x}_0^T\mathbf{x}_0 - \mathbf{x}_0^T\mathbf{x}_1' - \mathbf{x}_0^TA\mathbf{x}_0' - \mathbf{x}_1'^T\mathbf{x}_0 \\
&+ \mathbf{x}_1'^T\mathbf{x}_1' + \mathbf{x}_1'^TA\mathbf{x}_0' - \mathbf{x}_0'^TA^T\mathbf{x}_0 + \mathbf{x}_0'^TA^T\mathbf{x}_1' + \mathbf{x}_0'^TA^TA\mathbf{x}_0'
\end{aligned}$$

$$\begin{aligned}
\ell_1^2 =&2\ell_0^2 + \|\mathbf{x}_1'(\phi_0)\|^2 - 2\mathbf{x}_0(\phi_0,\sigma)\cdot\mathbf{x}_1'(\phi_0) - 2\mathbf{x}_0(\phi_0,\sigma)\cdot A(\phi_0)\mathbf{x}_0'(\phi_0,\sigma') \\
&+ 2\mathbf{x}_1'(\phi_0)\cdot A(\phi_0)\mathbf{x}_0'(\phi_0,\sigma').
\end{aligned} \tag{20}$$

This completes a schematic discussion of the Bridging Algorithm as applied to the study of the shapes of three-fold symmetric hexagons. In the next chapter, we will begin to make everything completely explicit.

CHAPTER 2

SOLVING THE BRIDGING ALGORITHM FOR HEXAGONS

The Bridging Algorithm has three distinct steps that allow us to calculate when values of $\ell_0, \ell_1, \theta_0, \theta_1, \sigma, \sigma'$ and ϕ_0 creates a three-fold symmetric hexagon. In this chapter, we will explicitly state the expressions that restrict and solve the first two steps of the Bridging Algorithm. Lastly, we will complete the third step of the Bridging Algorithm by calculating the equality (20).

2.1. EXPLICIT EXPRESSIONS FOR THE HEXAGON

When finding the properties of three-fold symmetric hexagons, we have to use the Z-System that we created in the last chapter.

In the Bridging Algorithm, we use $M(\phi_0)$, which is the coordinate transformation matrix. Now we must compute it for our hexagon. In section 1.3 of this thesis, we showed that $M(\phi_0)$ can be produced by the product of transformation matrices. These matrices are produced by finding a sequence of sites linking $r = (A_1'', A_0, A_1)$ to $r' = (A_0', A_1, A_0)$. This sequence is given below:

$$
\begin{array}{rcccccl}
r= & (A_1'', & & A_0, & & A_1) & \\
 & & \times & & & & T_1(\ell_1) \\
 & (A_0, & & A_1'', & & A_1) & \\
 & & & & \times & & T_2(\theta_0) \\
 & (A_0, & & A_1, & & A_1'') & \\
 & & & & & \downarrow & T_3(\phi_0) \\
 & (A_0, & & A_1, & & A_0') & \\
 & & \times & & & & T_1(\ell_0) \\
 & (A_1, & & A_0, & & A_0') & \\
 & & & & \times & & T_2(\theta_1) \\
 & (A_1, & & A_0', & & A_0) & \\
 & & \times & & & & T_1(\ell_1) \\
r'= & (A_0', & & A_1, & & A_0) &
\end{array}
$$

The $\times$s found between the two sites indicate a transposition of types **a** or **b** in section

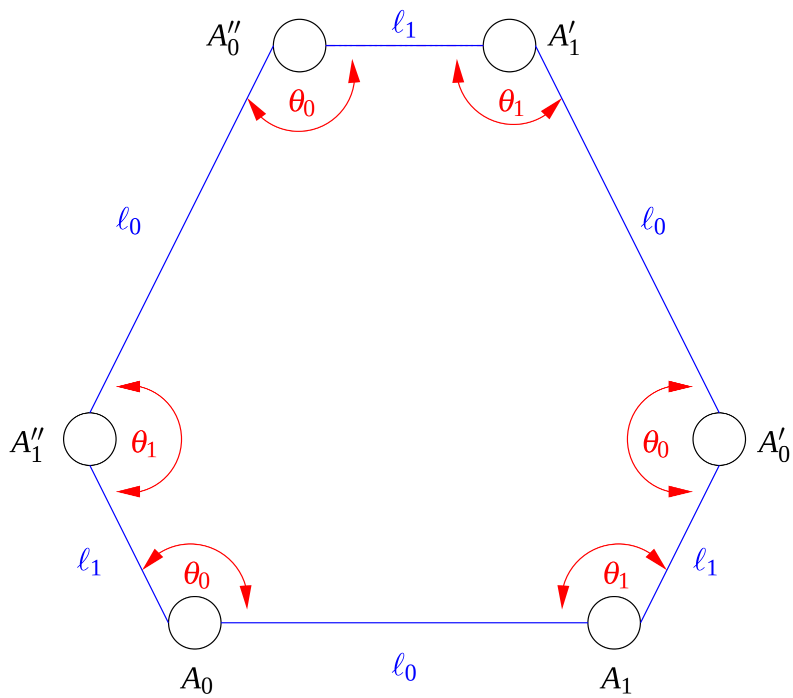

FIGURE 9. A General Three-Fold Symmetric Hexagon

1.3. The $\downarrow$ indicates a site transition of type **c**, again from section 1.3. To the right of each site transition, we have indicated the corresponding transformation matrix. Therefore, to transform site r to r', we found:

$$M(\phi_0) = T_1(\ell_1)T_2(\theta_0)T_3(\phi_0)T_1(\ell_0)T_2(\theta_1)T_1(\ell_1).$$

From this section forward, we will be using special notation to simplify our equations.

NOTATION 2.1.

$$c_0 = \cos\theta_0 \qquad c_1 = \cos\theta_1$$

$$s_0 = \sin\theta_0 \qquad s_1 = \sin\theta_1$$

$$c = \cos\theta \qquad s = \sin\theta$$

$$G = \sin\theta_0 \sin\theta_1 \cos\phi_0$$

$$a_1^2 = \ell_1^2 + \ell_0^2 - 2\ell_1\ell_0 c_1 \qquad a_0^2 = \ell_1^2 + \ell_0^2 - 2\ell_1\ell_0 c_0$$

All the subsequent equations were calculated using Maple as seen in hex.mw starting from line 7. When $M(\phi_0)$ is found using Maple (see worksheet line hex.mws 7), it is a matrix with 4 columns and 4 rows where :

$$M(\phi_0) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \ell_1 - \ell_0 c_0 + \ell_1 (c_0 c_1 - s_0 s_1 \cos\phi_0) & -c_0 c_1 + s_0 s_1 \cos\phi_0 & c_0 s_1 + c_1 s_0 \cos\phi_0 & -s_0 \sin\phi_0 \\ \ell_0 s_0 + \ell_1 (-c_1 s_0 - c_0 s_1 \cos\phi_0) & c_1 s_0 + c_0 s_1 \cos\phi_0 & -s_0 s_1 + c_0 c_1 \cos\phi_0 & -c_0 \sin\phi_0 \\ \ell_1 s_1 \sin\phi_0 & -s_1 \sin\phi_0 & -c_1 \sin\phi_0 & -\cos\phi_0 \end{pmatrix} \tag{21}$$

In section 1.4, we introduced new quantities A, $\mathbf{x}_1'$, and $\mathbf{x}_1$ which are found from $M(\phi_0) = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{x}_1'(\phi_0) & A \end{pmatrix}$ and $\mathbf{x}_1(\phi_0) = -A(\phi_0)^T \mathbf{x}_1'(\phi_0)$. Now we can explicitly compute these values to be:

$$A = \begin{pmatrix} -c_0 c_1 + s_0 s_1 \cos\phi_0 & c_0 s_1 + c_1 s_0 \cos\phi_0 & -s_0 \sin\phi_0 \\ c_1 s_0 + c_0 s_1 \cos\phi_0 & -s_0 s_1 + c_0 c_1 \cos\phi_0 & -c_0 \sin\phi_0 \\ -s_1 \sin\phi_0 & -c_1 \sin\phi_0 & -\cos\phi_0 \end{pmatrix} \tag{22}$$

$$\mathbf{x}_1' = \begin{pmatrix} x_1' \\ y_1' \\ z_1' \end{pmatrix} = \begin{pmatrix} \ell_1 - \ell_0 c_0 + \ell_1 (c_0 c_1 - s_0 s_1 \cos\phi_0) \\ \ell_0 s_0 + \ell_1 (-c_1 s_0 - c_0 s_1 \cos\phi_0) \\ \ell_1 s_1 \sin\phi_0 \end{pmatrix} \tag{23}$$

$$\mathbf{x}_1 = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} = -A(\phi_0)^T \mathbf{x}_1'(\phi_0) = \begin{pmatrix} \ell_1 - \ell_0 c_1 + \ell_1 (c_0 c_1 - s_0 s_1 \cos\phi_0) \\ \ell_0 s_1 + \ell_1 (-c_0 s_1 - c_1 s_0 \cos\phi_0) \\ \ell_1 s_0 \sin\phi_0 \end{pmatrix}. \tag{24}$$

In lemma 1.1 and 1.2, we have the assumed constraint that $[y_1'(\phi_0)]^2 + [z_1'(\phi_0)]^2 > 0$ and $[y_1(\phi_0)]^2 + [z_1(\phi_0)]^2 > 0$. We will denote these positive quantities as K' and K respectively. Now that we have explicit forms for y_1, y_1', z_1 and z_1', we can compute the restraints.

$$K' = y_1'^2 + z_1'^2 = a_1^2 - (c_0(\ell_0 - \ell_1 c_1) + \ell_1 G)^2 \tag{25}$$

$$K = y_1^2 + z_1^2 = a_0^2 - (c_1(\ell_0 - \ell_1 c_0) + \ell_1 G)^2 \tag{26}$$

Lemma 1.1 and 1.2 give values of the angles α and α' through equations created from the law of cosines. These equations can now be simplified to give us the explicit forms of

$\cos\alpha$ and $\cos\alpha'$.

$$\cos\alpha = \frac{a_1^2 - 2(\ell_1 - \ell_0 c_1)(c_0(\ell_0 - \ell_1 c_1) + \ell_1 G)}{2\ell_0 s_1 \sqrt{K'}}$$
$$\cos\alpha' = \frac{a_0^2 - 2(\ell_1 - \ell_0 c_0)(c_1(\ell_0 - \ell_1 c_0) + \ell_1 G)}{2\ell_0 s_0 \sqrt{K}}$$

However, the values of the $\sin\alpha$ and $\sin\alpha'$ are needed to solve for the values of y_0, y_0', z_0, and z_0'. We can find these values to be $\sin\alpha = \sqrt{1-\cos^2\alpha}$ and $\sin\alpha' = \sqrt{1-\cos^2\alpha'}$. This gives us the equations for $\sin\alpha$ and $\sin\alpha'$ below (see Maple worksheet hex.mws, lines 27-30):

$$\sin\alpha = \frac{\sqrt{H'}}{2\ell_0 s_1 \sqrt{K'}} \tag{27}$$
$$\sin\alpha' = \frac{\sqrt{H}}{2\ell_1 s_0 \sqrt{K}} \tag{28}$$

where

$$\begin{aligned} H' &= 4\ell_0^2(1-c_1^2)K' - \{a_1^2 - 2(\ell_1 - \ell_0 c_0)[c_0(\ell_0 - \ell_1 c_1) + \ell_1 G]\}^2 \\ &= a_1^2\big(-4\ell_1^2 G^2 + 4\ell_1(\ell_1 + 2\ell_1 c_0 c_1 - \ell_0 c_1 - 2\ell_0 c_0)G \\ &\qquad - \ell_1^2 + 8\ell_0\ell_1 c_0^2 c_1 + 4\ell_0\ell_1 c_0 c_1^2 + 4\ell_1\ell_0 c_0 + 2\ell_0\ell_1 c_1 \\ &\qquad + 3\ell_0^2 - 4\ell_0^2 c_1^2 - 4\ell_0^2 c_0 c_1 - 4\ell_1^2 c_0^2 c_1^2 - 4\ell_1^2 c_0 c_1 - 4\ell_0^2 c_0^2\big) \\ &= -a_1^2\big(2\ell_1 G - \ell_1(1+2c_1c_0) + \ell_0(c_1 + 2c_0 - \sqrt{3}s_1)\big) \\ &\qquad \big(2\ell_1 G - \ell_1(1+2c_0c_1) + \ell_0(c_1 + 2c_0 + \sqrt{3}s_1)\big) \end{aligned} \tag{29}$$

$$\begin{aligned} H &= 4\ell_0^2(1-c_1^2)K - \{a_0^2 - 2(\ell_1 - \ell_0 c_1)[c_1(\ell_0 - \ell_1 c_0) + \ell_1 G]\}^2 \\ &= a_0^2\big(-4\ell_1^2 G^2 + 4\ell_1(\ell_1 + 2\ell_1 c_0 c_1 - \ell_0 c_0 - 2\ell_0 c_1)G \\ &\qquad - \ell_1^2 + 8\ell_0\ell_1 c_1^2 c_0 + 4\ell_0\ell_1 c_1 c_0^2 + 4\ell_1\ell_0 c_1 + 2\ell_0\ell_1 c_0 \\ &\qquad + 3\ell_0^2 - 4\ell_0^2 c_0^2 - 4\ell_0^2 c_0 c_1 - 4\ell_1^2 c_0^2 c_1^2 - 4\ell_1^2 c_0 c_1 - 4\ell_0^2 c_1^2\big) \end{aligned} \tag{30}$$

$$= -a_0^2\big(2\ell_1 G - \ell_1(1+2c_0c_1) + \ell_0(c_0+2c_1-\sqrt{3}s_0)\big)$$
$$\big(2\ell_1 G - \ell_1(1+2c_1c_0) + \ell_0(c_0+2c_1+\sqrt{3}s_0)\big)$$

Now that we have given specific values for all the restrictions and values of lemma 1.1 and 1.2, we can now solve for the values of $\mathbf{x}_0$ and $\mathbf{x}_0'$.

$$\mathbf{x}_0' = \begin{pmatrix} x_0' \\ y_0' \\ z_0' \end{pmatrix} = \frac{1}{\sqrt{K}} \begin{pmatrix} \ell_0 c_0 \sqrt{K} \\ y_1 \ell_0 s_0 \cos\alpha' - \sigma' z_1 \ell_0 s_0 \sin\alpha' \\ z_1 \ell_0 s_0 \cos\alpha' + \sigma' y_1 \ell_0 s_0 \sin\alpha' \end{pmatrix} \tag{31}$$

$$\mathbf{x}_0 = \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} = \frac{1}{\sqrt{K'}} \begin{pmatrix} \ell_0 c_1 \sqrt{K'} \\ y_1' \ell_0 s_1 \cos\alpha - \sigma z_1' \ell_0 s_1 \sin\alpha \\ z_1' \ell_0 s_1 \cos\alpha + \sigma y_1' \ell_0 s_1 \sin\alpha \end{pmatrix} \tag{32}$$

Using these equations, we can learn more about the three fold symmetric hexagon. During the rest of this paper, we will investigate how to solve the third step of the Bridging Algorithm for our three-fold symmetric hexagon.

2.2. RESTRICTIONS ON $\ell_0, \ell_1, \theta_0, \theta_1$ AND ϕ_0

Lemma 1.1 solves for the values of the end point $\mathbf{R}_{A_0''}$ when the bonds and angles satisfy $K' > 0$ and inequality (9) . Lemma 1.2 obtains the values of the other end point $\mathbf{R}_{A_1'}$ when the bonds and angle satisfy $K > 0$ and inequality (15). We can simplify these restrictions using our new notations and our explicit values found in the section 2.1.

From the definitions (25) and (26), $K \geq 0$ and $K' \geq 0$. $K' = 0$ exactly when A_0, A_1'' and A_0' are collinear. $K = 0$ exactly when A_1, A_0', A_1'' are collinear. These situations must be excluded for the Bridging Algorithm to work. We are given the restrictions of $K > 0$ and $K' > 0$ to insure that the values of $\mathbf{x}_0$ and $\mathbf{x}_0'$ exist. When we solve for there values, we must divide by K and K', therefore we prevent dividing by zero of the expressions for $\mathbf{x}_0$ and $\mathbf{x}_0'$. The inequalities (9) and (15) insure that the values of $\cos\alpha$ and $\cos\alpha'$ satisfy $-1 \leq \cos\alpha \leq 1$, and $-1 \leq \cos\alpha' \leq 1$.

We can find the restrictions on $\cos\phi_0$ by solving H and H' for $\cos\phi_0$. Let $u_1 = \ell_1(1 + 2c_0c_1) - \ell_0(c_1 + 2c_0 - \sqrt{3}s_1)$ and $u_2 = \ell_1(1 + 2c_0c_1) - \ell_0(c_0 + 2c_1 - \sqrt{3}s_0)$. If

$$c_1 - c_0 + \sqrt{3}(s_1 - s_0) \geq 0,$$

then the upper bound of $2\ell_1 G$ is u_2 otherwise it will be u_1.

We can also find the lower bound of $2\ell_1 G$. Let $\psi_1 = \ell_1(1+2c_0c_1) - \ell_0(c_1 + 2c_0 + \sqrt{3}s_1)$ and $\psi_2 = \ell_1(1 + 2c_0c_1) - \ell_0(c_0 + 2c_1 + \sqrt{3}s_0)$. If

$$c_1 - c_0 - \sqrt{3}(s_1 - s_0) \geq 0,$$

then the lower bound of $2\ell_1 G$ is ψ_1 otherwise it will be ψ_2.

From these restrictions, we can tell when a candidate value for ϕ_0 can possibly come from an actual hexagon.

2.3. QUARTIC

Since we have solved the first two steps of the Bridging Algorithm for $\mathbf{x}_0$ and $\mathbf{x}_0'$, we can derive an explicit form of equality (20). In section 2.1, we gave the full expression of $A, \mathbf{x}_0(\phi_0, \sigma)$ and $\mathbf{x}_0'(\phi_0, \sigma')$. By placing these values into equality (20), we derive an equation with variables $\ell_0, \ell_1, \theta_0, \theta_1, \sigma, \sigma'$, and ϕ_0 (see Maple worksheet hex.mw). Some simplifications can be made in this equation. First we notice that $\frac{1}{2KK'}$ can be factored out. Since one of the restrictions in lemma 1.1 and lemma 1.2 state that $K, K' > 0$, we can cancel the fraction from our equation without effecting the resulting solutions. This simplifies our version of (20) to be (see hex.mws line 22):

$$\begin{aligned} 0 =& C_1G^4 + C_2G^3 + C_3G^2 + C_4G + C_5 + \sigma\sigma'\sqrt{H}\sqrt{H'}(C_6G^2 + C_7G + C_8) \\ &+ \ell_0 s_0 s_1 \sin\phi_0 \left(\sigma\sqrt{H'}(C_9G^2 + C_{10}G + C_{11}) + \sigma'\sqrt{H}(C_{12}G^2 + C_{13}G + C_{14})\right) \end{aligned} \tag{QUARTIC}$$

where C_i for $i = 1..14$ are the coefficients of G (see Appendix A for explicit values of these coefficients). These coefficients depend only on ℓ_0, ℓ_1, c_0, c_1. From the definition of H and

H', this means the value of $\sqrt{HH'}$ can not generally be simplified, and the QUARTIC can not be factored without further manipulation.

The ϕ_0 values for our QUARTIC equation can have the range of $(-180^\circ, 180^\circ]$. Therefore, we must study what happens when $\phi_0 \leq 0$ and when $\phi_0 \geq 0$. Since $\cos\phi_0 = \cos(-\phi_0)$, the values of C_i for all i will not change when ϕ_0 is replaced by $-\phi_0$. However $\sin(-\phi_0) = -\sin\phi_0$, therefore the only terms of QUARTIC that change when ϕ_0 is replaced by $-\phi_0$ are the terms involving $\sin\phi_0$. Notice that $\sin\phi_0$ is multiplied by σ or σ'. If $(\phi_0, \sigma, \sigma')$ is replaced by $(-\phi_0, -\sigma, -\sigma')$ then the terms involving $\sin\phi_0$ are not changed. Notice that when we do change the signs of both σ and σ', it will not change the term containing $\sigma\sigma'$. Therefore, we have a strict relationship between the solutions with positive ϕ_0 and negative ϕ_0.

THEOREM 2.2. *When* $[\ell_0, \ell_1, \theta_1, \theta_0, \sigma, \sigma', \phi_0]$ *is a solution of QUARTIC, then so is* $[\ell_0, \ell_1, \theta_1, \theta_0, -\sigma, -\sigma', -\phi_0]$.

Therefore for arbitrary σ and σ', we only need to study the case $\phi_0 \geq 0$.

2.4. SQUARED QUARTIC

We know that QUARTIC has 7 variables $(\ell_0, \ell_1, \theta_1, \theta_0, \phi_0, \sigma, \sigma')$. This makes the factoring more difficult because each variable has many different values that it could satisfy.

The first obstacle that will be addressed is making all values of ϕ_0 in terms of the cosine function. Therefore, the only way to eliminate the sine factors is by squaring. We must subtract the sine term from both sides of QUARTIC to prepare the equation to be squared.

$$\begin{aligned} C_1G^4 + C_2G^3 + C_3G^2 + C_4G + C_5 + \sigma\sigma'\sqrt{H}\sqrt{H'}(C_6G^2 + C_7G + C_8) \\ = -\ell_0 s_0 s_1 \sin\phi_0 \left(\sigma\sqrt{H'}(C_9G^2 + C_{10}G + C_{11}) + \sigma'\sqrt{H}(C_{12}G^2 + C_{13}G + C_{14})\right) \end{aligned}$$

where

$$A(G) = C_1G^4 + C_2G^3 + C_3G^2 + C_4G + C_5,$$

$$B(G) = C_6G^2 + C_7G + C_8,$$

$$E(G) = C_9G^2 + C_{10}G + C_{11}, \text{and}$$

$$F(G) = C_{12}G^2 + C_{13}G + C_{14}.$$

Therefore,

$$A(G) + \sigma\sigma'\sqrt{H}\sqrt{H'}B(G) = -\ell_0 s_0 s_1 \sin\phi_0(\sigma\sqrt{H'}E(G) + \sigma'\sqrt{H}F(G)).$$

Once we square both sides, we no longer have our $\sin\phi_0$ terms, but we could introduce extraneous solutions into our equation.

Since $G = s_1 s_0 \cos\phi_0$, all values of ϕ_0 are in the form of $\cos\phi_0$ once we square both sides of the equation above. After squaring, we obtain:

$$A(G)^2 + 2A(G)B(G)\sigma\sigma'\sqrt{H}\sqrt{H'} + HH'B(G)^2$$
$$= \ell_0^2 s_0^2 s_1^2 \sin^2\phi[H'E(G)^2 + 2\sigma\sigma'\sqrt{H}\sqrt{H'}E(G)F(G) + HF(G)^2].$$

This can be rearanged to make the squared QUARTIC be:

$$A(G)^2 + 2A(G)B(G) + HH'B(G)^2 - \ell_0^2(s_0^2 s_1^2 - C$$

$$+\sigma\sigma'\sqrt{H}\sqrt{H'}(2A(G)B(G) - \ell_0^2(s_0^2 s_1^2 - G^2)2E(G)F(G)).$$

We can expained this formula to find:

$$0 = D_1G^8 + D_2G^7 + D_3G^6 + D_4G^5 + D_6G^4 + D_7G^3 + D_8G^2 + D_9G + D_{10}$$
$$+ \sigma\sigma'\sqrt{H}\sqrt{H'}(D_{11}G^6 + D_{12}G^5 + D_{13}G^4 + D_{14}G^3 + D_{15}G^2 + D_{16}G + D_{17}).$$

where the coefficients D_i for $i = 6, 7, ..17$. (see Maple worksheet hex.mw) Each of the D_i are independent of σ, σ', and only depend on ℓ_0, ℓ_1, c_0, and c_1.

By squaring our QUARTIC, we were able to eliminate our sine function, but we are still left with a square root in our equation. We can not solve our squared QUARTIC for ϕ_0 until we can simplify this equation further.

The way we can try to simplify our squared QUARTIC is by guessing the factors. We can study this equation with its square root by setting $\ell_0 = \ell_1$ or $\theta_0 = \theta_1$. Through the use of Maple programming, we are able to set $\ell_0 = \ell_1$ in our squared QUARTIC equation. Maple is able to factor this quantity, and we can notice that both K and K' appear in Maple's factorization. Next, we can set $\theta_0 = \theta_1$ in our Maple program, and ask the computer to factor that quantity. It also contains K and K' as factors. Therefore, we can guess that K and K' should factor from our general squared QUARTIC equation. Through long division using Maple, we are able to see that KK' divides evenly into the general squared QUARTIC. Since we are given the restriction of $K > 0$ and $K' > 0$, we can cancel out our coefficients since it will not effect the resulting solutions. This leaves us with the general squared QUARTIC equation:

$$0 \;=\; (\mathbb{D}_1 G^4 \;+\; \mathbb{D}_2 G^3 \;+\; \mathbb{D}_3 G^2 \;+\; \mathbb{D}_4 G \;+\; \mathbb{D}_5 \;+\; \tau\sqrt{H}\sqrt{H'}(\mathbb{D}_6 G^2 \;+\; \mathbb{D}_7 G \;+\; \mathbb{D}_8)) \tag{Squared QUARTIC}$$

where $\tau = \sigma\sigma'$. Let us define

$$\begin{aligned}\mathbb{A}(G) =& \mathbb{D}_1 G^4 + \mathbb{D}_2 G^3 + \mathbb{D}_3 G^2 + \mathbb{D}_4 G + \mathbb{D}_5,\\ \mathbb{B}(G) =& \mathbb{D}_6 G^2 + \mathbb{D}_7 G + \mathbb{D}_8.\end{aligned}$$

Therefore squared QUARTIC becomes

$$\mathbb{A}(G) + \tau\sqrt{H}\sqrt{H'}\mathbb{B}(G) = 0.$$

Suppose $\ell_0, \ell_1, \theta_0, \theta_1, \phi_0, \sigma$, and σ' satisfies $(K > 0), (K' > 0), (H \geq 0)$, and $(H' \geq 0)$, and solves QUARTIC. Then $\ell_0, \ell_1, \theta_0, \theta_1$, and τ must solve squared QUARTIC. Conversely, if $\ell_0, \ell_1, \theta_0, \theta_1, \phi_0,$ and τ satisfies $(K > 0), (K' > 0), (H \geq 0),$ and $(H' \geq 0),$ and solve squared QUARTIC, then multiplying both side by KK' and substituting $\sigma\sigma'$ for τ creates:

$$\begin{aligned}&\sigma\sigma'\sqrt{H}\sqrt{H'}[2A(G)B(G)-2\ell_0^2(s_0^2s_1^2-G^2)E(G)F(G)]\\&=\ell_0^2(s_0^2s_1^2-G^2)[H'E(G)^2+HF(G)^2]-A(G)^2-HH'B(G)^2.\end{aligned}$$

By rearrangement, we receive

$$\begin{aligned}&A(G)^2+2A(G)B(G)\sigma\sigma'\sqrt{H}\sqrt{H'}+HH'B(G)^2\\&=\ell_0^2s_0^2s_1^2\sin^2\phi[H'E(G)^2+2\sigma\sigma'\sqrt{H}\sqrt{H'}E(G)F(G)+HF(G)^2].\end{aligned}$$

We can factor this equation to be:

$$(A(G)+\sigma\sigma'\sqrt{H}\sqrt{H'}B(G))^2=(\ell_0s_0s_1\sin\phi[\sigma\sqrt{H'}E(G)+\sigma'\sqrt{H}F(G)])^2.$$

Note if (σ,σ') is replaced by $(-\sigma,-\sigma')$ the quantity $\tau=\sigma\sigma'$ remains unchanged. Thus, there is a unique choice of (σ,σ') such that $\tau=\sigma\sigma'$ and

$$A(G)+\sigma\sigma'\sqrt{H}\sqrt{H'}B(G)=-\ell_0s_0s_1\sin\phi_0[\sigma\sqrt{H'}E(G)+\sigma'\sqrt{H}F(G)].$$

(Rearranged QUARTIC)

Thus for this σ,σ', we obtain a solution $\ell_0,\ell_1,\theta_0,\theta_1,\phi_0,\sigma$, and σ' of QUARTIC. Using this correspondence, we gain no extraneous solutions by focusing on squared QUARTIC.

2.5. Twice Squared QUARTIC

Squared QUARTIC can be rearranged to be

$$\mathbb{A}(G)=-\tau\sqrt{H}\sqrt{H'}\mathbb{B}(G).$$

Squaring both sides we get $\mathbb{A}(G)^2=\tau^2HH'\mathbb{B}(G)^2$. Through rearrangement, we obtain twice squared QUARTIC to be:

$$\mathbb{A}(G)^2-HH'\mathbb{B}(G)^2=0.$$

Therefore, if $(\ell_0, \ell_1, \theta_0, \theta_1, \phi_0, \tau)$ and $H, H' > 0$, and solves twice squared QUARTIC, then $(\ell_0, \ell_1, \theta_0, \theta_1, \phi_0)$ will solve squared QUARTIC. Conversely, if $(\ell_0, \ell_1, \theta_0, \theta_1, \phi_0)$ satisfies $H, H' > 0$ and solve twice squared QUARTIC, then it is always possible to choose exactly one value of τ so that $(\ell_0, \ell_1, \theta_0, \theta_1, \phi_0, \tau)$ solves squared QUARTIC. This correspondence shows that we gain no extraneous solution of squared QUARTIC by focusing attention on twice squared QUARTIC.

Twice squared QUARTIC is an eight degree polynomial in G. Maple can factor this equation as follows:

$$\begin{aligned} 0 =& (E_1G^6 + E_2G^5 + E_3G^4 + E_4G^3 + E_5G^2 + E_6G + E_7) \qquad \text{(Twice Squared QUARTIC)} \\ & (2\ell_1^2G^2 + (-\ell_0^2 + (4c_1 + 4c_0)\ell_1\ell_0 + (-3 - 4c_0c_1)\ell_1^2)G + (-1 + 3c_0c_1 \\ & + 2c_1^2 + 2c_0^2)\ell_0^2 + (-2c_1 - 2c_0 - 4c_1c_0^2 - 4c_1^2c_0)\ell_1\ell_0 + (1 + 3c_0c_1 + 2c_0^2c_1^2)\ell_1^2). \end{aligned}$$

Let us name $E_1G^6 + E_2G^5 + E_3G^4 + E_4G^3 + E_5G^2 + E_6G + E_7$ Six Degree, and our quadratic equation FACTOR.

In the next chapter, we will discover an interpretation of the quadratic FACTOR.

CHAPTER 3

HEXAGONS WITH AN AXIS OF THREE-FOLD ROTATIONAL SYMMETRY

We will use geometry to find a special case of our three-fold symmetric hexagon. In this chapter, we will study when our hexagon is knotted and unknotted around an axis of rotational symmetry. We will refer to a hexagon with an axis of three-fold rotational symmetry as a *symmetric* hexagon.

3.1. KNOTTED

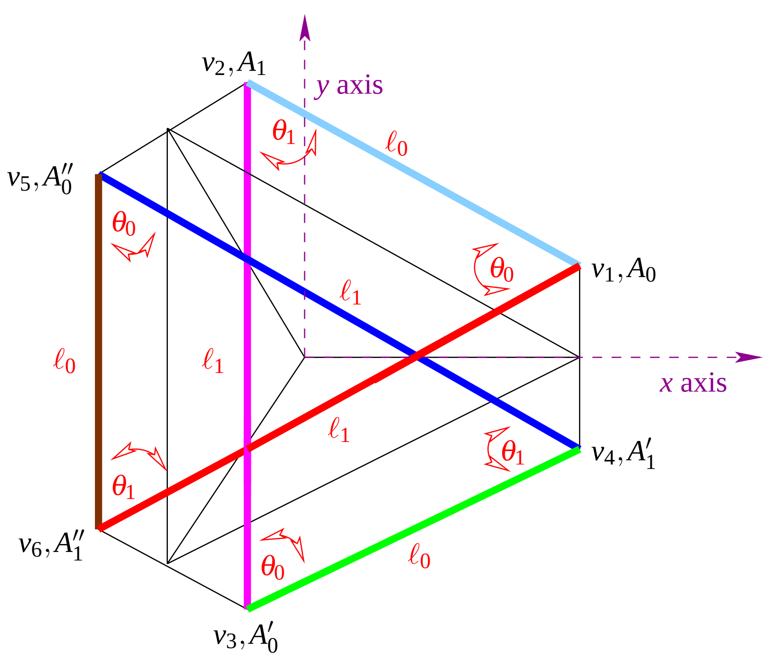

FIGURE 10. A Diagram of a Knotted Symmetric Hexagon

Let us study when a three-fold symmetric hexagon is knotted and symmetric. From figure 10, which views the hexagon projected along the z-axis, we can notice a relationship between the points $(v_1, v_4), (v_2, v_5)$ and (v_6, v_3). To create a knotted shape, their z-axis values must be of the same value with opposite signs. Their x and y coordinates must vary by the different variables of ε and δ to generate the different lengths and angles involving those two points. This gives explicit values for the vertices:

$$v_1 = \begin{pmatrix} a \\ \varepsilon \\ b \end{pmatrix}, \qquad v_4 = \begin{pmatrix} a \\ -\delta \\ -b \end{pmatrix} \tag{*}$$

$$v_5 = \begin{pmatrix} -\frac{a}{2} - \frac{\varepsilon\sqrt{3}}{2} \\ \frac{a\sqrt{3}}{2} - \frac{\varepsilon}{2} \\ b \end{pmatrix}, \qquad v_2 = \begin{pmatrix} -\frac{a}{2} + \frac{\delta\sqrt{3}}{2} \\ \frac{a\sqrt{3}}{2} + \frac{\delta}{2} \\ -b \end{pmatrix}$$

$$v_3 = \begin{pmatrix} -\frac{a}{2} + \frac{\varepsilon\sqrt{3}}{2} \\ \frac{-a\sqrt{3}}{2} - \frac{\varepsilon}{2} \\ b \end{pmatrix}, \qquad v_6 = \begin{pmatrix} -\frac{a}{2} - \frac{\delta\sqrt{3}}{2} \\ \frac{-a\sqrt{3}}{2} + \frac{\delta}{2} \\ -b \end{pmatrix}.$$

Suppose $v_1 = \mathbf{R}_{A_0}, v_2 = \mathbf{R}_{A_1}, v_3 = \mathbf{R}_{A'_0}, v_4 = \mathbf{R}_{A'_1}, v_5 = \mathbf{R}_{A''_0}$, and $v_6 = \mathbf{R}_{A''_1}$. This creates a family of knotted three-fold symmetric hexagons parameterized by a, b, ε, and δ. However, our general hexagon was described in terms of $\ell_0, \ell_1, \theta_0, \theta_1, \sigma, \sigma'$ and ϕ_0. Therefore, we must find the values of those variables in terms of a, b, ε, and δ. We can find these values using the distance formula and the law of cosines. We know from the law of cosines that :

$$(v_3 - v_4) \cdot (v_5 - v_4) = \frac{3a^2}{2} - \frac{\delta^2}{2} - \varepsilon\delta + \varepsilon^2 + 4b^2 = \ell_0 \ell_1 c_1 \tag{33}$$

$$(v_2 - v_1) \cdot (v_6 - v_1) = \frac{3a^2}{2} - \frac{\varepsilon^2}{2} - \varepsilon\delta + \delta^2 + 4b^2 = \ell_0 \ell_1 c_0. \tag{34}$$

From the distance equations, we can find:

$$(v_2-v_1)\cdot(v_2-v_1)=3a^2-a\delta\sqrt{3}+\delta^2-a\sqrt{3}\varepsilon-\delta\varepsilon+\varepsilon^2+4b^2=\ell_0^2 \tag{35}$$

$$(v_6-v_1)\cdot(v_6-v_1)=3a^2+a\delta\sqrt{3}+\delta^2+a\sqrt{3}\varepsilon-\delta\varepsilon+\varepsilon^2+4b^2=\ell_1^2. \tag{36}$$

These calculations came from the Maple worksheet abed.mw from lines $13-17$. From these vertices, we are also able to compute $\cos\phi_0$. According to [**4**], define

$$\begin{aligned}
E_1 =&(v_6-v_1)-\frac{v_2-v_1}{\|v_2-v_1\|}\Big(\frac{v_2-v_1}{\|v_2-v_1\|}\cdot(v_6-v_1)\Big),\\
E_2 =&(v_3-v_2)-\frac{v_2-v_1}{\|v_2-v_1\|}\Big(\frac{v_2-v_1}{\|v_2-v_1\|}\cdot(v_3-v_2)\Big),\\
\text{and } E_3 =&\frac{v_2-v_1}{\|v_2-v_1\|};
\end{aligned}$$

then

$$\begin{aligned}
\cos\phi_0 =& \frac{E_1}{\|E_1\|}\cdot\frac{E_2}{\|E_2\|} \qquad (**)\\
=&\Big(-2\delta\varepsilon^3+5\delta^2\varepsilon^2+3\varepsilon^2a^2-8b^2\delta\varepsilon-12a^2\delta\varepsilon-2\delta^3\varepsilon\\
&+8ab^2\varepsilon\sqrt{3}+3a^2\delta^2+8a^2b^2+9a^4+8ab^2\delta\sqrt{3}\Big)\\
&\cdot\Big(\big((3a^2+\delta^2-2\varepsilon\delta)^2+16b^2(a^2+\delta^2)\big)\\
&\big((3a^2+\varepsilon^2-2\varepsilon\delta)^2+16b^2(a^2+\varepsilon^2)\big)\Big)^{-\frac{1}{2}}.
\end{aligned}$$

and

$$\sin\phi_0=\frac{E_1}{\|E_1\|}\times\frac{E_2}{\|E_2\|}\cdot E_3$$

$$
\begin{aligned}
=&\Big(4\sqrt{3}b(-3a^2+\sqrt{3}a\varepsilon+\sqrt{3}a\delta+3\delta\varepsilon)\\
&\cdot\sqrt{3a^2-\sqrt{3}a\delta+\delta^2-\sqrt{3}a\varepsilon-\delta\varepsilon+\varepsilon^2+4b^2}\Big)\cdot\\
&\Big(\big((3a^2+\delta^2-2\varepsilon\delta)^2+16b^2(a^2+\delta^2)\big)\cdot\\
&\big((3a^2+\varepsilon^2-2\varepsilon\delta)^2+16b^2(a^2+\varepsilon^2)\big)\Big)^{-\frac{1}{2}}
\end{aligned}
$$

Since the value under the square root is always positive in $\cos\phi_0$, we notice that the value of $\cos\phi_0$ can never be imaginary. Also, we notice that the sign of ϕ_0 is the sign of the $\sin\phi_0$. The sign of $\sin\phi_0$ depends on its numerator:

$$
b(-\sqrt{3}a^2+a(\varepsilon+\delta)+\sqrt{3}\varepsilon\delta). \tag{37}
$$

Therefore, we can find the sign of ϕ_0 by finding the sign of the above expression.

Now we need to find the value of σ and σ' in our symmetric case. If we take our vertices from the knotted case, we can plug them into our inequalitiy (4) and (8) to find the value of σ and σ' to be:

$$
\sigma = \text{sign}\ \det\begin{pmatrix} 1 & 1 & 1 & 1 \\ v_6 & v_1 & v_3 & v_5 \end{pmatrix} = sign\big(3\sqrt{3}b(a^2+\varepsilon^2)\big),
$$

and

$$
\sigma' = \text{sign}\ \det\begin{pmatrix} 1 & 1 & 1 & 1 \\ v_1 & v_2 & v_6 & v_4 \end{pmatrix} = \text{sign}\big(3\sqrt{3}b(a^2+\delta^2)\big).
$$

Thus, $\sigma=\sigma'=\text{sign}(b)$. From these formulas, it is clear that the σ and σ' are dependent on the b value. If b is positive, then $\sigma=\sigma'=1$. If b is negative, then $\sigma=\sigma'=-1$. Therefore, we know all possible values of (σ,σ') for our knotted symmetric case.

Using this information, we can solve for a,b,ε, and δ in terms of ℓ_0,ℓ_1,θ_0 and θ_1 in the Maple worksheet abed.mw. The expressions for a,b,ε, and δ are not obviously easily simplified. However when a,b,ε, and δ have real solutions, we can plug them into $(**)$

(see abed.mw) to find:

$$\cos\phi_0 = \frac{1}{4\ell_1^2 s_1 s_0}\left(\ell_0^2 - 4(c_1+c_0)\ell_1\ell_0 + (4c_0c_1+3)\ell_1^2 \right.$$
$$\left. + \sqrt{\ell_0^4 - 8(c_0+c_1)\ell_1\ell_0^3 + 2(8c_0c_1+7)\ell_1^2\ell_0^2 - 8(c_0+c_1)\ell_1^3\ell_0 + \ell_1^4}\right). \tag{38}$$

The $\sin\phi_0$ function was also not easily simplified. Therefore, we can find the sign of ϕ_0 from the non square root values of equation (37):

$$\begin{aligned}&(\ell_1^4 + 6\ell_0\ell_1^3c_0 + 6\ell_0\ell_1^3c_1 - 14\ell_1^2\ell_0^2 - 16\ell_0^2\ell_1^2c_1c_0\\ &\quad - \ell_1^2SQ + 2\ell_0\ell_1c_0SQ + 10\ell_0^3\ell_1c_0 + 2\ell_0\ell_1c_1SQ + 10\ell_0^3\ell_1c_1 - 3\ell_0^2SQ - 3\ell_0^4)\\ &\cdot(-2\ell_0\ell_1c_1 + 2\ell_1^2 - 2\ell_0\ell_1c_0 + 2\ell_0^2 + SQ)^{(-1)}\end{aligned}$$

where

$$SQ = \sqrt{\ell_0^4 - 8\ell_0^3\ell_1c_0 - 8\ell_0^3\ell_1c_1 + 14\ell_1^2\ell_0^2 + 16\ell_0^2\ell_1^2c_1c_0 - 8\ell_0\ell_1^3c_0 - 8\ell_0\ell_1^3c_1 + \ell_1^4}$$

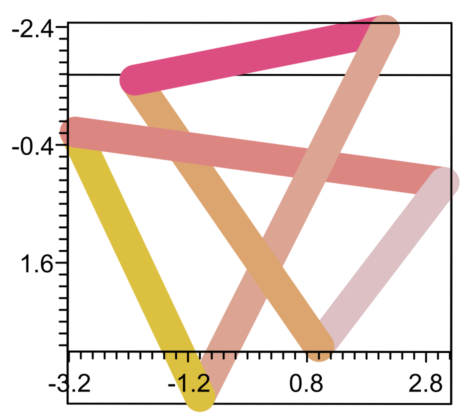

FIGURE 11. A Knotted Hexagon with Three-Fold Symmetry

From this information, we can use our Maple program hexplot.mw to create a three dimensional model of the knotted hexagon as specified in Apendix B. However, this model gives a different embedding than the described in $(*)$. In Figure 11, there is an example of this knotted family where $\theta_0 = 0.6826197291$, $\theta_1 = 0.6826197291$, $\ell_0 = 1$, $\ell_1 = 1.303369776, \sigma = 1, \sigma' = 1$ and $\phi_0 = 0.3322960944$. We can first check to see if the restrictions hold for these values. $K = K' = 0.4442868602$, therefore the restriction that $K, K' > 0$ holds. $c_1 - c_0 + \sqrt{3}(s_1 - s_0) = 1.732050808$ and $c_1 - c_0 + \sqrt{3}(s_1 - s_0) = -1.732050808$, therefore $-.424513652 < \cos\phi_0 < 1.682086412$. Our $\cos\phi_0 = 0.9452958170$, therefore is in the range. We also need to check the values of a, b, ε and δ. From Maple worksheet abed.mw, we find that $a = .4036783441$, $b = .4466801395$, $\varepsilon = 0.2498503168$, and $\delta = 0.2498503168$. Since these values are positive and real, we can find a knotted hexagon with our given $\ell_0, \ell_1, \theta_0, \theta_1, \sigma, \sigma'$ and ϕ_0. From this information, we can find:

ϕ_0	ϕ_1	ϕ_1''	σ	σ'	*Figure*
0.3322960944	−1.330419102	1.330419102	1	1	11
−0.3322960944	−1.358031864	1.358031864	−1	−1	11

See Maple worksheet rot.mw line 11 to rotate this three dimensional figure.

3.2. UNKOTTED

Now let us consider the unknotted hexagon with an axis of rotational symmetry. We can create this polygon by connecting the vertices $v_1, \ldots, v_6$ in a different manner. This allows us to use the same vertices as we found in our knotted case, but they will appear in a different order. In this configuration, $v_1 = \mathbf{R}_{A_0}, v_2 = \mathbf{R}_{A_1}, v_5 = \mathbf{R}_{A_0'}, v_6 = \mathbf{R}_{A_1'}, v_3 = \mathbf{R}_{A_0''}$ and $v_4 = \mathbf{R}_{A_1''}$. We must find the values of ℓ_0, ℓ_1, θ_0 and θ_1 in terms of a, b, ε, and δ. The new expressions from Maple worksheet abed2.mw are:

$$(v_1 - v_2)\cdot(v_1 - v_2) = 3a^2 - a\delta\sqrt{3} + \delta^2 + \varepsilon^2 - a\varepsilon\sqrt{3} - \delta\varepsilon + 4b^2 = \ell_0^2$$

$$(v_1 - v_4)\cdot(v_1 - v_4) = \delta^2 + 2\delta\varepsilon + \varepsilon^2 + 4b^2 = \ell_1^2$$

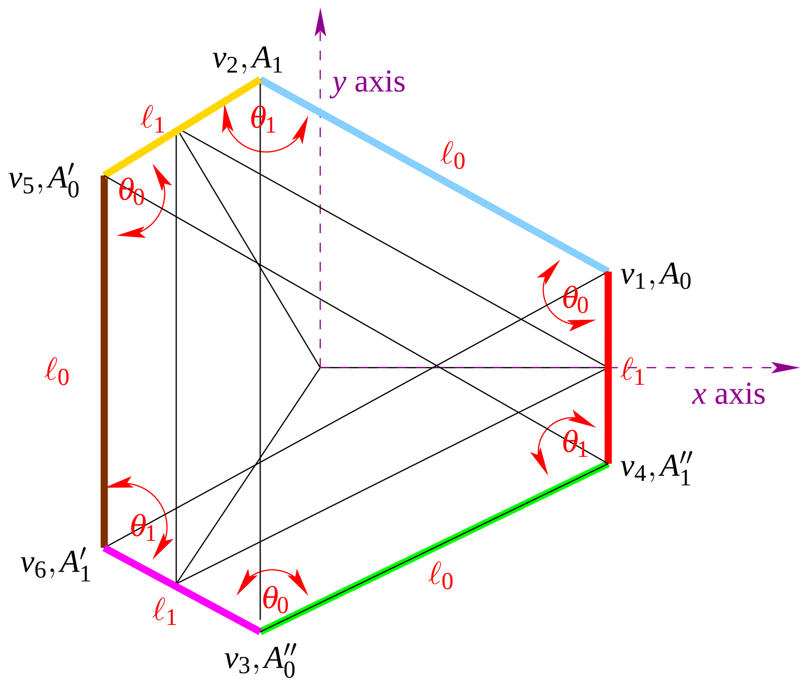

FIGURE 12. A Diagram of a Unknotted Symmetric Hexagon

$$(v_1 - v_2) \cdot (v_5 - v_2) = -\frac{a\delta\sqrt{3}}{2} - \frac{\varepsilon a\sqrt{3}}{2} + \delta^2 + \frac{\delta\varepsilon}{2} - \frac{\varepsilon^2}{2} + 4b^2 = \ell_0\ell_1 c_1$$

$$(v_2 - v_1) \cdot (v_4 - v_1) = -\frac{\delta^2}{2} + \varepsilon^2 - \frac{a\delta\sqrt{3}/2}{2} + \frac{\delta\varepsilon}{2} - \frac{a\varepsilon\sqrt{3}}{2} + 4b^2 = \ell_0\ell_1 c_0.$$

Again, we can compute a value for $\cos\phi_0$ where as in [**4**], we define

$$\begin{aligned}
E_1 =& (v_4 - v_1) - \frac{v_2 - v_1}{\|v_2 - v_1\|}\left(\frac{v_2 - v_1}{\|v_2 - v_1\|} \cdot (v_4 - v_1)\right), \\
E_2 =& (v_5 - v_2) - \frac{v_2 - v_1}{\|v_2 - v_1\|}\left(\frac{v_2 - v_1}{\|v_2 - v_1\|} \cdot (v_5 - v_2)\right), \\
\text{and } E_3 =& \frac{v_2 - v_1}{\|v_2 - v_1\|}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\cos\phi_0 &= \frac{E_1}{\|E_1\|}\cdot\frac{E_2}{\|E_2\|}\\
&= \big(6a^2\varepsilon\delta+\delta^3\varepsilon+2\delta^2\varepsilon^2-3\sqrt{3}a\varepsilon^2\delta+3\sqrt{3}a\delta^2\varepsilon+3a^2\delta^2\\
&\quad +3a^2\varepsilon^2-\sqrt{3}a\delta^3-16a^2b^2+16\delta\varepsilon b^2-\delta\varepsilon^3+\sqrt{3}a\varepsilon^3\big)\\
&\Big((\varepsilon^4-2\sqrt{3}a\varepsilon^3+2\varepsilon^3\delta-4\sqrt{3}a\varepsilon^2\delta+3a^2\varepsilon^2\\
&\quad +\varepsilon^2\delta^2+16\varepsilon^2b^2-2\sqrt{3}a\varepsilon\delta^2+6a^2\varepsilon\delta+3a^2\delta^2+16a^2b^2)\\
&\quad (\delta^4-2\sqrt{3}a\varepsilon^3+2\varepsilon\delta^3-4\sqrt{3}a\varepsilon\delta^2+3a^2\delta^2+\varepsilon^2\delta^2\\
&\quad +16\delta^2b^2-2\sqrt{3}a\varepsilon^2\delta+6a^2\varepsilon\delta+3a^2\varepsilon^2+16a^2b^2)\Big)^{-(\frac{1}{2})}.
\end{aligned} \tag{39}$$

Also,

$$\sin\phi_0 = \frac{E_1}{\|E_1\|}\times\frac{E_2}{\|E_2\|}\cdot E_3$$

$$\begin{aligned}
&= 8ab(\delta+\varepsilon)\sqrt{3a^2-\sqrt{3}a\delta+\delta^2-\sqrt{3}a\varepsilon-\varepsilon\delta+\varepsilon^2+4b^2}\\
&\quad\Big((\varepsilon^4-2\sqrt{3}a\varepsilon^3+2\varepsilon^3\delta-4\sqrt{3}a\varepsilon^2\delta+3a^2\varepsilon^2\\
&\quad +\varepsilon^2\delta^2+16\varepsilon^2b^2-2\sqrt{3}a\varepsilon\delta^2+6a^2\varepsilon\delta+3a^2\delta^2+16a^2b^2)\\
&\quad (\delta^4-2\sqrt{3}a\varepsilon^3+2\varepsilon\delta^3-4\sqrt{3}a\varepsilon\delta^2+3a^2\delta^2+\varepsilon^2\delta^2\\
&\quad +16\delta^2b^2-2\sqrt{3}a\varepsilon^2\delta+6a^2\varepsilon\delta+3a^2\varepsilon^2+16a^2b^2)\Big)^{-(\frac{1}{2})}
\end{aligned}$$

Again, we notice that the sign of ϕ_0 is the sign of the $\sin\phi_0$. The sign of $\sin\phi_0$ depends on its numerator:

$$a\delta(\delta+\varepsilon) \tag{40}$$

Therefore, we can find the sign of ϕ_0 by finding the sign of the above expression.

We can also find the values of σ and σ'. If we take our vertices from the unknotted case, we can plug them into our equations (4) and (8) for the σ and σ'. As in the knotted case:

$$\sigma = \text{sign}\ \det \begin{pmatrix} 1 & 1 & 1 & 1 \\ v_4 & v_1 & v_5 & v_3 \end{pmatrix} = \text{sign}(3\sqrt{3}b(a^2+\varepsilon^2)),$$

and

$$\sigma' = \text{sign}\ \det \begin{pmatrix} 1 & 1 & 1 & 1 \\ v_3 & v_2 & v_4 & v_6 \end{pmatrix} = \text{sign}(3\sqrt{3}b(a^2+\delta^2)).$$

Thus, $\sigma = \sigma' = \text{sign}(b)$.

We must solve for the values of a, b, ε, and δ in terms of $\ell_0, \ell_1, \theta_0, \theta_1$, and ϕ_0 (see Maple worksheet abed2.mws). As before, the expressions are complicated. When a, b, ε, and δ has real solutions, we can substituted them equation (38) the formula miraculously appears:

$$\cos\phi_0 = \frac{1}{4\ell_1^2 s_1 s_0}\Big(\ell_0^2 - 4(c_1+c_0)\ell_1\ell_0 + (4c_0c_1+3)\ell_1^2 \\ - \sqrt{\ell_0^4 - 8(c_0+c_1)\ell_1\ell_0^3 + 2(8c_0c_1+7)\ell_1^2\ell_0^2 - 8(c_0+c_1)\ell_1^3\ell_0 + \ell_1^4}\Big). \tag{41}$$

Comparing this equation to (37), the only difference is the sign in front of the square root. From this equation, we have found a symmetric non-knotted hexagon with three-fold symmetry.

We can find the sign of the ϕ_0 value by finding sign of the non square root values of (40).

$$\frac{(-\ell_1+\ell_0c_1)(\ell_0^2 - 2\ell_0\ell_1c_0 + \ell_1^2)}{-\ell_0^3c_1 + 2\ell_0^2\ell_1c_0c_1 + \ell_0^3c_0 + 13\ell_0\ell_1^2c_0 - \ell_0 ell_1^2c_1 - 8\ell_0^2\ell_1c_0^2 - 6\ell_1^3}$$

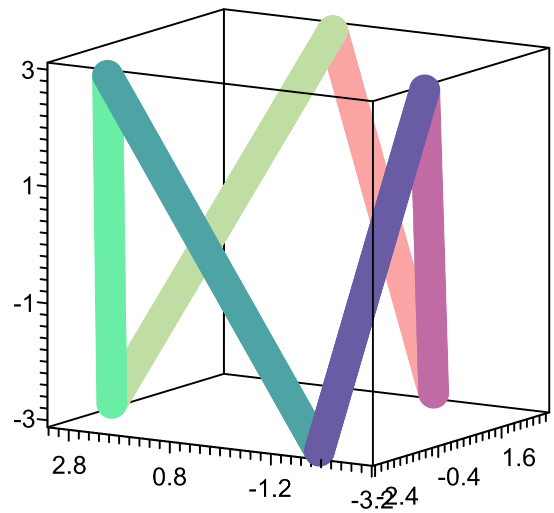

FIGURE 13. A Unknotted Symmetric Hexagon

Figure 13 is a good example of this family. In this figure, $\theta_0 = 1$, $\theta_1 = 1.303369776$, $\ell_0 = .6826197291$, and $\ell_1 = .6826197291$. From our equation, we obtain $\phi_0 = 2.368947425$. We can check to see if the restrictions hold for these values. $K = K' = .5316074064$, therefore the restriction that $K, K' > 0$ holds. $c_1 - c_0 + \sqrt{3}(s_1 - s_0) = 1.732050808$ and $c_1 - c_0 + \sqrt{3}(s_1 - s_0) = -1.732050808$, therefore $-.424513652 < \cos\phi_0 < 1.682086412$. Our $\cos\phi_0 = 0.1699147542$, therefore is in the range. We can calculate:

ϕ_0	ϕ_1	ϕ_1''	σ	σ'	*Figure*
1.400053162	−1.638255513	1.638255514	1	1	13
−1.400053162	−1.672169761	1.672169761	−1	−1	13

.

See Maple worksheet rot.mw line 5 to rotate this three dimensional figure.

It will be useful to have a single quadratic equation in G which characterize the rotationally symmetric case. When a, b, ε, and δ has real solutions, from (37) and (39) we get

$$\begin{aligned} 0 =& 2\ell_1^2 G^2 + (-\ell_0^2 + (4c_1 + 4c_0)\ell_1\ell_0 + (-3 - 4c_0c_1)\ell_1^2)G \\ &+ (-1 + 3c_0c_1 + 2c_1^2 + 2c_0^2)\ell_0^2 + (-2c_1 - 2c_0 - 4c_1c_0^2 - 4c_1^2c_0)\ell_1\ell_0 \\ &+ (1 + 3c_0c_1 + 2c_0^2c_1^2)\ell_1^2. \end{aligned} \tag{FACTOR}$$

This quadratic will be referred to as FACTOR. Notice that FACTOR is our quadratic equation that we found that factored out of our twice squared QUARTIC in section 2.5.

3.3. Hexagons with an Axis of Rotational Symmetry where $\theta_0 = \theta_1$

Looking at the formulas for θ_0 and θ_1 in terms of a, b, ε, and δ we see that if $\varepsilon = \delta$ then $\theta_0 = \theta_1$. Conversely, using the Maple expressions for a, b, ε, and δ in terms of ℓ_0, ℓ_1, θ_0 and θ_1, we see that if $\theta_0 = \theta_1$ then $\varepsilon = \delta$. Thus in the family of symmetric hexagons $\theta_0 = \theta_1$ if and only if $\varepsilon = \delta$.

The solutions of $a, b, \varepsilon = \delta$ are easily reduced in the knotted hexagon to be:

$$a = \frac{1}{12}\left(\sqrt{12a^2 + 6\sqrt{3}(\ell_0^2 - \ell_1^2)} + \sqrt{12a^2 - 6\sqrt{3}(\ell_0^2 - \ell_1^2)}\right)$$

$$b = \frac{1}{12}\left(-\sqrt{12a^2 + 6\sqrt{3}(\ell_0^2 - \ell_1^2)} + \sqrt{12a^2 - 6\sqrt{3}(\ell_0^2 - \ell_1^2)}\right)$$

$$\varepsilon = \delta = \frac{1}{12}\left(-6(\ell_0^2 + \ell_1^2) + 48\ell_0\ell_1 c - \sqrt{12a^2 + 6\sqrt{3}(\ell_0^2 - \ell_1^2)} \cdot \sqrt{12a^2 - 6\sqrt{3}(\ell_0^2 - \ell_1^2)}\right)^{\left(\frac{1}{2}\right)}$$

Therefore, we can produce a knotted hexagon when $a, b, \varepsilon = \delta$ are real. There are a couple of restrictions that insure that $a, b, \varepsilon = \delta$ exist:

$$2a^2 + \sqrt{3}(\ell_0^2 - \ell_1^2) > 0 \text{ and } 2a^2 - \sqrt{3}(\ell_0^2 - \ell_1^2) > 0.$$

For b to exist, we must insure that

$$-6(\ell_0^2 + \ell_1^2) + 48\ell_0\ell_1 c > \sqrt{12a^2 + 6\sqrt{3}(\ell_0^2 - \ell_1^2)} \cdot \sqrt{12a^2 - 6\sqrt{3}(\ell_0^2 - \ell_1^2)}.$$

We can simplify this inequality to:

$$(6\ell_0\ell_1 c - a^2)^2 - (12a^2 + 6\sqrt{3}(\ell_0^2 - \ell_1^2)) \cdot (12a^2 - 6\sqrt{3}(\ell_0^2 - \ell_1^2)) > 0.$$

This equation has many cancellations leaving us with the restriciton that

$$12\ell_0^2\ell_1^2(4c^2-1) > 0.$$

Since $\cos\theta > 0$, we have found that knotted hexagons around an axis of symmetry must have $0 < \theta \leq \frac{\pi}{3}$.

This informations allows us to find the simplified formula for $\cos\phi_0$ for this case. We can solve for these values easily by setting $\theta_0 = \theta_1 = \theta$. When the given values satisfy $2a^2 + \sqrt{3}(\ell_0^2 - \ell_1^2) > 0$, $2a^2 - \sqrt{3}(\ell_0^2 - \ell_1^2) > 0$, and $0 < \theta \leq \frac{\pi}{3}$, the wedge angle of the knotted hexagon will be:

$$\begin{aligned}\cos\phi_0 = \frac{1}{4\ell_1^2 s^2}\Bigg(&\ell_0^2 - 8\ell_1\ell_0 c + (3+4c^2)\ell_1^2 \\ &+ \sqrt{\ell_0^4 - 16\ell_1\ell_0^3 c + (14+16c^2)\ell_1^2\ell_0^2 - 16\ell_1^3\ell_0 c + \ell_1^4}\Bigg).\end{aligned} \tag{42}$$

The solutions for $a, b, \varepsilon = \delta$ in the unknotted hexagon produce different values which are found to be:

$$\begin{aligned}a =&\frac{\sqrt{3}}{72(\ell_0 c - \ell_1)\ell_1}\cdot\left(-a^2 - \sqrt{12a^2+6\sqrt{3}(\ell_0^2-\ell_1^2)}\right)\cdot\sqrt{12a^2-6\sqrt{3}(\ell_0^2-\ell_1^2)})\cdot \\ &\sqrt{42\ell_1^2 - 48\ell_0\ell_1 c + 6\ell_0^2 - 6\sqrt{12a^2+6\sqrt{3}(\ell_0^2-\ell_1^2)}\cdot\sqrt{12a^2-6\sqrt{3}(\ell_0^2-\ell_1^2)}} \\ b =&\frac{1}{12}\sqrt{-6\ell_1^2 + 48\ell_0\ell_1 c - 6\ell_0^2 + 6\sqrt{12a^2+6\sqrt{3}(\ell_0^2-\ell_1^2)}\cdot\sqrt{12a^2-6\sqrt{3}(\ell_0^2-\ell_1^2)}} \\ \varepsilon = \delta =&\frac{1}{12}\sqrt{42\ell_1^2 - 48\ell_0\ell_1 c + 6\ell_0^2 - 6\sqrt{12a^2+6\sqrt{3}(\ell_0^2-\ell_1^2)}\cdot\sqrt{12a^2-6\sqrt{3}(\ell_0^2-\ell_1^2)}}\end{aligned}$$

To insure, that the values of $a, b, \varepsilon = \delta$ are real for the unknotted hexagon:

$$(2a^2 + \sqrt{3}(\ell_0^2 - \ell_1^2)) \cdot (2a^2 - \sqrt{3}(\ell_0^2 - \ell_1^2)) > 0.$$

Also, we must check that the other values under the square roots of a, and $\varepsilon = \delta$ are real by:

$$(42\ell_1^2 - 48\ell_0\ell_1 c + 6\ell_0^2)^2 > 36(12a^2 + 6\sqrt{3}(\ell_0^2 - \ell_1^2)) \cdot (12a^2 - 6\sqrt{3}(\ell_0^2 - \ell_1^2)).$$

After expanding this value, and moving the whole quantity on one side, we recieve that

$$1728\ell_1^2(\ell_0 c - \ell_1)^2 > 0.$$

This statement is always true, therefore, a and $\varepsilon = \delta$ do not need any more restrictions to make their quantities real. Now, we must check that b is real by:

$$(-6\ell_1^2 + 48\ell_0\ell_1 c - 6\ell_0^2)^2 > -36(12a^2 + 6\sqrt{3}(\ell_0^2 - \ell_1^2)) \cdot (12a^2 - 6\sqrt{3}(\ell_0^2 - \ell_1^2)).$$

When we simplify this quantity, we recieve the restriction that

$$72a^4 + 432\ell_0\ell_1(-2\ell_0^2 c + \ell_0\ell_1 + 6\ell_0\ell_1 c^2 - 2\ell_1^2 c) > 0.$$

This gives us our two restrictions that allow us to find if an unknotted symmetric hexagon can be produced when the size angles are all the same.

We can plug in these values of $a, b, \varepsilon = \delta$ into equation (41) . When our restrictions are satisfied, we can find the wedge angle of the unknotted hexagon to be:

$$\cos\phi_0 = \frac{1}{4\ell_1^2 s^2}\left(\ell_0^2 - 8\ell_1\ell_0 c + (3+4c^2)\ell_1^2 \right. \\ \left. - \sqrt{\ell_0^4 - 16\ell_1\ell_0^3 c + (14+16c^2)\ell_1^2\ell_0^2 - 16\ell_1^3\ell_0 c + \ell_1^4}\right). \tag{43}$$

We can find the quadratic FACTOR of θ that satifies these two equations to be:

$$2\ell_1^2 G^2 + (-\ell_0^2 + 8\ell_1\ell_0 c + (-4c^2 - 3)\ell_1^2)G + (-1+7c^2)\ell_0^2 \\ + (-4c - 8c^3)\ell_1\ell_0 + (1 + 2c^4 + 3c^2)\ell_1^2 \tag{FACTOR of θ}$$

We can use this factor when we look at the special case of hexagons where $\theta_0 = \theta_1$ to help us solve for new families of solutions.

CHAPTER 4

θ CASE

The special case of a three-fold symmetric hexagon where $\theta_1 = \theta_0 = \theta$ is referred to as the θ case. By setting our angles equal to each other where $\cos\theta = c$ and $\sin\theta = s$, we note that $H = H' = \mathbb{H}$ and $E(G) = F(G) = \mathbb{E}$, and QUARTIC becomes:

$$A(G) + \sigma\sigma'\mathbb{H}B(G) = -\ell_0 s^2 \sin\phi_0 \sqrt{\mathbb{H}}(\sigma' + \sigma)\mathbb{E}.$$

where $a^2 = \ell_0^2 + \ell_1^2 - 2\ell_0\ell_1 c$ and

$$\begin{aligned} H = H' = \mathbb{H} = &- a^2\left(2\ell_1 G - \ell_1(1+2c^2) + \ell_0(3c - \sqrt{3}s)\right) \\ &\left(2\ell_1 G - \ell_1(1+2c^2) + \ell_0(3c + \sqrt{3}s)\right) \\ = &- a^2[(2\ell_1 G - \ell_1(1+2c^2) + 3\ell_0 c)^2 - 3\ell_0^2(1-c^2)]. \end{aligned}$$

This simplified version of our QUARTIC shows that the values of σ and σ' play a major role in finding the solutions to this equation. Therefore, we must study four separate situations of σ and σ' to obtain all solutions of the ϕ_0. The four situations are when $(\sigma = 1, \sigma' = 1), (\sigma = -1, \sigma' = -1), (\sigma = -1, \sigma' = 1)$, and $(\sigma = 1, \sigma' = -1)$. In this chapter, we will study these four separate cases of our sigma values and find what families are produced in each situation.

4.1. $\tau = \sigma\sigma'$ IS LESS THAN ZERO

When the σ and σ' have different signs in our special QUARTIC, our term $(\sigma' + \sigma)$ in the coefficient of $\sin\phi_0$ equals zero. Also, we notice that the only other coefficient with the values of σ and σ' in the QUARTIC appear as $\tau = \sigma\sigma'$. Thus when $\tau = -1$, we get

$$A(G) - \mathbb{H}B(G) = 0 \tag{Special QUARTIC}$$

Therefore both cases when $(\sigma = -1, \sigma' = 1)$ and $(\sigma = 1, \sigma' = -1)$ both have the same solution ϕ_0 to the QUARTIC. When we use Maple to factor Special QUARTIC, we receive

$$\begin{aligned} 0 &= -(\ell_1 - \ell_0)(\ell_1 + \ell_0)\Big(2\ell_1^2 G^2 + (-4c^2\ell_1^2 + 3\ell_0^2 + \ell_1^2)G - \ell_1^2 - 3\ell_0^2 + 2\ell_1^2 c^4 + 3\ell_0^2 c^2 \\ &\qquad - c^2\ell_1^2\Big)\Big(\ell_1^2 G^2 + (2\ell_1\ell_0 c - 2c^2\ell_1^2)G + 2\ell_1\ell_0 c + \ell_0^2 c^2 - \ell_0^2 + \ell_1^2 c^4 - 2c^3\ell_1\ell_0 - \ell_1^2\Big) \\ &= -(\ell_1 - \ell_0)(\ell_1 + \ell_0) BOAT\,\mathbb{K} \end{aligned} \tag{44}$$

where $\mathbb{K} = K = K' = a^2 - (c(\ell_0 - \ell_1 c) + \ell_1 G)^2$ and

$$BOAT = \Big(2\ell_1^2 G^2 + (-4c^2\ell_1^2 + 3\ell_0^2 + \ell_1^2)G - \ell_1^2 - 3\ell_0^2 + 2\ell_1^2 c^4 + 3\ell_0^2 c^2 - c^2\ell_1^2\Big)$$

.

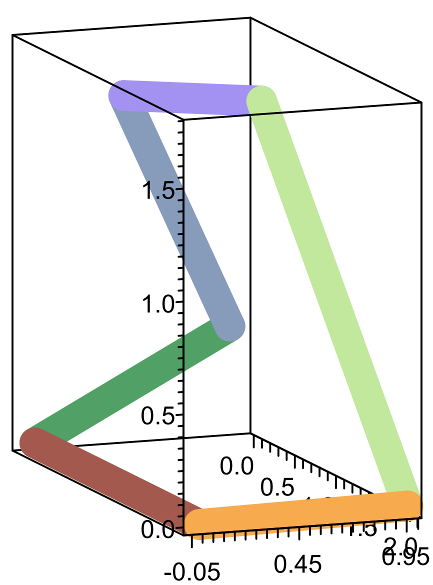

FIGURE 14. A Boat-Shaped Hexagon where $\theta_1 = \theta_0$

Since we are given the restriction that $\mathbb{K} > 0$, we can find values of ϕ_0 by setting $BOAT = 0$. The two solutions for ϕ_0 from BOAT are

$$\cos\phi_0 = \frac{1}{4\ell_1^2 s^2}(4c^2\ell_1^2 - 3\ell_0^2 - \ell_1^2 + \sqrt{-48\ell_1^2\ell_0^2c^2 + 9\ell_0^4 + 30\ell_0^2\ell_1^2 + 9\ell_1^4}) \tag{45}$$

$$\cos\phi_0 = \frac{1}{4\ell_1^2 s^2}(4c^2\ell_1^2 - 3\ell_0^2 - \ell_1^2 - \sqrt{-48\ell_1^2\ell_0^2c^2 + 9\ell_0^4 + 30\ell_0^2\ell_1^2 + 9\ell_1^4}) \tag{46}$$

Using these results, we can study what families of solutions can be produced by equations (45) and (46). In our Maple program, we can observe that equation (45) and (46) create the same family of solutions where equation (45)'s value of ϕ_0 is equations (46)'s value of ϕ_0'. These solutions for ϕ_0 creates a boat-shaped hexagon. This family is also unknotted, and does not have an axis of three-fold rotational symmetry. In Figure 14, $\theta_0 = \frac{\pi}{2}$, $\theta_1 = \frac{\pi}{2}$, $\ell_0 = 1$, and $\ell_1 = 2$. From equation (45), we obtain $\phi = 0.9333197962$. This solution exist since the restrictions hold where $K = K' = 4.220620882 > 0$ and $-.6160254040 < G < 1.116025404$. This solution from equation (46) fails to satisfy the restrictions.

In QUARTIC, we have found that when $(\ell_0 = \ell_1)$ our equation (44) will always be solved. This shows that we have a "*flexible*" family of solutions.

THEOREM 4.1. *When $\ell_0 = \ell_1, \theta_0 = \theta_1$, and $\sigma = -\sigma'$, there exists a three-fold symmetric hexagon for all the ϕ_0 values satisfing our restrictions as discussed in* [**6**].

This family was discussed in [**6**], but now we have now shown those solutions are not extraneous.

4.2. $\tau = \sigma\sigma'$ IS GREATER THAN ZERO

We have studied what happened when the signs of σ and σ' were different. Now we must investigate what happens when the signs are the same. However, this process becomes more difficult because the coefficients of $\sin\phi_0$ are still present. This leaves us with $\sqrt{\mathbb{H}}$, which cannot be factored. Therefore, we must use the squared QUARTIC equation to find the solutions for our θ case.

In the theta case, we will find our squared QUARTIC equation from section 2.4 to be:

$$\mathbb{A}(G)+\tau\mathbb{H}\mathbb{B}(G)=0.$$

To simplify our squared QUARTIC, we can plug the $\tau=1$ into our equation. We obtain that squared QUARTIC factors as follows:

$$\begin{aligned}
0 = &\Big(2\ell_1^2G^2+(-\ell_0^2+8\ell_1\ell_0c+(-4c^2-3)\ell_1^2)G+(-1+7c^2)\ell_0^2 \\
&+(-4c-8c^3)\ell_1\ell_0+(1+2c^4+3c^2)\ell_1^2\Big) \\
&\Big(2\ell_1^2(-8\ell_1\ell_0c+3\ell_0^2-2\ell_0\ell_1+3\ell_1^2)(-8\ell_1\ell_0c+3\ell_0^2+2\ell_0\ell_1+3\ell_1^2)G^2 \\
&+(-9\ell_0^6+72\ell_0^5c\ell_1+(-9-324c^2)\ell_1^2\ell_0^4+(144c+576c^3)\ell_1^3\ell_0^3 \\
&\quad+(-19-472c^2-256c^4)\ell_1^4\ell_0^2+(168c+192c^3)\ell_1^5\ell_0+(-27-36c^2)\ell_1^6)G \\
&+(6c^2-9)\ell_0^6+(-360c^3+36c)\ell_1\ell_0^5+(690c^4-21+141c^2)\ell_1^2\ell_0^4 \\
&+(-480c^5-624c^3+24c)\ell_1^3\ell_0^3+(128c^6+444c^4+249c^2-11)\ell_1^4\ell_0^2 \\
&+(-60c-168c^3-96c^5)\ell_1^5\ell_0+(27c^2+18c^4+9)\ell_1^6\Big) \\
=&FACTOR\cdot CHAIR.
\end{aligned}$$

Notice that the first quadratic factor is FACTOR of θ. Therefore, we can verify that our equations for the knotted and unknotted hexagons with rotational three-fold symmetry are correct. Using this information, we can focus our attention on the other quadratic factor that is called CHAIR. CHAIR's roots are:

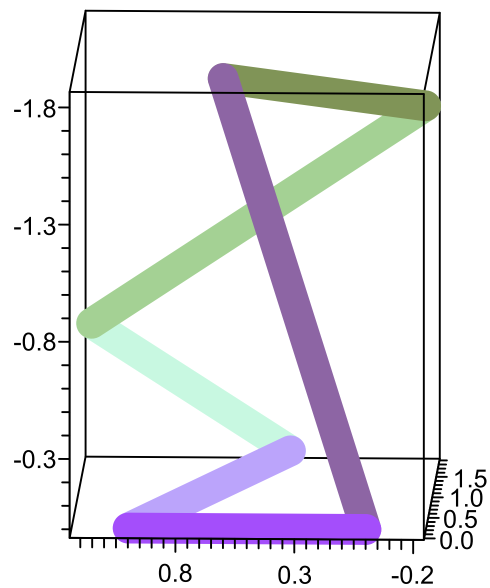

FIGURE 15. A Chair-Shaped Hexagon where $\theta_1 = \theta_0$

$$\cos\phi_0 = \frac{1}{4\ell_1^2(3\ell_0^2+(-8c-2)\ell_1\ell_0+3\ell_1^2)(3\ell_0^2+(-8c+2)\ell_1\ell_0+3\ell_1^2)s^2} \cdot \Big(9\ell_0^6 - 72c\ell_0^5\ell_1 + (9+324c^2)\ell_1^2\ell_0^4 + (-144c-576c^3)\ell_1^3\ell_0^3 + (19+472c^2+256c^4)\ell_1^4\ell_0^2 + (-168c-192c^3)\ell_1^5\ell_0 + (27+36c^2)\ell_1^6 + (3\ell_0^4 - 24\ell_1\ell_0^3c + (10+32c^2)\ell_1^2\ell_0^2 - 24\ell_1^3\ell_0c + 3\ell_1^4) \cdot \sqrt{3(3\ell_0^4+(-16c^2+10)\ell_1^2\ell_0^2+3\ell_1^4)} \Big) \tag{47}$$

$$\cos\phi_0 = \frac{1}{4\ell_1^2(3\ell_0^2+(-8c-2)\ell_1\ell_0+3\ell_1^2)(3\ell_0^2+(-8c+2)\ell_1\ell_0+3\ell_1^2)s^2} \cdot \\ \Bigg(9\ell_0^6 - 72c\ell_0^5\ell_1 + (9+324c^2)\ell_1^2\ell_0^4 + (-144c-576c^3)\ell_1^3\ell_0^3 \\ + (19+472c^2+256c^4)\ell_1^4\ell_0^2 + (-168c-192c^3)\ell_1^5\ell_0 + (27+36c^2)\ell_1^6 \\ - (3\ell_0^4 - 24\ell_1\ell_0^3c + (10+32c^2)\ell_1^2\ell_0^2 - 24\ell_1^3\ell_0c + 3\ell_1^4) \cdot \\ \sqrt{3(3\ell_0^4+(-16c^2+10)\ell_1^2\ell_0^2+3\ell_1^4)}\Bigg) \tag{48}$$

We know that a ϕ_0 exists for a given values of bonds and angles for equations 45 and 46 when

$$3\ell_0^4 + (-16c^2+10)\ell_1^2\ell_0^2 + 3\ell_1^4 > 0.$$

Chair's factors produce ϕ_0 that create a non-knotted polygons without any rotational symmetry along an axis. However, they do create a chair shaped polygon. In Figure 15, we can see an example of a hexagon in this family whose ϕ_0 was calculated by equation (46). When $\ell_0 = 1$, $\ell_1 = 2$, $\theta_0 = \frac{\pi}{4}$, and $\theta_1 = \frac{\pi}{4}$, we obtain $\phi = 1.288564606$ in our Figure 15. This solution exist since the restrictions hold where $K = K' = 3.377241071 > 0$ and $-0.04809079475 < G < 1.7755483092$. Equation 45 and 46 are related because they both form the same polygon. However, they take a different perspective on the hexagon. Equation 46 produces a ϕ_0, and equation 4 creates another ϕ_0 that is equal to equation 45 ϕ_0'.

Now that we have found all the families of hexagons that are created when $\theta_1 = \theta_0$, we can see that we have specific restrictions on knotted hexagons. In our examples, we only saw one family of solutions that create a knotted hexagon. This leads ut to the following.

CONJECTURE 4.2. *Every knotted three-fold symmetric hexagon with $\theta_1 = \theta_0$ contains an axis of rotational symmetry.*

We have learned that there are 4 different families of hexagons where $\theta_1 = \theta_0$. All of our families exist and produce beautiful graphs as shown in our Figures. We will use this information to learn more about our general hexagon with three-fold symmetry.

4.3. Learning from θ Case

We have already seen that our QUARTIC can be simplified in our θ case to become:

$$A(G) + \sigma\sigma'\mathbb{H}B(G) = -\ell_0 s^2 \sin\phi_0 \sqrt{\mathbb{H}}(\sigma' + \sigma)\mathbb{E}.$$

We can square this equation to produce squared QUARTIC from section 2.4.

$$0 = \mathbb{A}(G) + \tau\mathbb{H}\mathbb{B}(G).$$

We know that our squared QUARTIC in the θ case simplifies when $\tau = 1$ to

$$0 = FACTOR \cdot CHAIR.$$

When $\tau = -1$, QUARTIC factored into

$$A(G) - \mathbb{H}B(G) = (\ell_0 - \ell_1)(\ell_0 + \ell_1)BOAT\,\mathbb{K}$$

, and then squared QUARTIC is

$$0 = (\ell_0 - \ell_1)^2(\ell_0 + \ell_1)^2 BOAT^2.$$

We can study the θ case in our twice squared QUARTIC equation. This equation is very similar to our general twice squared QUARTIC which was found in section 2.5. In this situation, twice squared QUARTIC reduces to

$$\mathbb{A}(G)^2 = \mathbb{H}^2\mathbb{B}(G)^2.$$

This simplifies into

$$0 = (\mathbb{A}(G) - \mathbb{H}\mathbb{B}(G)) \cdot (\mathbb{A}(G) + \mathbb{H}\mathbb{B}(G)).$$

In our θ case, our equations for the twice square QUARTIC becomes

$$0 = (\ell_0 - \ell_1)^4(\ell_0 + \ell_1)^4 FACTOR \cdot CHAIR \cdot BOAT^2.$$

Therefore, in the θ case our $SIXDEGREE = (\ell_0 - \ell_1)^4(\ell_0 + \ell_1)^4 CHAIR \cdot BOAT^2$.

In the future, we can use this information to help us generalize our general hexagon with three-fold symmetry.

CONCLUSION

For any given values of $\ell_0, \ell_1, c_0, c_1, \sigma, \sigma'$ and ϕ_0, we can find all roots of G of the twice squared QUARTIC. Two of these roots are solutions of the quadratic equation $FACTOR = 0$. If the restrictions hold, they yield symmetric hexagons. However, we can also find numerically all six roots of SIXDEGREE, and systematically check each one to see if the restrictions hold. In this way, we find all shapes of the three-fold symmetric hexagon except those where either $\{\mathbf{R}_{A_0}, \mathbf{R}_{A_1''}, \mathbf{R}_{A_0'}\}$ or $\{\mathbf{R}_{A_1}, \mathbf{R}_{A_0'}, \mathbf{R}_{A_1''}\}$ are collinear (i.e. $K = 0$ or $K' = 0$).

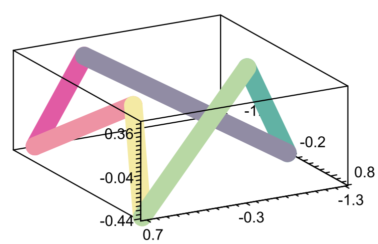

FIGURE 16. A General Unknotted Symmetric Hexagon

For example, we can take $\ell_0 = 1, \ell_1 = 2, \theta_0 = \frac{\pi}{2}, \theta_1 = \frac{\pi}{4}$. First we must find what restriction occur on our G. Since $c_1 - c_0 + \sqrt{3}(s_1 - s_0) = -1.214412$ and $c_1 - c_0 - \sqrt{3}(s_1 - s_0) = -.19980084$, we find that our G must satisfy

$$-.2865660925 \leq G \leq 0.6294095228.$$

For $K' > 0$, $G \neq 0.7368128792$. For $K > 0$, $G \neq 0.7644805979$.

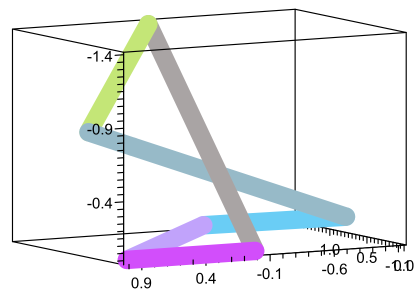

FIGURE 17. A Boat-Shaped Hexagon with $G = .50872361$

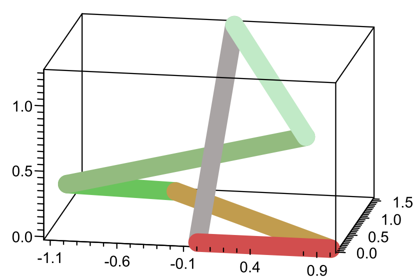

FIGURE 18. A Negative Boat-Shaped Hexagon with $G = .50872361$

Our twice squared QUARTIC has the factor of FACTOR that yields:

$$(G - .71229494)(G - .2055982705).$$

We can notice when $G = .71229494$ the restrictions do not hold, therefore we only have one solution from FACTOR, when $G = .2055982705$. We first must check if a, b, ε, and δ are real for this value of G. Therefore, we plug in this G into Maple worksheet abed.mw in lines 10-14 to find $a = .5678098193, b = .4430212407, \varepsilon = .6336005322$, and $\delta = 1.159421699$. Since these values are real and positive, this solution produces an unknotted hexagon rotated around an axis of symmetry as seen in our figure 16. We know from the construction of symmetric hexagons that the values of σ and σ' must be the same. Therefore, we only

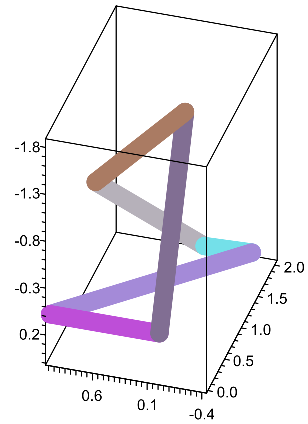

FIGURE 19. A Chair-Shaped Hexagon with $G = .27213284$

need to plug our given values into the QUARTIC to find the values of σ and σ'. When we plug in those values, we find that our $\sigma = \sigma' = 1$ for our unknotted symmetric hexagons.

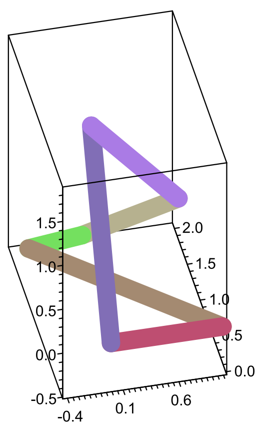

FIGURE 20. A Negative Chair-Shaped Hexagon with $G = .27213284$

If we let $\ell_0, \ell_1, \theta_0, \theta_1$ be the same values as before in SIXDEGREE from twice squared QUARTIC, we recieve the other solutions, which are:

$$0 = -.000011(G + 6.6644690)(G + .72381880)(G - .27213284)$$
$$(G - .50872361)(G - .55106963)(G - .77428261).$$

Since $G = -6.6644690, -.72381880, .77428261$ do not satisfy our restrictions, we must only study our other three values to find out which families they produce. When $G =$

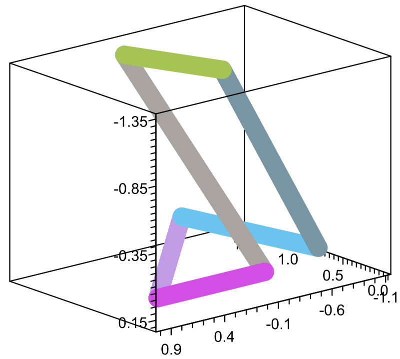

FIGURE 21. A Boat-Shaped Hexagon with $G = 0.5510696$

$0.5510696, 0.50872361$, squared QUARTIC is solved when $\tau = -1$. By plugging in these values into QUARTIC, we find that when $G = 0.50872361, .5510696358$, $\sigma = 1$ and $\sigma' = -1$. When $G = .27213284$, squared QUARTIC is solved when $\tau = 1$. When we plug this value into QUARTIC, we find that when $G = .27213284$, $\sigma = -1$ and $\sigma' = -1$. These solutions are summerized in the following table and figures :

G	σ	σ'	ϕ_0	ϕ_1	ϕ_1''	*Figure*
.2055982705	1	1	1.275775411	2.851722140	.2907598626	16
.2055982705	-1	-1	-1.275775411	-2.851722140	$-.2907598626$	16
.27213284	-1	-1	1.175746744	.305802540	-2.647968569	19
.27213284	1	1	-1.175746744	$-.305802540$	2.647968569	20
0.50872361	1	-1	0.7677951047	$-.330852634$	0.089803675	17
0.50872361	-1	1	-0.7677951047	.330852634	-0.08980367520	18
0.5510696	1	-1	0.6772002174	$-.581026714$	0.207126169	21
0.5510696	-1	1	-0.6772002174	.581026714	-0.207126169	22

Therefore, we have found all the solutions.

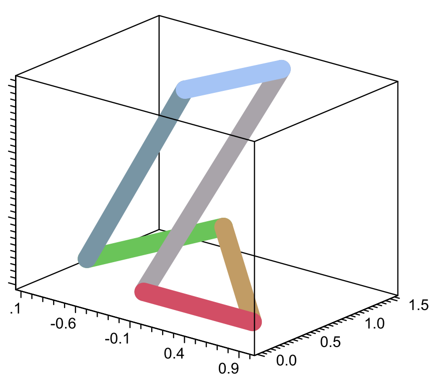

FIGURE 22. A Negative Boat-Shaped Hexagon with $G = 0.5510696$

We hope in the future we can get an explicit factorization of the six degree polynomial SIXDEGREE from the twice squared QUARTIC equation to get a more general understanding of our general three-fold symmetric hexagon. Perhaps we can use the property that whenever ϕ_0 solves twice squared QUARTIC so does ϕ_0' and ϕ_0''. Therefore, this thesis is concluded with a question. Can our six degree polynomial be solved, and what kinds of families of three-fold symmetric hexagons can those solutions produce?

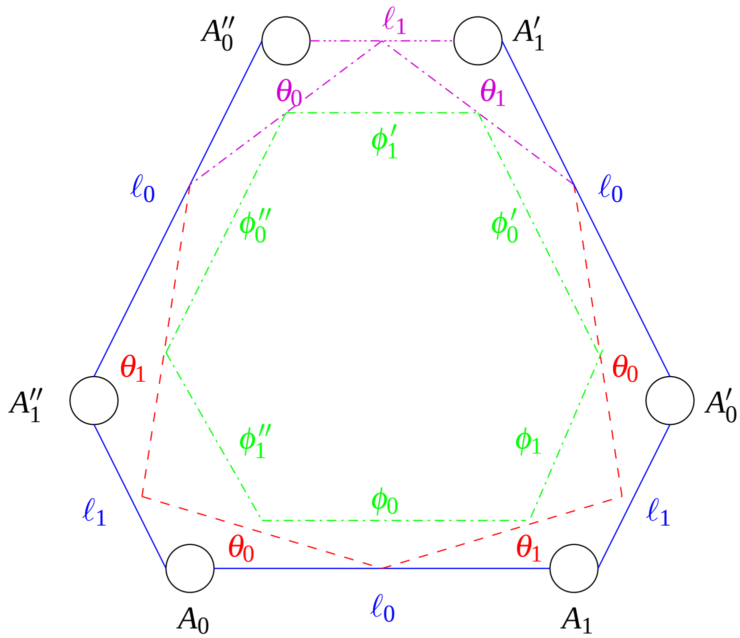

FIGURE 23. Labeled Hexagon with ϕ_0', ϕ_1',and ϕ_0''

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APPENDIX A

QUARTIC

$$
\begin{aligned}
0 =& C_1G^4+C_2G^3+C_3G^2+C_4G+C_5+\sigma\sigma'\sqrt{H}\sqrt{H'}(C_6G^2+C_7G+C_8)\\
&+\sin\phi s_1s_0\ell_0(\sigma\sqrt{H'}(C_9G^2+C_{10}G+C_{11})+\sigma'\sqrt{H}(C_{12}G^2+C_{13}G+C_{14}))
\end{aligned}
$$

$$C_1=-2\ell_1^4(3\ell_0^2-2\ell_1\ell_0c_1-2\ell_1\ell_0c_0+\ell_1^2)$$

$$
\begin{aligned}
C_2 =& \ell_1^2(\ell_0^4+(-16c_1-16c_0)\ell_1\ell_0^3+(10+40c_1c_0+12c_1^2+12c_0^2)\ell_1^2\ell_0^2\\
&+(-12c_0-16c_1c_0^2-12c_1-16c_1^2c_0)\ell_1^3\ell_0+(5+8c_1c_0)\ell_1^4)
\end{aligned}
$$

$$
\begin{aligned}
C_3 =& -\ell_1((-3c_1-3c_0)\ell_0^5+(16c_1^2-4+16c_0^2+35c_1c_0)\ell_1\ell_0^4\\
&+(-10c_1-12c_0^3-12c_1^3-68c_1^2c_0-68c_1c_0^2-10c_0)\ell_1^2\ell_0^3\\
&+(36c_1^3c_0+16c_0^2+36c_0^3c_1+34c_1c_0+84c_0^2c_1^2+16c_1^2)\ell_1^3\ell_0^2\\
&+(-3c_0-24c_1^3c_0^2-24c_1^2c_0^3-3c_1-36c_1^2c_0-36c_1c_0^2)\ell_1^4\ell_0+(12c_0^2c_1^2+15c_1c_0)\ell_1^5)
\end{aligned}
$$

$$
\begin{aligned}
C_4 =& (2c_0^2+2c_1^2+5c_0c_1)\ell_0^6+(-6c_1^3+3c_0-6c_0^3-24c_1^2c_0+3c_1-24c_1c_0^2)\ell_1\ell_0^5\\
&+(-1-2c_0c_1-4c_0^2+4c_1^4+36c_1c_0^3+75c_1^2c_0^2+4c_0^4-4c_1^2+36c_1^3c_0)\ell_1^2\ell_0^4\\
&+(-88c_1^2c_0^3-2c_1^3+8c_1+8c_0-2c_0^3-24c_0^4c_1-2c_1^2c_0-88c_1^3c_0^2-2c_1c_0^2\\
&-24c_1^4c_0)\ell_1^3\ell_0^3+(-6c_1^2-6c_0^2+38c_1^2c_0^2+32c_1c_0^3-6+36c_1^2c_0^4+32c_1^3c_0
\end{aligned}
$$

$$-39c_0c_1+72c_0^3c_1^3+36c_0^2c_1^4)\ell_1^4\ell_0^2+(-16c_1^4c_0^3+13c_1-6c_1^2c_0-36c_1^2c_0^3$$

$$-16c_1^3c_0^4-6c_1c_0^2-36c_1^3c_0^2+13c_0)\ell_1^5\ell_0+(-5+8c_0^3c_1^3+15c_1^2c_0^2)\ell_1^6$$

$$C_5=(-3-3c_1^2c_0^2+3c_0^2+3c_1^2)\ell_0^6+(13c_1^2c_0^3+13c_1^3c_0^2+6c_0-8c_0^3-13c_1^2c_0$$

$$-13c_1c_0^2+2c_1^4c_0+2c_0^4c_1+6c_1-8c_1^3)\ell_1\ell_0^5+(-4-4c_1^5c_0-20c_0^2c_1^4$$

$$+6c_0^2+4c_1^4+26c_1c_0^3-3c_0c_1-20c_1^2c_0^4+4c_0^4+24c_1^2c_0^2+6c_1^2-41c_0^3c_1^3$$

$$-4c_1c_0^5+26c_1^3c_0)\ell_1^2\ell_0^4+(-8c_1^3c_0^2+36c_1^4c_0^3+2c_0^4c_1-34c_1c_0^2$$

$$+2c_1^4c_0-8c_1^2c_0^3+12c_1^5c_0^2-8c_1^3+12c_1^2c_0^5-8c_0^3-34c_1^2c_0+36c_1^3c_0^4)\ell_1^3\ell_0^3$$

$$+(7c_0^2+6c_1c_0^3-22c_1^4c_0^4-12c_1^5c_0^3-16c_1^2c_0^4+7c_1^2+26c_0c_1+1-12c_1^3c_0^5$$

$$+39c_1^2c_0^2+6c_1^3c_0-16c_0^2c_1^4-14c_0^3c_1^3)\ell_1^4\ell_0^2+(12c_1^3c_0^4-13c_1^2c_0$$

$$+12c_1^4c_0^3-6c_1-6c_0-13c_1c_0^2+3c_1^3c_0^2+3c_1^2c_0^3+4c_1^4c_0^5+4c_1^5c_0^4)\ell_1^5\ell_0$$

$$+(2-5c_0^3c_1^3+5c_0c_1-2c_1^4c_0^4)\ell_1^6$$

$$C_6=\ell_1^2$$

$$C_7=-\ell_0^2+(c_0+c_1)\ell_1\ell_0-2c_0\ell_1^2c_1$$

$$C_8=\ell_1(-1+c_0c_1)((-c_1-c_0)\ell_0+(c_0c_1+1)\ell_1)$$

$$C_9=2\ell_1^3$$

$$C_{10}=\ell_1(-\ell_0^2+(4c_1+4c_0)\ell_1\ell_0+(-3-4c_0c_1)\ell_1^2)$$

$$C_{11} = (-2c_0 - c_1)\ell_0^3 + (2c_1^2 + 1 + 4c_0^2 + 5c_0c_1)\ell_1\ell_0^2$$
$$+ (-4c_1^2c_0 - 4c_1c_0^2 - 3c_1 - 4c_0)\ell_1^2\ell_0 + (1 + 3c_0c_1 + 2c_0^2c_1^2)\ell_1^3$$

$$C_{12} = 2\ell_1^3$$

$$C_{13} = \ell_1(-\ell_0^2 + (4c_0 + 4c_1)\ell_1\ell_0 + (-3 - 4c_1c_0)\ell_1^2)$$

$$C_{14} = (-2c_1 - c_0)\ell_0^3 + (2c_0^2 + 1 + 4c_1^2 + 5c_1c_0)\ell_1\ell_0^2$$
$$+ (-4c_0^2c_1 - 4c_0c_1^2 - 3c_0 - 4c_1)\ell_1^2\ell_0 + (1 + 3c_1c_0 + 2c_1^2c_0^2)\ell_1^3$$

Appendix B

To investigate our three-fold symmetric hexagon, we can create polygons within Maple to view the family of three fold symmetric hexagons. Using the Z-System formation of our hexagon, we can define each of the six vertices of our figure in space. In this program, you must give a specific value of the length of the bonds ℓ_0 and ℓ_1, angles θ_0 and θ_1, as well as the signs of the σ and σ' values. This program will create the hexagon in a three dimensional graph with the values of ϕ_0. We calculated the values of ϕ_1'' and ϕ_1 to be

$$\phi_1'' = -\arg(s_0\ell_0 + \ell_1(-s_0c_1 - c_0\cos\phi_0 s_1 - i\sin\phi_0 s_1)) - \sigma\alpha$$

$$\phi_1 = -\arg(s_1\ell_0 + \ell_1(-s_1c_0 - c_1\cos\phi_0 s_0 - i\sin\phi_0 s_0)) - \sigma'\alpha'$$

In this program, we defined the six atoms from their poses by starting with $\mathbf{R}_{A_0} = E_{r_0} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix}^T = \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}^T$ where $E_{r_0} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$, and we can use transformation matricies to find the other five poses. We can obtain these poses from the permutation:

$$\begin{array}{rlllllll}
r_0 = & (A_0, & & A_1, & & A_0') & & \\
 & & \times & & & & & T_1(\ell_0) \\
r_1 = & (A_1, & & A_0, & & A_0') & & \\
 & & & & \times & & & T_2(\theta_1) \\
 & (A_1, & & A_0', & & A_0) & & \\
 & & \times & & & & & T_1(\ell_1) \\
r_0' = & (A_0', & & A_1, & & A_0) & & \\
 & & & & & \downarrow & & T_3(-\phi_1) \\
 & (A_0', & & A_1, & & A_1') & & \\
 & & & & \times & & & T_2(\theta_0) \\
 & (A_0', & & A_1', & & A_1) & & \\
 & & \times & & & & & T_1(\ell_0) \\
r_1' = & (A_1', & & A_0', & & A_1) & &
\end{array}$$

To the right of each site transition, we have indicated the corresponding transformation matrices. Therefore, to transform vertex r_0 to r_1,r'_0,r'_1, we found to be:

$$\mathbf{R}_{A_1} = E_{r_0} \cdot T_1(\ell_0) \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix}^T$$

$$\mathbf{R}_{A'_0} = E_{r_0} \cdot T_1(\ell_0) \cdot T_2(\theta_1) \cdot T_1(\ell_1) \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix}^T$$

$$\mathbf{R}_{A'_1} = E_{r_0} \cdot T_1(\ell_0) \cdot T_2(\theta_1) \cdot T_1(\ell_1) \cdot T_3(-\phi_1) \cdot T_2(\theta_0) \cdot T_1(\ell_0) \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix}^T$$

We must find the other two poses by the transition:

$$\begin{array}{rlllll}
r_0 = & (A_0, & A_1, & A'_0) & & \\
 & & & \downarrow & T_3(-\phi_0) & \\
 & (A_0, & A_1, & A''_1) & & \\
 & & \times & & T_2(\theta_0) & \\
 & (A_0, & A''_1, & A_1) & & \\
 & & & \downarrow & T_3(\phi''_1) & \\
 & (A_0, & A''_1, & A''_0) & & \\
 & \times & & & T_1(\ell_1) & \\
r''_1 = & (A''_1, & A_0, & A''_0) & & \\
 & & \times & & T_2(\theta_1) & \\
 & (A''_1, & A''_0, & A_0) & & \\
 & \times & & & T_1(\ell_0) & \\
r''_0 = & (A''_0, & A''_1, & A_0) & &
\end{array}$$

Therefore, to transform vertex r_0 to r''_1 and r''_0, we found to be:

$$\mathbf{R}_{A''_1} = E_{r_0} \cdot T_3(-\phi_0) \cdot T_2(\theta_0) \cdot T_3(\phi''_1) \cdot T_1(\ell_1) \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix}^T$$

$$\mathbf{R}_{A''_0} = E_{r_0} \cdot T_3(-\phi_0) \cdot T_2(\theta_0) \cdot T_3(\phi''_1) \cdot T_1(\ell_1) \cdot T_2(\theta_1) \cdot T_1(\ell_0) \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix}^T$$

Using these transformation matrices explained in section 1.3, we are able to find the coordinates of all six atoms, and we can create a three dimensional polygon by ploting those atoms using the Maple command polygonplot3d.