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ORIGINAL PAPER

Three-dimensional chiral objects and their star graph representations

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Abstract Planar chirality properties can be analysed using n-polyominoes and graphs. In this paper we study graph representations of three-dimensional chiral objects and discuss the generalization of planar case. We show that graph representations of three-dimensional chiral objects can be star graphs.

Keywords Chirality · 3D Jordan property · Graph representations

1 Introduction

Chirality in the ordinary, three-dimensional space plays a key role in many fields of the natural sciences, especially in biology, chemistry, pharmacology and medical cosmetology. In chemistry, *chirality* is a property of molecules having a non superimposable mirror image.

In mathematics, *chirality* of an object S in the three-dimensional space $\mathbb{R}^3$ means, that it cannot produce a perfect overlap with its mirror image $S^\diamond$ within $\mathbb{R}^3$. Otherwise S is said to be *achiral* in $\mathbb{R}^3$.

The simplest approach of chirality is to say that a 3D object (or a molecule) is either chiral or achiral. One can think that there is no other possibility. On the other hand a few scientists recognized that it is possible to measure the degree of chirality. For example Frank Harary, R.W. Robinson, P.G. Mezey, A.I. Kitaigorodski, K. Mislow,

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J. Siegel, G. Gilat, D. Avnir and A.Y. Meyer (see [3,10,4,9,12,14,13,11,15,7,5]) have important contributions in this field.

Following the idea introduced and developed by the above listed authors and generalizing the 2-dimensional case discussed in our paper [2] and Mezey's result (see [14]) we consider here the 3-dimensional case. We are going to show that there always exist special star-graph representations for 3D chiral objects.

2 Basic notions

Many two-dimensional chirality problems can be studied by so called lattice animals (see e.g. [2], [12], [14] and [13]). Now, we are going to use the same idea in the 3-dimensional space.

Let us consider in the three-dimensional space a Cartesian grid of the first octant of size $n \times n \times n$ consisting of $(n-1)^3$ small unit cube cells. This means that we took the nth regular subdivision of the interval $[0,n]$ of each coordinate axis: $[0,1], [1,2], \dots, [n-1,n]$. Every cell in the grid can be labeled by an ordered triplet (i, j, k) where the "coordinates" indicate the positions of orthogonal projections of the cell onto the coordinate axis. For example $(2, 3, 1)$ means that the orthogonal projection of the unit cube cell onto x-axis is the second subinterval $[1,2]$ of x-axis, the orthogonal projection onto y-axis is the third subinterval $[2,3]$ of y-axis and the orthogonal projection onto z-axis is the first subinterval $[0,1]$.

Definition 2.1 Two faces (belonging to the same cube or to different cubes) are called *adjacent* if they have exactly one common edge.

Definition 2.2 Two cells (unit solid cubes) are called *adjacent* if they have exactly one common face.

Definition 2.3 Let us denote by $\mathcal{A}$ a connected set resulted by the union of an arbitrary number of adjacent solid cells. The *boundary* of $\mathcal{A}$ is defined as the union all faces which belong to exactly one cell of $\mathcal{A}$.

Definition 2.4 A union of (finite number of) adjacent cells is called three-dimensional *solid animal* if it is connected and it does not contain "hole".

In this paper we deal with solid animals only. It means that they consist of all faces and all interior points of the cubic cells as ordinary point sets in the 3D space. Thus we'll omit the attribute "solid" further on. The boundaries of these animals are non-self-intersecting continuous simple closed surfaces in the 3D space. They divide the space into an "interior" region and an "exterior" region. This property is often called 3D *Jordan property*.

Definition 2.5 The *interior* of $\mathcal{A}$ is defined as the interior region determined by the boundary B of $\mathcal{A}$.

3 New results

Let us consider an arbitrary 3D animal $\mathcal{A}$ with boundary B and its mirror image $\mathcal{A}^{\diamondsuit}$ with boundary $B^{\diamondsuit}$. Assume that $\mathcal{A}$ and $\mathcal{A}^{\diamondsuit}$ are positioned in the three-dimensional space so that the intersection of their interior $Int(\mathcal{A}) \cap Int(\mathcal{A}^{\diamondsuit})$ has maximum possible volume, i.e.

$$\text{Volume}\left[Int(\mathcal{A}) \cap Int(\mathcal{A}^{\diamondsuit})\right] = \text{maximum}.$$

We denote the union of B and $B^{\diamondsuit}$ satisfying condition of maximum intersection by $B \oplus B^{\diamondsuit}$. Note that $B \oplus B^{\diamondsuit}$ contains only the faces of the boundaries B and $B^{\diamondsuit}$. Grid faces of $B \cap B^{\diamondsuit}$ are considered *double faces* and in the figures of the paper they are denoted by bold lines. Object $B \oplus B^{\diamondsuit}$ partitions $\mathbb{R}^3 \setminus \left(B \oplus B^{\diamondsuit}\right)$ into $k+1$ disjoint subsets, namely $S_0, S_1, \ldots, S_k$ where S_0 is the unbounded exterior part of the space lying outside of both 3D Jordan-property surfaces B and $B^{\diamondsuit}$. Let us keep the notations of [14] and [2], considering $S_1 = Int(\mathcal{A}) \cap Int(\mathcal{A}^{\diamondsuit})$ and for $i = 2, 3, \ldots, k$ let S_i be the maximum connected subset of the partition which belongs to the interior of precisely one of $\mathcal{A}$ or $\mathcal{A}^{\diamondsuit}$ having no common points with any of $S_0, S_1, \ldots, S_{i-1}$. Observe that S_1 may be the union of more disjoint components, but $S_2, S_3, \ldots, S_k$ are all connected components.

If $B \oplus B^{\diamondsuit}$ is not unique, one with the smallest k must be chosen ("minimum k condition").

Now we are going to associate to the partition $S_1, \ldots, S_k$ a graph $\mathcal{G}$ with node set $V(\mathcal{G}) = \{1, \ldots, k\}$. Each node i of the graph $\mathcal{G}$ corresponds to a subset S_i, $i = 1, \ldots, k$. Adjacency of nodes in $\mathcal{G}$ will be defined as follows.

Definition 3.1 Nodes i and j are adjacent in the graph $\mathcal{G}$ if the corresponding subsets S_i and S_j of the partition are separated by a set of connected adjacent simple faces, i.e. double grid faces from $B \oplus B^{\diamondsuit}$ are excluded. Such a separating (hole-free) union of adjacent simple grid faces is called *wall* further on.

As an example for the above mentioned notions let us consider a special $3D$ chiral animal $\mathcal{A}$ and its mirror image $\mathcal{A}^{\diamondsuit}$ with boundaries B respectively $B^{\diamondsuit}$ (Fig. 1). (Here the dotted line represents the mirror-plane.)

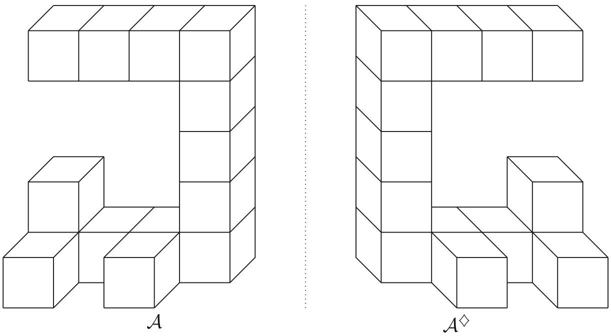

Fig. 1 $\mathcal{A}$ and its mirror image $\mathcal{A}^{\diamondsuit}$

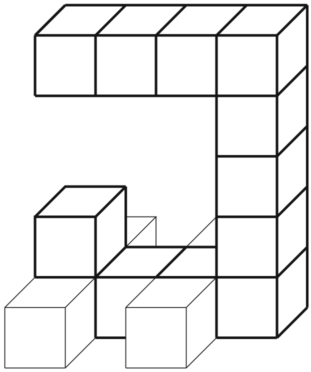

Fig. 2 $B \oplus B^{\diamond}$ of our example

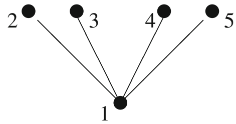

Fig. 3 The graph associated to $\mathcal{A}$ in our example

Considering condition of maximum intersection we obtain $B \oplus B^{\diamond}$ as shown in Fig. 2.

We can associate a graph to $\mathcal{A}$ as shown in Fig. 3.

3.1 Minimum k condition

We are going to illustrate the importance of "minimum k condition" by the following example. Consider now the animal $\mathcal{C}$ shown in Fig. 4.

This chiral object $\mathcal{C}$ from Fig. 4 consists of 13 unit cubes. One can reach the maximum intersection with its mirror image in two different ways. There are 9 common cubes in both cases. Figure 5 shows one possibility. In this case $k = 3$.

The graph associated to the object considered in Case 1) is shown in Fig. 6

Another possibility to get the maximum intersection has shown in Fig. 7.

Notice that Case 2) from Fig. 7 cannot be considered because of the minimum k condition.

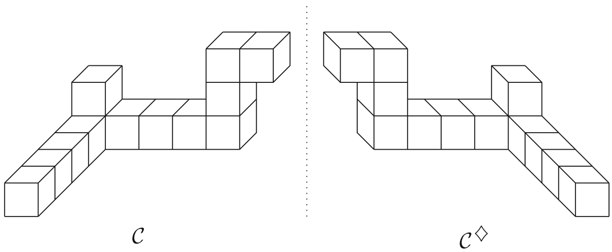

Fig. 4 A chiral object $\mathcal{C}$ and its mirror image $\mathcal{C}^{\diamond}$

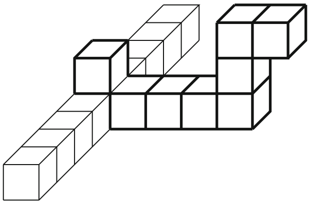

Fig. 5 Case 1) Maximum intersection of $\mathcal{C}$ and $\mathcal{C}^{\diamond}$ when $k = 3$

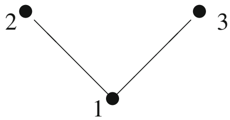

Fig. 6 Case 1) graph representation of $\mathcal{C}$

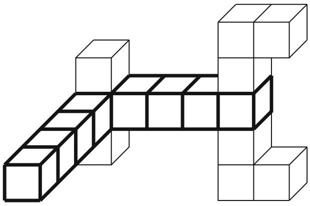

Fig. 7 Case 2) maximum intersection of $\mathcal{C}$ and $\mathcal{C}^{\diamond}$ when $k = 5$

3.2 New theorems

Let us consider now an arbitrary animal $\mathcal{A}$ in the 3 dimensional space with boundary B and its mirror image $\mathcal{A}^{\diamond}$ with boundary $B^{\diamond}$.

Imagine we color the grid faces of B by red color and those of $B^{\diamond}$ by blue. All other faces of the grid are considered uncolored.

Lemma 3.1 *Neither $\mathcal{A}$ nor $\mathcal{A}^{\diamond}$ crosses any S_i, for $i = 1, 2, \ldots, k$.*

Proof Neither $\mathcal{A}$ nor $\mathcal{A}^{\diamond}$ crosses S_1, because $S_1 = Int(\mathcal{A}) \cap Int(\mathcal{A}^{\diamond})$, so lemma 3.1 holds for $i = 1$. In case of $i \in \{2, 3, \ldots, k\}$ suppose indirectly, that $\mathcal{A}$ or $\mathcal{A}^{\diamond}$ crosses S_i. By definition S_i belongs to the interior of precisely one of $\mathcal{A}$ or $\mathcal{A}^{\diamond}$. If the other one crosses S_i that contradicts to the condition Volume $\left[Int(\mathcal{A}) \cap Int(\mathcal{A}^{\diamond})\right] =$ maximum. □

Lemma 3.1 implies that $Int(S_i)$ can contain only "uncolored" grid faces for $i = 1, 2, \ldots, k$. Boundaries B and $B^{\diamond}$ are surfaces with 3D Jordan properties, so Lemma 3.1 also implies that two adjacent partition sets S_i and S_j can be separated only by a monochromatic wall.

Theorem 3.1 *If S_i and S_j are adjacent, then either $i = 1$ or $j = 1$.*

Proof Suppose indirectly that there exist i and j, $(i, j \in \{2, 3, \ldots, k\})$ such that S_i and S_j are adjacent partition sets. One of them belongs to $Int(\mathcal{A}) \backslash Int(\mathcal{A}^{\diamond})$ and the other to $Int(\mathcal{A}^{\diamond}) \backslash Int(\mathcal{A})$. (Otherwise $i = j$ would be, or we have a monochromatic wall in $Int(\mathcal{A}) \backslash Int(\mathcal{A}^{\diamond})$ or $Int(\mathcal{A}^{\diamond}) \backslash Int(\mathcal{A})$ that is a contradiction with the condition of maximum intersection.) This contradicts the fact that the wall separating adjacent S_i and S_j cannot contain double grid faces. □

Theorem 3.2 *For each $i \in \{2, \ldots, k\}$ S_i and S_1 are adjacent partition sets.*

Proof Suppose indirectly that there exists an $i \in \{2, \ldots, k\}$ such that S_1 and S_i are not adjacent sets. Theorem 3.1 implies that there is no adjacent partition set for S_i.

B and $B^{\diamond}$ have 3D Jordan-property, thus Lemma 3.1 implies that a wall of double faces separates S_i from the other partition sets situated in its neighborhood, that is a superposition of B with its mirror image $B^{\diamond}$, so we obtain a contradiction with the fact that B is chiral. □

We can summarize our results for the graph representation of B in the following theorem:

Theorem 3.3 *The graph representation of a chiral surface with 3D Jordan-property is a star graph, i.e. it contains a node that is adjacent to all other nodes and there are no other adjacent nodes in the graph.*

4 Conclusion

Several "measures" of chirality have been proposed earlier. For example Frank Harary and Paul Mezey wrote remarkable papers in this field (see [4], [12] and [14]). Here we must mention Harary and Robinson's pioneer work (see [9]) and significant contributions of A.I. Kitaigorodski, K. Mislow, J. Siegel, G. Gilat, D. Avnir and A.Y. Meyer (see [11,15,7,5,6,1,8]).

In our earlier work [2] we proved that a chiral object in the 2 dimensional space can be represented with a star graph. The number of nodes of the graph measures the degree of chirality of an object. In this paper we show that the idea can be extended to the 3-dimensional objects, i.e. a 3-dimensional chiral object can be represented by a star graph which also provides solution for the quantification problem of chirality in $\mathbb{R}^3$.

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