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# Graph Representations of Three-dimensional Chiral Objects

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***Abstract*—Chirality of objects is a problem with important applications in biology, pharmacology, medical cosmetology, organic chemistry, inorganic chemistry, supramolecular chemistry, biochemistry, and other branches of science.**

**In this paper we provide a solution for quantification problem of chirality for three-dimensional objects.**

***Index Terms*—Chirality, graph representations, 3D Jordan property .**

## I. Introduction

CHIRALITY in chemistry is a property of molecules having a non-superimposable mirror image. The concept of chirality was introduced by Louis Pasteur who first separated left-handed and right-handed tartaric acid crystals in 1849.

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

For example, a right glove is different from a left glove, the left hand is a non-superimposable mirror image of the right hand. The Greek word "kheir" means "hand." So chirality indeed means "handedness".

A chiral object $S$ and its mirror image $S^\diamondsuit$ are said to be *enantiomorphs* (i.e. "opposite forms" in Greek language) or *enantiomers* when referring to molecules.

Usually chemical and physical properties of enantiomers are the same, but interestingly their biological properties can be completely different. A well known tragic event was the Thalidomide disaster in the late 1950-es and early 60-es :

"Thalidomide is a sedative drug that was prescribed to pregnant women. It was present in at least 46 countries under different brand names. When taken during the first trimester of pregnancy, Thalidomide prevented the proper growth of the foetus, resulting in horrific birth defects in thousands of children around the world. Why? The Thalidomide molecule is chiral. There are left and right-handed Thalidomides. The drug that was marketed was a 50/50 mixture. One of the molecules, say the left one, was a sedative, whereas the right one was found later to cause foetal abnormalities." (see [3])

This event shows why chirality plays a key role in pharmacology and chemistry.

Considering the study of the relative spatial arrangement of atoms forming a molecule, the simplest approach is to say that the above mentioned molecule is chiral or achiral. One can think that there is no other case. On the other hand a few scientists recognized that it is possible to measure the degree of chirality. Several "measures" of chirality have been proposed earlier. For example Frank Harary and Paul Mezey wrote remarkable papers in this field (see [4], [6] and [7]). Here we must mention Harary and Robinson's pioneer work (see [5]) and significant contributions of A.I. Kitaigorodski, K. Mislow, J. Siegel, G. Gilat,

D. Avnir, R.S. Cahn, C.K. Ingold, A.Y. Meyer and V. Prelog (see [8-14]) .

We are going to generalize the graph construction introduced in [7] and our result from [1] about graph representations of two-dimensional chiral objects giving a theoretical tool for quantification problem of chirality of three-dimensional objects.

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## II. Main definitions

Two-dimensional chirality problems can be studied by so called lattice animals (see e.g. [1], [6], [7] and [8]). Generalizing this idea for 3D problems we consider in the three-dimensional space $R^3$ a Cartesian grid of the first octant of size $n \times n \times n$ consisting of $(n-1)^3$ small unit cube cells.

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

*Definition 2.2:* Two cells (solid unit cubes) are *adjacent* if they have a common face.

*Definition 2.3:* A union of (finite number of) adjacent cells (considered with their interior) is called three-dimensional *solid animal* if it does not contain "hole".

Note that the boundary of any 3D solid animal is a non-self-intersecting continuous simple closed surface that divides the space into an "interior" region and an "exterior" region. This property is often called 3D *Jordan property*.

## III. Graph representation of 3D solid animals

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

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

We denote the union of $B$ and $B^\diamondsuit$ satisfying condition of maximum intersection by $B \oplus B^\diamondsuit$. This object $B \oplus B^\diamondsuit$ partitions $R^3 \setminus \left(B \oplus B^\diamondsuit\right)$ into $k+1$ disjoint subsets, namely $P_0, P_1, \ldots, P_k$ where $P_0$ is the unbounded exterior part of the space lying outside of both 3D Jordan-property surfaces $B$ and $B^\diamondsuit$.

Let us generalize the result of [1] and [7], considering $P_1 = Int(B) \cap Int(B^\diamondsuit)$ and for $i = 2, 3, \ldots, k$ let $P_i$

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be the maximum connected subset of the partition which belongs to the interior of precisely one of $B$ or $B^{\diamondsuit}$ having no common points with any of $P_0$, $S_1$, ..., $P_{i-1}$. Observe that $P_1$ may be the union of more disjoint components, but $P_2$, $P_3$, ..., $P_k$ are all connected components.

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

Let us consider now $\mathcal{A}$ and its mirror image $\mathcal{A}^{\diamondsuit}$ from Figure 1 (here the dotted line represents the mirror-plane).

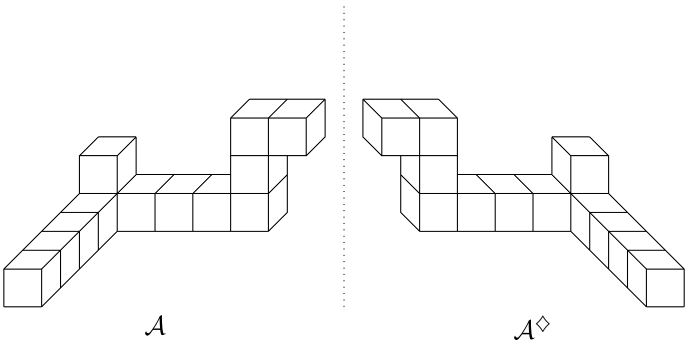


Fig. 1. A 3D solid animal $\mathcal{A}$ with 13 cells and its mirror image $\mathcal{A}^{\diamondsuit}$

Figures 2 and 3 show that minimum $k$ condition is essential. Here we consider two cases that satisfy condition of maximum intersection. Grid edges from $B \cap B^{\diamondsuit}$ are denoted by bold lines. Both figures show an intersection of 9 cells, but only case a) satisfies the minimum $k$ condition, having $k = 3$.

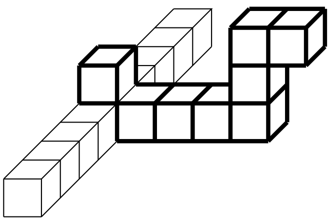

Fig. 2. Case a) Maximum intersection of $\mathcal{A}$ and $\mathcal{A}^{\diamondsuit}$ when $k = 3$.

Another possibility (case b) to get the maximum intersection has shown in Figure 3.

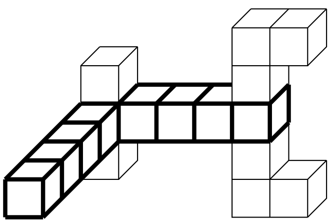

Fig. 3. Case b) Maximum intersection of $\mathcal{A}$ and $\mathcal{A}^{\diamondsuit}$ when $k = 5$.

Notice that case b) cannot be considered because minimum $k$ condition is not satisfied.

Now we are ready to associate a graph for the partition $P_0$, $P_1, \ldots, P_k$. Let us consider the node set $\{1, 2, \ldots, k\}$. By definition nodes $i$ and $j$ are adjacent if the corresponding subsets $P_i$ and $P_j$ of the partition are separated by a simple sequence of adjacent faces, i.e. the separating sequence of faces does not contain "double" grid faces from $B \oplus B^{\diamondsuit}$. This means that the graph representation of the 3D solid animal $\mathcal{A}$ from Figure 1 is the graph of Figure 4.

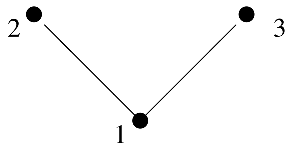


Fig. 4. Cherry graph representation of $\mathcal{A}$

Following the idea of [7], the number $k - 1$ when $k$ is the number of nodes of the associated graph is denoted by $gtk(\mathcal{A})$ and is defined as the *geometrical - topological chirality measure of* $\mathcal{A}$.

Evidently, for an achiral solid animal we have a perfect overlap between $\mathcal{A}$ and its mirror image $\mathcal{A}^{\diamondsuit}$, thus $k = 1$ and $gtk(\mathcal{A}) = 0$ (i.e. the graph representation is an isolated node).

We can summarize our generalized results for 3D chiral solid animals in the following theorem:

*Theorem 3.1:* For any arbitrary given three-dimensional solid animal $\mathcal{A}$ there exists a graph representation such that the number of nodes measures the chirality of $\mathcal{A}$.

## IV. Conclusion

In this paper we discussed and illustrated by examples graph representations of three-dimensional solid objects, giving a combined geometrical - topological chirality "measure" generalizing the results of two-dimensional case ([1] , [7]).

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