J Math Chem (2012) 50:1514–1520
DOI 10.1007/s10910-012-9986-9

ORIGINAL PAPER

Star graph representations of chiral objects in graph theory

Béla Barabás · Ottilia Fülöp

Received: 12 December 2011 / Accepted: 17 February 2012 / Published online: 15 March 2012

Abstract Planar chirality of objects is a problem with important applications in many fields of natural sciences, especially in chemistry and pharmacology. The analysis of chirality properties can be studied using n-polyominoes and planar graphs. In this paper we show that graph representations of chiral objects can be star-graphs.

Keywords Chirality · Jordan curve · Graph representations

1 Introduction

Chirality, as an expression was introduced by Louis Pasteur who discovered molecular chirality. The Greek word "kheir" means "hand." So chirality indeed means "handedness". Chirality is a property of asymmetry.

In chemistry, chirality is a property of molecules having a non-superimposable mirror image.

In mathematics, chirality of an object A means that it cannot produce a perfect overlap with its mirror image $A^{\diamond}$.

If a molecule can be made coincident with its mirror image by translations and rotations in the 3D space than it is called "*achiral*" in the specified space. Otherwise the molecule is called "*chiral*" in the 3D space. There are many stable organic molecules with existing and stable mirror image. These are called *enantiomers*. Usually their chemical and physical properties are the same, but interestingly their biological

B. Barabás (✉) · O. Fülöp
Institute of mathematics, Budapest University of Technology and Economics, Egry J. U. 1., 1111 Budapest, Hungary
e-mail: belab@math.bme.hu

O. Fülöp
e-mail: otti@math.bme.hu

properties can be completely different. A well known tragic event was the Thalidomide case 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 [1])

This event illustrates the main reason, why chirality plays a key role in chemistry and pharmacology. Considering the chemical chirality, the simplest approach is to say that a 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 [2,4] and [5]). Here we must mention Harary and Robinson's pioneer work (see [3]) and important contributions of Kitaigorodski, Mislow, Siegel, Gilat, Rassat, Avnir and Meyer (see [7–14]).

Following the idea introduced by the above mentioned authors, we consider the 2 dimensional case. Here we also refer to an early work of Cahn et al. [15]. The acceleration of research in nanotechnology has led to the focal point of interest in the one molecular layers of a surface, thus the importance of characterization of planar chirality increased. We are going to summarize briefly Mezey's results (see [5]) about graph representations of chiral objects.

We show that there always exist special star-graph representations for these objects.

2 Basic concepts and previous results

Definition 2.1 An object A embedded in an n-dimensional Euclidean space E^n is *chiral* if it cannot produce a perfect overlap with its mirror image $A^\diamond$ within E^n. Otherwise A is said to be *achiral* in the specified space.

Note, that chirality and achirality of objects are always dependent on n. An object A that is chiral if embedded in a given n-dimensional Euclidean space E^n is achiral if embedded in a higher dimensional Euclidean space. This implies that chirality of A may occur only in the lowest dimension space where the specified object is embeddable (see [6] and [5]).

Many two-dimensional chirality problems can be studied by so called *lattice animals*. We start with some graph theoretical concepts used in this paper.

Let us consider in the plane a square grid of size $n \times n$, consisting of $(n-1)^2$ small equal squares. Let $G = (V, E)$ be the graph with node set V formed by the n^2 grid points and the edge set E containing all sides of $(n-1)^2$ squares (i.e. all grid edges).

Definition 2.2 A *Jordan cycle* C of the graph G is a cycle that is a connected subgraph of G having only two-degree nodes.

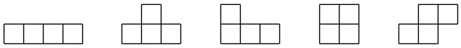


Fig. 1 Tetrominoes in $\mathbb{R}^2$

Definition 2.3 A subgraph A of G is called *animal* if it contains all the nodes and edges of that fall on a Jordan cycle C of G or within the interior of C.

Definition 2.4 A *cell* C of an animal A is a 4-cycle contained in A.

Note that the perimeter of an arbitrary animal A is a Jordan curve. Let us denote this curve by $J(A)$.

Definition 2.5 Animals with n cells are called *n-polyominoes* or *n-ominoes*.

For example, the 4-ominoes (tetrominoes) are the “straight”, “T”, “L”, square and skew tetrominoes (See Fig. 1).

Let us consider an arbitrary animal A. We will denote shortly the Jordan curve $J(A)$ by J and its mirror image by $J^{\diamond}$. Assume that they are positioned so that the intersection of their interior $Int(J)$ and $Int(J^{\diamond})$ has the maximum possible area, i.e. area $[Int(J) \cap Int(J^{\diamond})]$=maximum. We denote the union of J and $J^{\diamond}$, satisfying condition of maximum intersection by $J \oplus J^{\diamond}$.

This object $J \oplus J^{\diamond}$ partitions the plane into $k+1$ disjoint subsets, namely $S_0, S_1, \ldots S_k$, where S_0 is the unbounded exterior part of the plane lying on the outside of both Jordan curves J and $J^{\diamond}$. Let us consider $S_1 = Int(J) \cap Int(J^{\diamond})$ 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 J or $J^{\diamond}$ having no common points with any of $S_0, S_1, \ldots S_{i-1}$. (S_1 may be the union of more disjoint components, and $S_2, S_3, \ldots, S_k$ are connected components.) If $J \oplus J^{\diamond}$ is not unique, one with the smallest k is chosen. (“minimum k condition”)

In [5] it is shown that the condition of maximum intersection and minimum k condition for $J \oplus J^{\diamond}$ are essential.

The integer $k-1$ denoted by $gtk(J)$ in [5] is an important attribute of chirality of Jordan curve J. In the above mentioned paper the author defines the graph representation $g\left(J \oplus J^{\diamond}\right)$ of a Jordan curve as follows.

Definition 2.6 Let us consider a graph with node set $\{1, 2, \ldots, k\}$. By definition nodes i and j are adjacent if the corresponding subsets S_i and S_j of the partition are separated by a line segment (i.e. sequence of grid edges) of $J \oplus J^{\diamond}$ of positive length.

3 Our results

Definition 3.1 In this paper we consider nodes i and j *adjacent* if the corresponding subsets S_i and S_j of the partition introduced in Sect. 2 are separated by a *simple* line segment of $J \oplus J^{\diamond}$ of positive length (so ”parallel” grid edges from $J \cap J^{\diamond}$ are excluded). In this case partition sets S_i and S_j are also called *adjacent*.

As an example let us consider the chiral Jordan curve J and its mirror image $J^{\diamond}$ from Fig. 2.

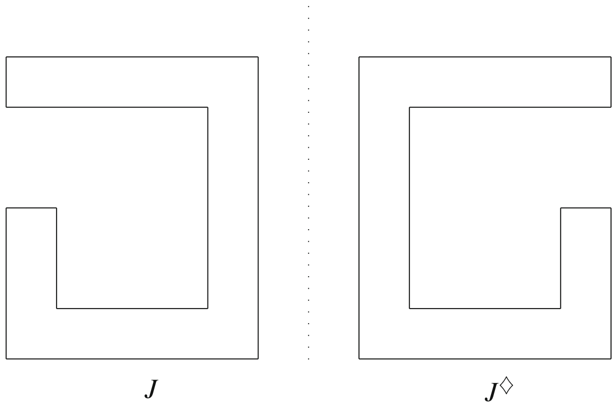


Fig. 2 J and its mirror image $J^{\diamondsuit}$

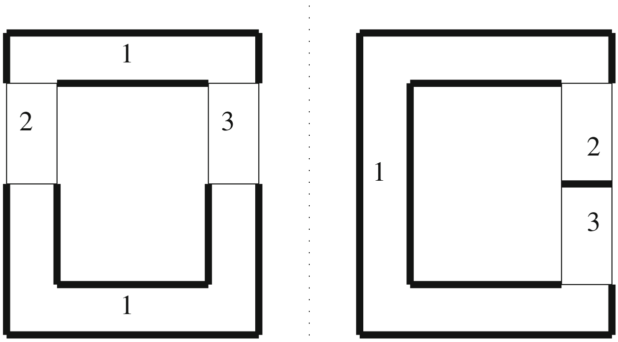
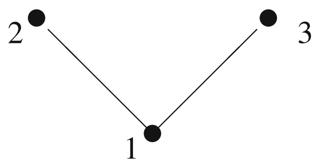


Fig. 3 On the right figure J is rotated by 180°, on *the left* one S_1 is not connected

Fig. 4 Graph representation of J from Fig. 2



Notice that in this paper we consider graph representation of a Jordan curve $J(A)$ based on adjacency from Definition 3.1. Assume that J and $J^{\diamondsuit}$ from Fig. 2 are positioned so that the intersection of their interiors $Int(J) \cap Int(J^{\diamondsuit})$ has the maximum possible area.

$J \oplus J^{\diamondsuit}$ in this case is not unique because both objects from Fig. 3 satisfy condition of maximum intersection and the minimum k condition.

The graph representation of J (defined using adjacency from Definition 3.1) denoted by $g\left(J \oplus J^{\diamondsuit}\right)$ following the notations of [5] in both cases is a "cherry graph" as shown in Fig. 4.

Nodes 2 and 3 are not adjacent for the second object of Fig. 3, because S_2 and S_3 are separated by a "parallel" line segment (grid edges from $J \cap J^{\diamondsuit}$ are denoted by bold lines).

Consider an arbitrary animal A in the plane, $J := J(A)$ the Jordan curve determined by the perimeter of A and its mirror image $J^{\diamondsuit}$. For simplicity, let us call the grid edges of Jordan curve J red ones and the edges from $J^{\diamondsuit}$ blue ones. The other edges of the square grid are considered uncolored.

Lemma 3.1 *Neither red nor blue grid edges exist in $Int(S_i)$ for all $i = 1, 2, \ldots, k$.*

Proof If $i = 1$, $S_1 = Int(J) \cap Int(J^{\diamondsuit})$. Observe that $Int(J)$ doesn't contain red edges and $Int(J^{\diamondsuit})$ doesn't contain blue grid edges because J and $J^{\diamondsuit}$ are Jordan curves. Thus S_1 can contain only uncolored grid edges.

Let us suppose indirectly that there exist $i \in \{2, \ldots, k\}$ such that $Int(S_i)$ contains a colored edges "e". If "e" is red then $S_i \subseteq Int(J^{\diamondsuit})$.

J is a Jordan curve that crosses S_i , thus $F := Int(J) \cap Int(S_i) \neq \emptyset$. We have $\emptyset \neq F \subseteq Int(J) \cap Int(J^{\diamondsuit})$, that is a contradiction with the condition of maximum intersection. If "e" is a blue edge (i.e. belongs to the Jordan curve $J^{\diamondsuit}$) we get similarly a contradiction with the condition of maximum intersection. □

Corollary 3.1 *Any line segment separating two adjacent partition sets contains only edges of the same color. (All of them are red or all of them are blue ones.)*

Proof $J \oplus J^{\diamondsuit}$ partitions the plane into sets $S_0, S_1, S_2, \ldots, S_k$ thus the simple line segment that separates two arbitrary adjacent partition sets S_i and S_j cannot contain uncolored grid edges. If we suppose indirectly that this line segment contains both red and blue grid edges (i.e. edges from both Jordan curves J and $J^{\diamondsuit}$) let us consider two different colored grid edges with a common endpoint. J and $J^{\diamondsuit}$ are Jordan curves, thus at least one of them crosses S_i or S_j, contradiction with Lemma 3.1. □

Corollary 3.2 *Any two adjacent partition sets S_i and S_j different from S_1 belong two the interior of different Jordan curves (one of them belongs to $Int(J) \setminus Int(J^{\diamondsuit})$ and the other to $Int(J^{\diamondsuit}) \setminus Int(J)$).*

Proof Suppose indirectly that there exist adjacent partition sets S_i and S_j different from S_1 that belong to $Int(J) \setminus Int(J^{\diamondsuit})$. (If they belong to $Int(J^{\diamondsuit}) \setminus Int(J)$ the proof is similar.) S_i and S_j are separated by a blue line segment (because J is a Jordan curve). Then $J^{\diamondsuit}$ crosses J such that either S_i or S_j belongs to $Int(J) \cap Int(J^{\diamondsuit})$, that is a contradiction with the condition of maximum intersection. □

Theorem 3.1 *If S_i and S_j $(i, j \in \{1, 2, \ldots, k\})$ are adjacent, then one of them is S_1.*

Proof This theorem says that two partition sets S_i and S_j $(i \neq j)$ different from S_1 cannot be adjacent.
Suppose indirectly that there exist $i \neq j$ $(i, j \in \{2, 3, \ldots, k\})$ such that S_i and S_j are adjacent. Assume that $S_i \in Int(J) \setminus Int(J^{\diamondsuit})$. Corollary 3.2 implies that $S_j \in Int(J^{\diamondsuit}) \setminus Int(J)$.

Corollary 3.1 guarantees that the line segment that separates S_i and S_j is monochromatic. Suppose it is blue. Let us consider an endpoint E of this blue separating line segment. J and $J^\diamond$ are Jordan curves thus all grid edges incident to E are colored (red or blue). Any coloration of them lead us to a contradiction with $S_i \in Int(J)$ or with the condition of maximum intersection. □

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. J and $J^\diamond$ are Jordan curves, thus Lemma 3.1 implies that parallel line segments separates S_i from the other partition sets situated in its neighborhood, that is a superposition of J with its mirror image $J^\diamond$, contradiction with the fact that J is chiral.

We can summarize our results for $g\left(J \oplus J^\diamond\right)$ in the following theorem:

Theorem 3.3 *The graph representation $g\left(J \oplus J^\diamond\right)$ of a chiral Jordan curve J 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 Summary

Star graph representations presented in this paper provide graph theoretical tools for the quantification problem of chirality of objects in $\mathbb{R}^2$. In this contribution we show that introducing a more rigorous definition for adjacency (Definition 3.1) in the graphs relative to P.G. Mezey's definition [5] we obtain star graph representations of planar chiral objects.

References

1. http://www.thalidomide.ca/
2. F. Harary, P.G. Mezey, *Chiral and Achiral Square-cell Configurations; The Degree of Chirality, New Develoments in Molecular Chirality* (Kluwer Academic Publisher, Dordrecht, 1991), pp. 241–256
3. F. Harary, R.W. Robinson, The number of achiral trees. J. Reine Angew. Math. **278**, 322–332 (1975)
4. P. G. Mezey, Similarity analysis in two and three dimensions using lattice animals and polycubes. J. Math. Chem. **11**, 27–45 (1992)
5. P.G. Mezey, Chirality measure and graph representations. Comput. Math. Appl. **34**(11), 105–112 (1997)
6. P.G. Mezey, *Shape in Chemistry An Introduction to Molecular Shape and Topology* (VCH Publishers, New York, 1993)
7. A.I. Kitaigorodski, *Organic Chemical Crystallography, Chapter 4* (Consultants Bureau, New York, 1961), pp. 75–100
8. K. Mislow, J. Siegel, Stereoisomerism and local chirality. J. Am. Chem. Soc. **106**, 3319–3328 (1984)
9. A. Rassat, Chimie organique physique—Un critère de classement des systèmes chiraux de points à partir de la distance au sens de Haussdorf. Compt. Rend. Acad. Sci. (Paris) II **299**, 53–55 (1984)
10. G. Gilat, On quantifying chirality—obstacles and problems towards unification. J. Math. Chem. **15**, 197–205 (1994)
11. G. Gilat, coefficient—a measure of the amount of structural chirality. J. Phys. A Math. Gen. **22**, L545–L550 (1989)
12. G. Gilat, On the quantification of asymetry in nature. Found. Phys. Lett. **3**, 189–196 (1990)
13. D. Avnir, A.Y. Meyer, Quantifying the degree of molecular shape distortion. A chirality measure. J. Mol. Struct. (Theochem) **226**, 211–222 (1991)

14. F. Harary, M. Lewinter, Spanning subgraphs of a hypercube. Int. J. Comput. Math. **25**(1), 1–4 (1988)
15. R.S. Cahn, C.K. Ingold, V. Prelog, Specification of molecular chirality. Angew. Chem. Int. Ed. Engl. **5**, 385–415 (1966)