*Symmetry: Culture and Science*
*Vol. 21, Nos.1-3, 27-36, 2010*

# CHIRALITY IN METRIC SPACES

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***Abstract:*** *A definition of chirality based on group theory is presented. It is shown to be equivalent to the usual one in the case of Euclidean spaces, and it permits to define chirality in metric spaces which are not Euclidean.*

2000 MSC code: 58D19 ; PACS code: 02.20.Bb

## 1. INTRODUCTION

The terms *chiral* and *chirality* were introduced by Lord Kelvin (Thomson 1904):

I call any geometrical figure, or group of points, chiral, and say that it has chirality if its image in a plane mirror, ideally realized, cannot be brought to coincide with itself.

Following the definition above, chirality is understood as a lack of mirror symmetry, and achirality means the existence of mirror symmetry. This kind of symmetry was known several millenaries ago: a number of ancient art images exhibiting mirror symmetry can be found in the book of Darvas (2007). Weyl (1952) related mirror symmetry to improper rotations, and it is now widely accepted that an object in the Euclidean space is achiral if it is identical to one of its images through an indirect isometry, an indirect isometry being the composition of translations, rotations, and of an odd number of mirror reflections. One of the simplest examples of chiral figures in the plane is any non-isoscele and non-degenerate triangle: it cannot be superimposed by composition of translations and *planar* rotations to its image generated by reflection around an arbitrary line (here, the mirror is a line). Conversely, any isoscele triangle is achiral in the plane. However, chiral triangles in the plane are achiral in the 3D space because it always exists a translation and a *spatial* rotation perfectly superposing the triangle on its image through an arbitrary plane (here, the mirror is a plane). In chemistry, chirality of molecules has a special importance due to its relation with optical phenomena, and involves sometimes complicated situations with flexible molecules. Nevertheless, it is still based on geometrical chirality in the 3D Euclidean space.

Clearly, the modern definition of chirality needs that we consider objects in the *d*-dimensional Euclidean space. A practical consequence of the definition is that a subdimensional object is achiral because it is identical to its image reflected in the (*d*–1)-hyperplane containing the object: e.g., a planar object in the 3D space is achiral, and a chiral 3D object plounged in the 4D space becomes achiral. Thus, the actual definition of chirality is intimately related to the dimension of the Euclidean space. In this paper, we propose a general definition of chirality which does not need any Euclidean space structure, and we show that it is equivalent to the usual definition in the case of an Euclidean space. We assume further in the text that a "non-Euclidean space" is just a space which is not Euclidean, and it is not assumed to have necessarily a geometric structure such as the one of hyperbolic spaces or other non-Euclidean spaces encountered in differential geometry and physics. In fact, the minimal geometric structure that we assume is induced by the existence of a distance, i.e. we work in metric spaces. The Euclidean space is also a metric space. Achirality is a particular instance of symmetry, so that we need a general definition of symmetry. The unifying one of Petitjean (2007) is retained: an object is a function having its input argument in the metric space, and objects are transformed via isometric transforms over the elements of this metric space. These isometries have a group structure. Thus, the idea is to relate the definition of achirality to the properties of the group. A chiral object is just an object which is not achiral.

## 2. GROUP STRUCTURE

Let $G$ be a group and $e$ its neutral element. Since there is no ambiguity, the symbol of the operation of the group will be omitted in expressions. The product of an element $a$ of $G$ by itself is noted $a^2$ and the inverse of $a$ is noted $a^{-1}$. Conventionnally, $a^0=e$. We define the set $G^+$ as the subset of $G$ generated by products of squared elements of $G$.

*Definition 1*: $G^+ = \left\{ r \in G / \exists k \in \mathrm{N}^*, \exists a_i \in G, i = 1,\ldots,k, r = \prod_{i=1}^{i=k} a_i^2 \right\}$

*Theorem 1*: $G^+$ is a subgroup of $G$. It is called the direct subgroup of $G$.

Proof: $G^+$ is not empty because $e \in G$, and $G^+$ is closed under the group operation and is closed under inversion.

Now we define $G^-$ as being the complement of $G^+$ to $G$.

*Definition 2*: $G^{-}=G-G^{+}$

$G^{-}$ may be empty. E.g., the cyclic group isomorphic to $(\mathbb{Z}/n\mathbb{Z},+)$, when $n$ is odd, is such that $G^{+}=G$ and $G^{-}=\varnothing$ because $\forall p\in\{0,\ldots,n-1\}$, either $a^{p}=a^{p/2}a^{p/2}$ when $p$ is even, or $a^{p}=a^{(p+n)/2}a^{(p+n)/2}$ when $p$ is odd. However, when $n$ is even, $G^{+}$ contains the $n/2$ even powers of the generator $a$, and $G^{-}$ contains its $n/2$ odd powers.

We assume further that $G^{-}$ is not empty.

*Lemma 1*: $\forall r\in G^{+}$ and $\forall q\in G^{-}$, $rq\in G^{-}$ and $qr\in G^{-}$.

Proof: If we assume that $rq\in G^{+}$, then, multiplying on the left by $r^{-1}$ which is in $G^{+}$ would mean that $q\in G^{+}$, which is impossible. Same proof for $qr$ by multiplication on the right by $r^{-1}$.

So, the product of two elements of $G^{+}$ is in $G^{+}$, the product of an element of $G^{+}$ by an element of $G^{-}$ is in $G^{-}$ and conversely. In general, the product of two elements of $G^{-}$ may be either in $G^{+}$ or in $G^{-}$.

We also introduce the definition 3, which will be useful later.

*Definition 3*: When existing, the involutions of $G^{-}$ are called mirrors.

## 3. DEFINITION OF CHIRALITY

We refer to the general framework needed to define symmetry according to Petitjean (2007): $E$ being a metric space and $\delta$ being its associated distance, $F$ is the group of all bijections of $E$ onto $E$ preserving $\delta$. This group $F$ operates on $E$. Its neutral element is $I_F$. The elements of $F$ are isometries (in respect to $\delta$). Then, an object $Y$ is defined as a function having its input argument in $E$. The object $Y$ is symmetric if there is a bijection $U$ of $F$, with $U\neq I_F$, such that for all elements $x$ of $E$, $Y(Ux)=Y(x)$.

Let $F^{+}$ be the direct subgroup of $F$ and $F^{-}=F-F^{+}$.

*Definition 4*: The isometries of $F^{+}$ are called direct isometries, and when existing, the isometries of $F^{-}$ are called indirect isometries.

*Definition 5*: An object having symmetry due to a direct isometry has direct symmetry, and an object having symmetry due to an indirect isometry has indirect symmetry.

*Definition 6*: An object having indirect symmetry is called achiral and an object having no indirect symmetry is called chiral.

By extension, when $F^-$ is empty, a symmetric object may be called chiral.

Still by extension, a non symmetric object may be called chiral.

## 4. EUCLIDEAN SPACES

The definition of chirality given in the previous section is proved below to be equivalent with the usual one when the space is Euclidean. The distance δ is the usual Euclidean distance. The set $F$ of all isometries contains the translations, the rotations, and the orthogonal transformations composed by rotations and by an odd number of mirror inversions (i.e., the orthogonal matrices associated to these orthogonal transformations have a determinant equal to −1).

The translations are all elements of $F^+$, because a translation of vector $t$ is always the composition of two identical translations of vector $t/2$. Any $d$-dimensional rotation can be written as a product of $d(d-1)/2$ Givens rotations (see appendix), and each Givens rotation of angle θ is the square of two identical Givens rotations of angle θ/2. So, the rotations are elements of $F^+$. However, the orthogonal transformations composed by rotations and by an odd number of mirror inversions are elements of $F^-$, due to the sign of the determinant of their associated $d$-dimensional square matrix. As a particular example of these latter transformations, mirror inversions are involutions of $F^-$, and according to the definition 3, can be just called mirrors.

To summarize:
- Compositions of an even number of mirrors with translations and rotations are elements of $F^+$
- Compositions of an odd number of mirrors with translations and rotations are elements of $F^-$

It follows that the traditional definition of chirality and our definition 6 are equivalent in the case of Euclidean spaces.

## 5. NON EUCLIDEAN SPACES

The simplest situation is the case of finite strings of $n$ characters or $n$ symbols we like (bits, digits, etc.). We assume first that the $n$ positions are sequentially labelled $1,\cdots,n$. Owing to the definition of symmetry retained at the beginning of section 3, the group of isometries contains only two elements: the neutral element, represented by the identity permutation matrix, and the operator permuting the symbols at positions $i$ and $n+1-i$ for

$i$=1,$\cdots$,$n$. The permutation matrix associated to this operator is the antidiagonal matrix $J$, which is a mirror because $J^2 = I$. Any relabeling of the $n$ positions would be associated to a permutation matrix $P$ such that the mirror would be written $PJP'$, where $P'$ is the transposed of $P$, and we have again $(PJP')(PJP')=I$. It follows from our definition that palindromas are achiral, and non palindromic words are chiral. The existence of a mirror in a palindroma is obvious, although there is no Euclidean structure.

Infinite sequences of symbols in one direction have only one isometry, i.e. the neutral element. So they are never symmetric and are all chiral. Infinite sequences in both directions may be indiced by a set of signed integers isomorphic to $\mathbb{Z}$. For clarity, we assume that it is $\mathbb{Z}$itself, and $i$ is an index taking any value in $\mathbb{Z}$. The direct subgroup $F^+$ of isometries contains the operators $T_k$ translating all positions $i$ to $i+k$, $k$ taking any signed integer value. Its complement $F^-$ contains the mirrors $M_0(j)$ permuting all positions $j+i$ with $j+1-i$, $j$ taking any integer value, and the mirrors $M_1(j)$ permuting all positions $j+i$ with $j-i$, $j$ taking any integer value, and the compositions of the operators $T_k$ with odd numbers of mirrors. So, an infinite sequence such that ...ABCABCABC... is symmetric and chiral, and an infinite sequence such that ...ABCCBAABCCBA... or ...ABCBAABCBA... is symmetric and achiral.

Extensions to multidirectional lattices are possible, but are not constrained to follow some Euclidean-like structure, such as nodes in crystal lattices.

According to our definition of symmetry, a rectangular matrix $A$ of $m$ lines and $p$ columns is viewed as a function of a bicomponent index $x$ such that the first component of $x$ takes integer values in 1,$\cdots$,$m$ and the second component of $x$ takes integer values in 1,$\cdots$,$p$. The $mp$ values returned by the function are the $mp$ elements of the matrix, and are not necessarily numbers: they may be of any type. The distance between two bicomponent indices $x_1$ and $x_2$ is issued from the ordinary Euclidean norm, but applies here to two ordered pair of numbers: $\delta(x_1, x_2) = \|x_2 - x_1\|$. So, the group $F$ contains the following isometries: $(I_m, I_p)$, $(I_m, J_p)$, $(J_m, I_p)$, and $(J_m, J_p)$, where $I_m$ and $I_p$ are the identity permutations of respective sizes $m$ and $p$, and $J_m$ and $J_p$ are permuting respectively the lines $i$ and $m+1-i$ for $i$=1,$\cdots$,$m$ and the columns $j$ and $p+1-j$ for $j$=1,$\cdots$,$p$. In matricial form, the images of $A$ through these isometries are respectively $I_m A I_p'$, $I_m A J_p'$, $J_m A I_p'$, and $J_m A J_p'$. So $F^+ = \{(I_m, I_p)\}$, and $F^- = \{(I_m, J_p), (J_m, I_p), (J_m, J_p)\}$. The three elements of $F^-$ are mirrors, any of them being the product of the two other ones. In the Euclidean case, the product of two mirrors would not be a mirror. In this particular case, $F$ is a commutative group.

When $p=m$, $A$ is a square matrix, and $F^-$ contains four more mirrors. One corresponds to the usual matrix transposition (i.e. lines and columns are exchanged), and the three other ones correspond to the respective products of the transposition by the $(I_m, J_m)$, $(J_m, I_m)$, $(J_m, J_m)$, and $(J_m, J_p)$. Again, all products in $F$ are commutative: $F$ is a commutative group. The product of the transposition by ($J_m$, $J_m$) is the transposition through the antidiagonal of $A$. A matrix called symmetric in the usual sense, i.e. identical to its transpose, is thus achiral. A matrix usually said to be "non-symmetric" may be in fact either chiral or achiral (and thus symmetric), even if it is rectangular, depending of its structure.

It is pointed out that a matrix should not be confused with a rectangle or a square in the Euclidean plane, despite that we conventionnally draw matrices rectangularly: e.g., the mirror ($J_m$, $J_p$) should not be confused with the center of symmetry of a rectangle in the Euclidean plane, which is associated to a rotation of angle $\pi$, this latter being not a mirror. In fact, matrices and tensors are not geometrical figures, and when existing, their symmetry properties should not be confused with those of their graphical representations.

Graphs are nodes and edges structures of major importance in many areas, including mathematics, chemistry, econometrics, etc. According to Petitjean (2007), the isometries associated to a graph of $m$ nodes are the $m$! possible renumbering of the nodes, each renumbering being represented by a permutation matrix of size $m$. The group $F$ is the group of these $m$! permutations. Each permutation $P$ can be decomposed into $k$ independant cycles of lengths $m_1,...,m_k$ , with $m_1+\cdots+m_k=m$. To each cycle is associated a circular permutation $C_i$ of length $m_i$, $i=1,\cdots,k$. Then, $P=C_1C_2\cdots C_k$, and all elements of this latter product commute, although the product of permutations does not commute, in general. The smallest integer $K$ such that $P^K=I$ is the least common multiple of $m_1,...,m_k$ . A permutation containing exactly one cycle of length 2 is usually called a transposition, and is a mirror. Except the identity permutation $I$, all permutations $P$ composed of cycles of length 1 or 2 are mirrors. More generally, $P\in F^+$ if and only if all cycles of $P$ have an odd length.

Proof: if $P$ has at least one cycle $C_i$ of even length $m_i$, it can be written $P=\Pi C_i\,\Pi C_j$ , where $\Pi C_j$ is the product of odd length cycles (contains at least $I$). Assuming $P$ in $F^+$ would mean that $\Pi C_i$ would be in $F^+$ because each cycle of odd length $m_j$ is a square, i.e. $C_j = C_j^{(m_j+1)/2} C_j^{(m_j+1)/2}$ , and so the product $\Pi C_i = P(\Pi C_j)^{-1}$ would fall in $F^+$. But the determinant of each $C_i$ is $-1$, so that none of the $C_i$ is in $F^+$. If there is only one even length cycle $C_i$ in $P$, then $C_i\in F^-$, and thus $P\in F^-$. If there are at least two even length cycles in the expression of $P$, each of these even length cycles $C_i$ can be written as product of other permutations, but since the $C_i$ are independant, none of the permutations involved in the expression of one of the even length cycles can appear in the expression of an other one of the even length cycles, except the identity. So the product of the $C_i$ cannot exhibit any square apart $I$, and thus cannot be in $F^+$ unless $P=I$, in which case $P$ has only cycles of odd lengths 1.

In order to exemplify symmetry in graphs, we consider the graphs associated to some molecular structural formulas. E.g. the molecular graph of the water H-O-H contains three nodes and two edges. There are two automorphisms: one is associated to the identity permutation of order 3, and the other one is associated to a permutation exchanging the two hydrogens and leaving invariant the oxygen. This latter permutation is a mirror, and so the graph of the water is achiral. It is emphazised here that this achirality should not be confused with the geometrical achirality of the water molecule. The graph of the hydrochloric acid H-Cl is chiral because it has only one automorphism (the identity), although it is geometrically achiral. The graph of the methanol $CH_3$-O-H has 6 automorphisms, which constitute the subgroup isomorphic to all permutations of 3 elements (the hydrogens of the methyl group): this graph offers both direct and indirect symmetry (and so it is achiral). The hydrogen suppressed molecular graph of any linear alcane containing $n$ carbons ($n \geq 2$), C-C-...-C-C, has two automorphisms and is achiral.

Outside the field of chemistry, a graph containing $mp$ nodes ($m \geq 2$, $p > 2$) constituting a single ring of size $mp$ containing cyclically $m$ repetitions of the same ordered sequence of $p$ different nodes (e.g. $p$ different letters), has a symmetry group of $m$ automorphisms which is isomorphic to the subgroup of all circular permutations of $m$ elements and to ($Z/mZ$,+). When $m$ is even, the graph has both direct and indirect symmetry. When $m$ is odd, the graph has direct symmetry and is chiral.

## 6. DISCUSSION AND CONCLUSION

The main goal of this paper was to show that the concept of chirality/achirality is not attached to the existence of an Euclidean space. We have demonstrated that the existence of chirality or achirality is induced by the group structure of the isometries. This group of isometries is assumed to operate on a metric space rather than on the Euclidean space. This latter is a metric space, too, but all other requirements needed to build an Euclidean space are relaxed: we work under much less assumptions than in the Euclidean case, and thus it is a major progress. Furthermore, we have proved that our definition of chirality/achirality is indeed equivalent to the usual one in the Euclidean case. However, the usual sense of chirality involving orientation of space looses its original meaning: this is fortunate, because space orientation is undefined when the space is not Euclidean.

A practical consequence of our definition of chirality is that we can classify the symmetry operators of an object into two classes: the direct symmetry operators, and the indirect symmetry operators, which induce achirality. So, depending of its symmetry operators, a symmetric object can be either direct-symmetric and not indirect-symmetric (i.e. chiral), or indirect-symmetric (i.e. achiral) and not direct-symmetric, or both direct and indirect symmetric. This classification works in the non Euclidean case, but in this latter situation, we must keep in mind that we are dealing with objects in a space which is not Euclidean. It means that when we superimpose this model of symmetry to an

Euclidean model, each model of symmetry induces its own properties to the object. E.g., a graph for which the nodes receives cartesian coordinates has the symmetries due to the graph automorphisms, and has the Euclidean symmetries due to its geometrical representation. The symmetry groups of these two kinds of symmetries are not isomorphic, in general. If we would consider together these both kinds of symmetries, we would have to metrize the cartesian product of the Euclidean space by the metric space underlying the graph structure. A similar situation occurs in chemistry, where both the geometry of the molecule and the graph associated to the structural formula must be considered together. E.g. the bromo-chloro-fluoromethane Br-CHF-Cl, assuming that the carbon is at the center of a regular tetrahedron with each of the four other atoms lying at its vertices, is achiral in the Euclidean space, has a chiral graph (only one automorphism), and the whole molecule is chiral if we consider both the graph and the spatial geometry. Other examples of symmetry in product spaces have been presented by Petitjean (2002).

An other consequence of our definition of chirality is based on the partition of the group $F$ of isometries into two subsets, i.e. the direct subgroup $F^+$ and its complement $F^-=F-F^+$. The neutral element is always in $F^+$, and this fact enlights why the problems of building direct symmetry measures and building chirality measures may require different solutions (Petitjean 2003). The full discussion of symmetry measures being outside the scope of the present work, the reader is referred to the cited paper.

Several situations of interest have not been considered, such as hyperbolic spaces and Thurston geometries (Scott 1983, Thurston 1997, Molnár 1997, Molnár 2005, Molnár and Szirmai 2006). These geometries will be considered in a subsequent paper.

## ACKNOWLEDGMENTS

I thank very much Emil Molnár for having provided useful comments and references and I thank the anonymous reviewer for his helpful suggestions. I am grateful to György Darvas for his enlighting comments and for having managed the anonymous peer review process of this paper.

# APPENDIX: FACTORISATION OF ROTATIONS

Let $R$ be a $d$-dimensional rotation, $d>1$. A Givens rotation is represented by a matrix of the form:

$$G(j,k,\theta)=\begin{pmatrix} I & 0 & 0 & 0 & 0 \\ 0 & c & 0 & -s & 0 \\ 0 & 0 & I & 0 & 0 \\ 0 & s & 0 & c & 0 \\ 0 & 0 & 0 & 0 & I \end{pmatrix}$$

where $c=cos(\theta)$ and $s=sin(\theta)$ appear at the intersections $j^{th}$ and $k^{th}$ rows and columns, $1\le j<k\le d$, and the square blocks $I$ are identity matrices of respective sizes $j-1$, $k-1-j$, and $d-k$. Since the multiplication of any matrix of $d$ lines by $G(j,k,\theta)$ on the left affects only the lines $j$ and $k$, we restrict our attention to these lines. Given the reals $a$ and $b$, we can set θ in order to have:

$$\begin{pmatrix} c & -s \\ s & c \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}=\begin{pmatrix} r \\ 0 \end{pmatrix}$$

Practically, we set $s=-b/\sqrt{a^2+b^2}$ and $c=a/\sqrt{a^2+b^2}$, and we get $r=\sqrt{a^2+b^2}$. Applying successively Givens rotations to the $d(d-1)/2$ couples $(j,k)$, $j=1,\cdots,d-1$, $k=j+1,\cdots,d$, we factorize $R$ as a product of $d(d-1)/2$ Givens rotations by an upper triangular matrix $U$ (this is a particular case of the well-known QR decomposition). $U$ is itself a rotation matrice because $R$ is a rotation matrix. So, the diagonal elements of $U$ can contain only +1 and −1 values, and thus $U$ is diagonal because its columns are unit vectors. Since the process generates a non negative value at each intersection of the line $j$ and the column $j$ for $j=1,\cdots,d-1$, the $d-1$ first diagonal elements of $U$ take the value +1, and its last diagonal element receives the value of the determinant of $R$, i.e. +1 because $R$ is a rotation. Thus, $U=I$ and $R$ is factorized as the product of $d(d-1)/2$ Givens rotations.

*Remark*: $G(j,k,\theta)=G(j,k,\theta/2)G(j,k,\theta/2)$. So, any rotation can be expressed as a product of $d(d-1)/2$ squares of Givens rotations.

Other remark: in the literature, the Givens rotations matrices are often defined as being the transposed of the ones above. This difference is meaningless in our context. We just notice that when $d=2$, the Givens rotation matrix of angle θ we used here corresponds to a rotation of angle +θ when operating on the left of a column vector, which is the standard way to write this kind of product. The transposed rotation matrix corresponds to a rotation of angle −θ.

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