Geometric properties of chiral bodies

G. Gilat [a] and Y. Gordon [b]

[a] Department of Physics, [b] Department of Mathematics,
Technion - Israel Institute of Technology, Haifa 32000, Israel

Received 26 August 1993; revised 18 March 1994

The new developments concerning the possible metrization of structural chirality have drawn much attention recently. The main approach of such quantification is based on the maximal volume overlap between two enantiomorphs of a given chiral set. This approach raises an interesting problem concerning the shape of such a domain of overlap, namely, whether it is chiral or not. It is shown presently that for a two or three dimensional set if the maximal volume overlap is unique then it must be *achiral*. It is also shown that if a two-dimensional body is convex then by the Brünn–Minkowski theorem the maximal volume overlap of the body with its enantiomorph is *achiral*. In addition, universal upper bounds for chiral coefficients χ_n of convex sets in any dimension n are given, being $\chi_2 \leqslant 0.3954$ and $\chi_3 \leqslant 0.6977$ for dimensions two and three, respectively.

1. Introduction

In recent years there has been an ever-increasing interest and activity in the phenomenon of structural chirality, in particular, in the attempts of quantifying it [1–8]. These attempts are mainly based on two different approaches: (a) The method of Hausdorff distances introduced by Rassat [1] and (b) the method of maximal overlap of two enantiomorphs of the same chiral set [3], based on the original approach of Kitaigorodskii [9]. These two approaches differ from one another in the degree of dimensionality of the elements chosen for quantification, one being sub-dimensional and the second is equi-dimensional. In other words, the first approach is using distances between points, whereas the second approach is using volumes (areas in dimension 2), being of the same dimension as is the space to which it refers.

These features are discussed and analyzed in a recent article by the first author [10]. The main conclusion of this analysis is that the overlap method, based on an equi-dimensional element, i.e., the volume (area for 2d bodies) is of more general and substantial nature than the Hausdorff distances and hence more suitable for the purpose of quantifying chirality. Moreover, physical chiralities [3] are also accessible to metrization by the overlap approach [10], but not readily so for the Hausdorff distances approach.

It is the purpose of the present article to analyze general properties of chiral bodies that are relevant to the approach of maximal volume overlap of a given chiral body with its enantiomorph, being an arbitrarily displaced rotation of a mirror image of the body.

One of the main problems related to the overlap method concerns the possible shape of such an overlap between two enantiomorphs of the same body, or more specifically: "Is the shape of an overlap chiral or achiral?" It is quite feasible to guess that a general answer to such a question does not exist and that the shape of the maximal overlap depends on the nature of the given chiral body. Nevertheless, it is hereby claimed that for any 2-dimensional (2d) chiral convex body, the shape of the maximal overlap between it and its enantiomorph is *achiral*. The same conclusion holds true for 3d convex bodies provided we restrict the enantiomorph to take the form of translations of mirror images, and disallow rotations. In dimension 2 this is not a real restriction since a rotation does not play any role. This result is one of the conclusions of the present article and in order to obtain it we need to prove two auxiliary theorems. One of these has already been introduced [3,10] and it concerns the general statement that if the shape of an overlap is chiral, then there exist *two equal* maximal overlaps, one being the mirror image of another. The same conclusion is true for *any chiral intersection* between two enantiomorphs of the same chiral body. Moreover, in the case of any 2d body, the transition from one intersection to its mirror image can be accomplished by a linear translation of one enantiomorph of the given body with respect to another. The situation for 3d convex bodies is more complicated since an enantiomorph of a body allows a rotation and translation of the mirror image. Nevertheless, it can be generally stated that for any 2- or 3-dimensional bodies, not necessarily convex, if the maximal overlap is *unique* then it must be *achiral*. In the case of 2d convex sets it is possible to apply the Brünn–Minkowski theorem [11,12] to a linearly displaced set and show that the volume of intersection of the set with its enantiomorph is a concave [13] function of the amount of displacement. This is a conclusion derived from the second theorem, and it leads to the result that the maximal overlap of two enantiomorphs of a 2-dimensional convex chiral body cannot be chiral.

In addition to this general conclusion, we use volume-ratio estimates to obtain values for upper bounds of the chiral coefficient χ which is a measure of the amount of geometric chirality [3]. These values can be estimated for any n-dimensional convex chiral body and the results for $n = 2$ and 3 are $\chi \leqslant 0.3954$ and 0.6977, respectively.

In section 2 we state and prove the theorems necessary to show the achirality of the maximal overlap of two enantiomorphs of any 2- or 3-dimensional chiral body. In section 3 the numerical value for the upper bounds of χ are derived. The article is concluded in section 4.

2. Maximal volume overlap of chiral enantiomorphs

Let D be an arbitrary body in $\mathbb{R}^n, n = 2, 3$. Let $U = U_f$ denote a rotation operator with respect to some axis represented by a unit vector f. Let $\Phi = \Phi_e$ be the reflection operator defined by: $\Phi(x) = x - 2\langle x, e\rangle e$, for all $x \in \mathbb{R}^n$, where e is a unit vector and $\langle x, e\rangle = \sum_{i=1}^{n} x_i e_i$. Note that Φ is a reflection about the mirror-plane (line in dimension 2) orthogonal to e, $P_e = \{x = (x_1, \dots, x_n); \langle x, e\rangle = 0\}$. Let

$$D^* = U\Phi(D) + b \tag{1}$$

be an enantiomorph of D, and let us now consider the intersection

$$\Delta = D \cap D^* = D \cap \{U\Phi(D) + b\}. \tag{2}$$

Now we consider also Δ^*, the mirror-image of Δ given by

$$\Delta^* = \Phi(\Delta) = \Phi(D) \cap \{\Phi U\Phi(D) + \Phi(b)\}. \tag{3}$$

Let us observe that $\Phi^2 = I$, where I is the identity operator, and the matrix representing $\Phi = \Phi_e$ where $e = (e_1, e_2, e_3)$ is given by

$$\Phi = \begin{pmatrix} 1 - 2e_1^2 & -2e_1e_2 & -2e_1e_3 \\ -2e_1e_2 & 1 - 2e_2^2 & -2e_2e_3 \\ -2e_1e_3 & -2e_2e_3 & 1 - 2e_3^2 \end{pmatrix}, \tag{4}$$

and $\det(\Phi) = -1$. We now apply the rotation–translation map defined for $x \in \mathbb{R}^n$ by $W(x) = \Phi U\Phi(x) - \Phi U^{-1}(b)$ on Δ^*, to obtain

$$\begin{aligned} \Delta' &= \Phi U\Phi(\Delta^*) - \Phi U^{-1}(b) = \Phi U^{-1}(\Delta) - \Phi U^{-1}(b) \\ &= D \cap \{\Phi U^{-1}(D) - \Phi U^{-1}(b)\}. \end{aligned} \tag{5}$$

Δ' is a rotated-displaced variant of Δ^* and is therefore identical in volume to Δ. Both Δ and Δ' present various intersections between D and its enantiomorph D^*. Let M denote the maximal volume of Δ, namely

$$M = \max_{\{U,\Phi,b\}} \mathrm{vol}_n(\Delta) = \max_{\{U,\Phi,b\}} \mathrm{vol}_n(D \cap \{U\Phi(D) + b\}). \tag{6}$$

It is important to notice that if Δ is chiral, then M is not uniquely defined since the volume of $\Delta^* = \Phi(\Delta)$ is also equal to M. We shall call the pair of unit vectors (e,f) admissible if they are vectors in $\mathbb{R}^3$ such that $\langle e,f\rangle = 0$. Note that if we restrict the attention to $\mathbb{R}^2$ only, then rotation $U = U_f$ in the xy plane corresponds to a rotation with $f = (0, 0, 1)$ as axis, and reflection $\Phi = \Phi_e$ corresponds to reflection about the mirror-line $\{x = (x_1, x_2); \langle x, e\rangle = 0\}$, and in this case e is in the xy plane, so orthogonal to f.

LEMMA 1

If the pair (e, f) is admissible then $(\Phi_e U_f)^2 = I$ and there exists a unit vector $g \in P_f$, i.e. $\langle f, g\rangle = 0$, so that $\Phi_e U_f = \Phi_g$. Conversely, if $(\Phi_e U_f)^2 = I$ then either $U_f = I$, or $\Phi_e U_f = -I$, or (e,f) is an admissible pair.

Proof

The orthogonality condition is equivalent to saying that e lies in the plane P_f. Let us, without loss of generality, assume that $e = (1, 0, 0)$ and $f = (0, 0, 1)$ and let $U = U_f$ be the rotation in the xy plane by an angle θ and set $\Phi = \Phi_e$. In matrix notation then

$$U = \begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 \\ -\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \Phi = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{7}$$

If we choose now the vector $g = (\cos(\theta/2), \sin(\theta/2), 0)$, then

$$\Phi_g = \begin{pmatrix} -\cos(\theta) & -\sin(\theta) & 0 \\ -\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix} = \Phi U, \tag{8}$$

so that $(\Phi U)^2 = \Phi_g^2 = I$.

Conversely, suppose $(\Phi U)^2 = I$ where $U = U_f$ and $\Phi = \Phi_e$ for some arbitrary unit vectors f, e in $\mathbb{R}^3$. We may suppose that $f = (0, 0, 1)$ so that P_f is the xy plane, and assume that

$$U = \begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 \\ -\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{9}$$

where for the moment let $\sin(\theta) \neq 0$. We may also select the xy axes so that $e = (0, e_2, e_3)$, thus

$$\Phi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 - 2e_2^2 & -2e_2e_3 \\ 0 & -2e_2e_3 & 1 - 2e_3^2 \end{pmatrix}. \tag{10}$$

Then

$$\Phi U = \begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 \\ -(1 - 2e_2^2)\sin(\theta) & (1 - 2e_2^2)\cos(\theta) & -2e_2e_3 \\ 2e_2e_3\sin(\theta) & -2e_2e_3\cos(\theta) & 1 - 2e_3^2 \end{pmatrix}. \tag{11}$$

Now, $\Phi U = U^{-1}\Phi = U^*\Phi = (\Phi U)^*$, hence ΦU is a symmetric matrix, implying $2e_2e_3\sin(\theta) = 0$, i.e., $e_2e_3 = 0$. If $e_3 = 0$ then $e = (0, \pm 1, 0)$ which is orthogonal to f. If $e_2 = 0$ then $e = (0, 0, \pm 1)$, and in the case

$$\Phi U = \begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 \\ -\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{12}$$

but since $\Phi U = (\Phi U)^*$ it follows that $\sin(\theta) = 0$, which is impossible. To conclude, suppose now that $\sin(\theta) = 0$. Then either $\theta = 0$, i.e. $U = I$, or $\theta = \pi$. In the latter case, since the 23 and 32 entries of the matrix ΦU in eq. (11) are identical, it follows that $e_2 e_3 = 0$. So again either $e = (0, \pm 1, 0)$ which is orthogonal to f, or $e = (0, 0, \pm 1)$, and then the matrix $\Phi U = -I$, and this ends the proof in dimension 3.

In dimension 2 the proof is trivial, indeed, for any rotation U and reflection Φ in the xy plane there is a vector g so that $\Phi U = \Phi_g$, hence the reflection-rotation ΦU amounts to a reflection only, and of course, we cannot have $\Phi U = -I$ in the plane. □

An interesting general geometric result for $n = 2$ is presented in fig. 1. If we look at any union of $D \cup D^*$ and its mirror image $(D \cup D^*)^*$ and we perform an exact overlap of D of one union upon its enantiomorph, we obtain two identical bodies of D^* displaced from one another by a pure translation. The geometric reason behind this result has to do with the invariance of angles under reflection and rotation. This result does not hold in $\mathbb{R}^3$, but it is true for the special case of $(\Phi U)^2 = I$.

Let us now look for the maximum volume overlap M' of $D \cap \{\Phi(D) + b\}$ taken over all reflections Φ and vectors b,

$$M' = \max_{\{\Phi, b\}} \mathrm{vol}_n(D \cap \{\Phi(D) + b\}) . \tag{13}$$

Upon comparing M' and M (eq. (6)) it is clear that $M \geqslant M'$. In dimension 3, however, it is possible to construct a convex body D such that D is centrally (i.e. inversely) symmetric, meaning $D = -D$, and so that $M' < \mathrm{vol}_3(D)$, or equivalently, D is not identical with any of its mirror-images. For this body, if we choose $U\Phi = -I$ and $b = 0$, we obtain $\Delta = D$, hence $M = \mathrm{vol}_3(D) > M'$. Incidentally, a centrally symmetric body of odd-dimension is therefore achiral.

THEOREM 1

(i) When $n = 2, M = M'$.

(ii) If the maximum M is attained for a certain unique triple $\{U, \Phi, b\}$, then D has a rotation–translation symmetry, i.e. the rotation operator $(U\Phi)^2$ satisfies

$$D = (U\Phi)^2(D) + U\Phi(b) + b . \tag{14}$$

(iii) When $n = 3$, if the maximum M is unique and D has no rotation–translation symmetry, then either $M = M'$ or M is achieved for $U\Phi = -I$.

(iv) If the maximal volume intersection body is unique, then it is achiral.

Proof

(i) This is obvious because in dimension 2, every product $U\Phi$ of a rotation U and a reflection Φ is a reflection.

(ii) If M is attained uniquely, then by eqs. (2) and (5), $\Phi U^{-1}(D - b) = U\Phi(D) + b$, i.e. $D = (U\Phi)^2(D) + b + U\Phi(b)$. For $n = 2$, since $U\Phi$ is a reflection, $(U\Phi)^2 = I$,

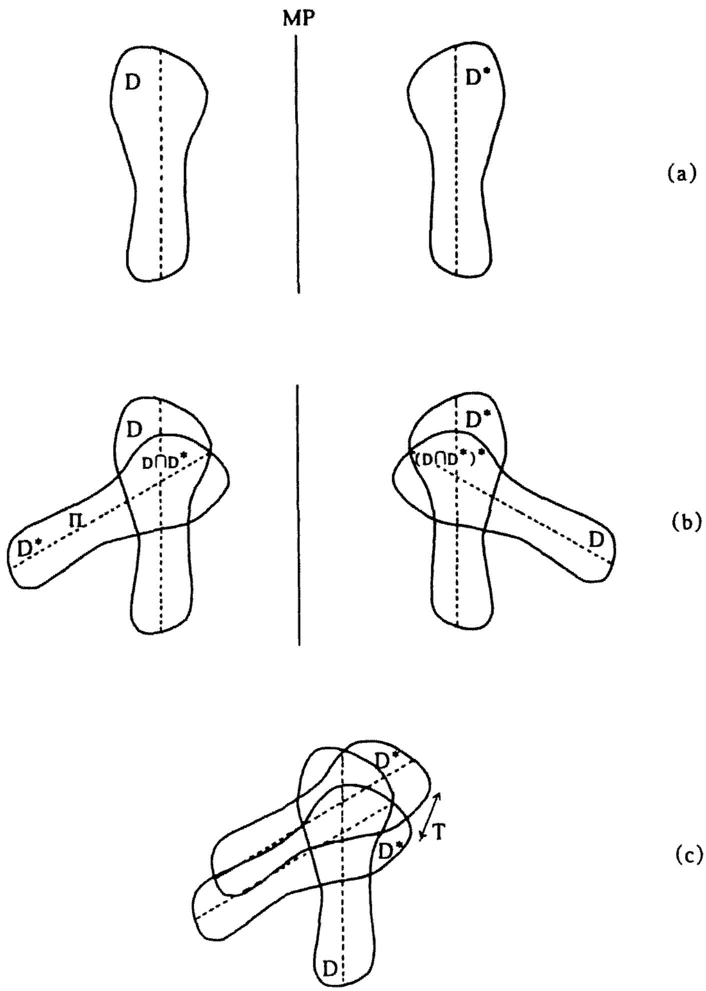

Fig. 1. (a) The two enantiomorphs D and D^* are schematically shown with reference to a mirror line MP, in a 2d space. An arbitrary line that intersects them is also shown. (b) $D \cap D^*$ and $(D \cap D^*)^*$, two mirror images of an arbitrary intersection of D and $D*$ are shown with respect to MP. (c) The right hand side (RHS) of (b) is transformed by a rotational-translation (RT) transformation onto the LHS of the same figure, so that D overlaps precisely D of the LHS. The enantiomorph D^* is seen to be displaced from the other D^* by a translation T. By angular conservation under reflection it becomes clear that linear intersections on both D^* must be parallel to one another.

so that $D = D + b + U\Phi(b)$ implies $b = -U\Phi(b)$, therefore if $b \neq 0$, then $U\Phi$ is the reflection operator about the mirror plane orthogonal to b.

(iii) In this case by eq. (14) $(U\Phi)^2 = I$ and $b + U\Phi(b) = 0$. By lemma 1, either $U = I$, then $M = M'$, or $U\Phi = -I$.

(iv) This is obvious because Δ of eq. (2) and Δ' of eq. (5) have the same volume, so by uniqueness, if Δ is maximal then it is identical to Δ'. We obtain

$$U\Phi(\Delta) = U\Phi(\Delta') = U\Phi(D \cap \{\Phi U^{-1} - \Phi U^{-1}(b)\}) = \Delta - b\,. \tag{15}$$

□

We now state the classical Brünn–Minkowski theorem [11,12], which we shall need in the sequel [14–16].

THEOREM 2

Let A, B be two compact sets in the n-dimensional Euclidean space $\mathbb{R}^n$. Then for all $0 \leqslant \lambda \leqslant 1$

$$\mathrm{vol}_n(\lambda A + (1-\lambda)B) \geqslant (\mathrm{vol}_n(A))^{\lambda}(\mathrm{vol}_n(B))^{1-\lambda}\,, \tag{16}$$

and [14]

$$(\mathrm{vol}_n(\lambda A + (1-\lambda)B))^{1/n} \geqslant \lambda(\mathrm{vol}_n(A))^{1/n} + (1-\lambda)(\mathrm{vol}_n(B))^{1/n}\,. \tag{17}$$

A brief word about the notation. The set $\lambda A + (1-\lambda)B$ denotes the convex combination $\{\lambda a + (1-\lambda)b; a \in A, b \in B\}$. We shall apply the theorem to a particular situation:

Let a_0, a_1, b_0, b_1 and A_0, A_1, B_0, B_1 be a collection of four points and four compact sets in $\mathbb{R}^n$. Consider the intersection $K_0 = (a_0 + A_0) \cap (b_0 + B_0)$ and $K_1 = (a_1 + A_1) \cap (b_1 + B_1)$ and for all $0 \leqslant \lambda \leqslant 1$, let $K_\lambda = (a_\lambda + A_\lambda) \cap (b_\lambda + B_\lambda)$, where $a_\lambda = \lambda a_1 + (1-\lambda)a_0$ and $A_\lambda = \lambda A_1 + (1-\lambda)A_0$, and the b_λ, B_λ are defined similarly. We claim that

PROPOSITION 1

For all $0 \leqslant \lambda \leqslant 1$

$$(\mathrm{vol}_n(K_0))^{1-\lambda}(\mathrm{vol}_n(K_1))^{\lambda} \leqslant \mathrm{vol}_n(K_\lambda)\,. \tag{18}$$

In particular,

$$\min\{\mathrm{vol}_n(K_0), \mathrm{vol}_n(K_1)\} \leqslant \mathrm{vol}_n(K_\lambda)\,. \tag{19}$$

Proof

We shall first show that any convex combination of the sets K_0 and K_1, i.e., $\lambda K_1 + (1-\lambda)K_0$, is contained in K_λ. Indeed, if $k_0 \in K_0$ and $k_1 \in K_1$, then they are of the form $k_0 = a_0 + \alpha_0$, and $k_1 = a_1 + \alpha_1$ where $\alpha_i \in A_i, (i = 0, 1)$. It follows that $\lambda k_1 + (1-\lambda)k_0 = a_\lambda + \lambda\alpha_1 + (1-\lambda)\alpha_0 \in a_\lambda + A_\lambda$, and similarly $\lambda k_1 + (1-\lambda)k_0 \in b_\lambda + B_\lambda$, implying that $\lambda K_1 + (1-\lambda)K_0 \subset K_\lambda$.

By the Brünn–Minkowski inequality [11,12] we obtain that

$$(\mathrm{vol}_n(K_0))^{1-\lambda}(\mathrm{vol}_n(K_1))^{\lambda} \leqslant \mathrm{vol}_n(\lambda K_1 + (1-\lambda)K_0) \leqslant \mathrm{vol}_n(K_\lambda)\,. \tag{20}$$

□

Remarks

1. If we denote by $f(\lambda)$ the function $(\mathrm{vol}_n(K_\lambda))^{1/n}$ then the inequality

$$f(\lambda) \geqslant (\mathrm{vol}_n(\lambda K_1 + (1-\lambda)K_0))^{1/n} \geqslant \lambda f(1) + (1-\lambda) f(0), \tag{21}$$

implies that the function $f(\lambda)$ is concave [13].

2. In the particular case where $A_0 = A_1 = A$ and $B_0 = B_1 = B$ are both convex bodies in $\mathbb{R}^n$, we have that $A_\lambda = A$ and $B_\lambda = B$ for all $0 \leqslant \lambda \leqslant 1$, and so taking $a_0 = b_0 = b_1 = 0$ (= the origin), it follows that: If for some point $a \in \mathbb{R}^n$ we have the equality $\mathrm{vol}_n(A \cap B) = \mathrm{vol}_n((a + A) \cap B)$, then for all points x inside the interval $[0, a]$, the rigid translation of A to x along the segment $[0, a]$ will have a larger intersection with B than at the end points 0 and a. This implies that the function $\mathrm{vol}_n((x + A) \cap B)$ for x ranging along *any* straight line L achieves only *one local maximum* value V_L in *one unique* interval I_L. Therefore, denoting by $V = \max_L V_L$, it follows that $\{x; \mathrm{vol}_n((x + A) \cap B) = V\}$ is a convex set in $\mathbb{R}^n$.

3. It is obvious that the proposition and the remarks above admit generalizations to intersections of convex combinations of an arbitrary number of sets.

As a conclusion of the above theorem, it can now be shown that there is an *achiral* maximal volume overlap of two enantiomorphs of a given convex chiral body D in $\mathbb{R}^2$; this result is due to the fact that $M = M'$ in dimension 2 and follows from:

THEOREM 3

Let $D \subset \mathbb{R}^n$ be a convex body, $n = 2, 3$. The maximum value M' is attained for an achiral intersection.

Proof

Using eqs. (2) and (5) with $U = I$, we have seen that $\mathrm{vol}_n(\Delta) = \mathrm{vol}_n(\Delta') = \mathrm{vol}_n(D \cap \{\Phi(D) - \Phi(b)\})$. Hence, by proposition 1, for any $\lambda \in [0, 1]$ the body

$$\Delta_\lambda = D \cap \{\Phi(D) - \lambda\Phi(b) + (1-\lambda)b\} \tag{22}$$

has volume at least M', hence equal to M' since M' is maximum.

Taking $\lambda = \frac{1}{2}$, and using the fact that $\Phi^2 = I$, we have that the set

$$\Delta_{\frac{1}{2}} - \tfrac{1}{2}b = (D - \tfrac{1}{2}b) \cap (\Phi(D) - \tfrac{1}{2}\Phi(b)) \tag{23}$$

has maximal volume M' and is invariant under the reflection Φ, hence is achiral, implying that $\Delta_{\frac{1}{2}}$ is achiral. Note that in dimension 2, $M = M'$. □

3. Universal bounds for chiral coefficients in all dimensions

The practical calculation of M, M' for chiral bodies is not straightforward and it may require tedious computations. It is, therefore, desirable to derive universal bounds for these values. This can be done for any dimension $n \geqslant 1$, and we now extend the definition of M described by eq. (6) for an arbitrary body $D \subset \mathbb{R}^n$, by

$$M_n(D) = \sup_{\{T \in \mathcal{O}_n; \det(T) = -1\}} \mathrm{vol}_n(D \cap \{T(D) + b\}), \tag{24}$$

where $\mathcal{O}_n$ denotes the group of orthogonal matrices. Note that $M_n(D)$ coincides with the value M defined by eq. (6) for dimensions 2, 3. Set now the *chiral coefficient* of D to be

$$\chi_n(D) = 1 - \frac{M_n(D)}{\mathrm{vol}_n(D)}. \tag{25}$$

Clearly, $0 \leqslant \chi_n(D) < 1$. Note that if n is an odd integer, and if $D = -D$ is a centrally symmetric body in $\mathbb{R}^n$, then $\chi_n(D) = 0$, since we may take $T = -I$ and $b = 0$. In general, we shall call a body $D \subset \mathbb{R}^n$ *achiral* if $\chi_n(D) = 0$. In 2d space this means that Δ coincides with its mirror-image about some line.

A reasonable approach to obtain upper bounds for $\chi_n(D)$ is to find a body K which is contained in D and retains it geometric shape under the application of $T \in \mathcal{O}_n$ satisfying $\det(T) = -1$, so that it is contained in $D^* = T(D)$ as well. Such convenient bodies are ellipsoids in $\mathbb{R}^n$ which are contained in D. Let us now look for the ellipsoid $\mathcal{E}$ (necessarily unique [17] when D is convex), of maximal volume that is contained in D. Since $\mathcal{E}$ retains its shape under all orthogonal transformations, then it is also contained in D^* and as such can be contained intersections between D and D^*, the volume of which must satisfy $\mathrm{vol}_n(\mathcal{E}) \leqslant \mathrm{vol}_n(D \cap D^*)$ and hence

$$\chi_n(D) \leqslant 1 - \frac{\mathrm{vol}_n(\mathcal{E})}{\mathrm{vol}_n(D)}. \tag{26}$$

The value $(\mathrm{vol}_n(D)/\mathrm{vol}_n(\mathcal{E}))^{1/n}$ is defined as the volume ratio of D and is denoted by $\mathrm{vr}(D)$. It was shown by Ball [18] that among all convex bodies D, $\mathrm{vr}(D)$ is maximal if, and only if, D is a tetrahedron. Since $\mathrm{vr}(D) = \mathrm{vr}(A(D))$ for any affine transformation A, we may take the tetrahedron to be the n-dimensional regular tetrahedron $\mathcal{T}_n$ which contains the n-dimensional unit ball B_2^n, where

$$B_2^n = \left\{ x \in \mathbb{R}^n; \sum_{i=1}^{n} x_i^2 \leqslant 1 \right\}. \tag{27}$$

For this case [18],

$$\mathrm{vol}_n(\mathcal{T}_n) = \frac{n^{n/2}(n+1)^{(n+1)/2}}{n!}, \tag{28}$$

$$\mathrm{vol}_n(B_2^n) = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)}, \tag{29}$$

and so [19],

$$\chi_n(D) \leqslant 1 - (\mathrm{vr}(D))^{-n} \leqslant 1 - (\mathrm{vr}(\mathcal{T}_n))^{-n} = 1 - \frac{\mathrm{vol}_n(B_2^n)}{\mathrm{vol}_n(\mathcal{T}_n)} \tag{30}$$

or, for any convex body $D \subset \mathbb{R}^n$

$$\chi_n(D) \leqslant 1 - \frac{\pi^{n/2} n!}{n^{n/2}(n+1)^{(n+1)/2}\Gamma(\frac{n}{2}+1)} \leqslant 1 - \left(\frac{c}{n}\right)^{n/2}, \tag{31}$$

where c is a positive universal constant. In particular, the numerical results for $n = 2, 3$ are

$$\chi_2(D) \leqslant 1 - \frac{\pi}{3\sqrt{3}} = 0.3954\ldots, \tag{32}$$

$$\chi_3(D) \leqslant 1 - \frac{\pi}{6\sqrt{3}} = 0.6977\ldots. \tag{33}$$

In addition to these results it is interesting to compare the upper bound obtained for convex centrally symmetric bodies, in 2-dimensional space. The best upper bound of χ for such a set is [20]

$$\chi_2(D) \leqslant 3 - 2\sqrt{2} = 0.172\ldots. \tag{34}$$

It is interesting to note that the same upper bound $3 - 2\sqrt{2}$ exists also for triangles [21]. This upper bound is considerable less than the value we obtain for a general convex 2-dimensional body.

For odd dimension n, we know that if D is a convex and centrally symmetric body, i.e. $D = -D \subset \mathbb{R}^n$, then $\chi_n(D) = 0$. But for even integers $n \geqslant 4$ it is possible to improve for such bodies the upper bound estimates for $\chi_n(D)$. It was shown by Ball [18] that among such bodies $\mathrm{vr}(D)$ is maximal if and only if D is a parallelepiped. Hence, denoting by Q_n the regular cube, perpendicular edges and side lengths equal to 2, which contains B_2^n, since $\mathrm{vol}_n(Q_n) = 2^n$, we obtain [19] for all centrally symmetric bodies:

$$\chi_n(D) \leqslant 1 - (\mathrm{vr}(D))^{-n} \leqslant 1 - (\mathrm{vr}(Q_n))^{-n} = 1 - \frac{\pi^{n/2}}{2^n\Gamma(\frac{n}{2}+1)}. \tag{35}$$

4. Conclusions

Among the main results of the present article is the one which proves that the maximal overlap of two enantiomorphs of any given *convex* 2-dimensional body is achiral. A special case of this result is the Giering theorem [22] that concerns triangles. It is also shown that this result holds true in dimension 3 as well if the maximal overlap pertains to applications of *mirror images*, where no rotations are allowed. For general bodies, not even necessarily convex or connected, in dimensions 2 and 3, this result is true when the maximal overlap, taken over all reflection, rotations and displacements, is *unique*. The main practical significance of these conclusions is that it may become helpful for the purpose of calculating the degree of chirality of arbitrary bodies in 2d or 3d space.

Another result brought here are upper bound estimates for the chiral coefficients χ_n, being $\chi_2(D) \leqslant 0.3954$ and $\chi_3(D) \leqslant 0.6977$, for all convex bodies D in dimension 2 and 3 respectively. These estimates improve earlier results based upon symmetric polyhedra [23]. We have also obtained universal upper bounds for $\chi_n(D)$ for any dimension n and convex bodies D.

Many of the results obtained in section 2 are readily extendable to n-dimensional spaces, but the physical practicality of the results is obviously limited to $n = 2, 3$ only. The treatment in the present context is applicable only to geometric chiralities. The subject of physical chiralities [3,10] cannot be treated in a similar context since in general a physical chiral set cannot be classified [10] as convex or otherwise. Physical chiralities are more meaningful in the context of "Chiral Interactions" that have been introduced recently [24].

Acknowledgements

The first author (G.G.) wishes to acknowledge helpful discussions with Professors H. Bacry and Y. Benyamini as well as with Dr. A. Resnikov. This research has been supported for both authors by the Fund for the Promotion of Research at the Technion.

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