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Chirality and general aspects of symmetry

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Abstract

The phenomenon of chirality is described in terms of symmetry and *via* symmetry operators.

1. Introduction

Since the time that Lord Kelvin (1904) coined chirality as a property of an object to be nonsuperposable on its mirror image, the formal basis of this phenomenon still remains unclarified despite the unique clarity of the definition and the ready possibility of its instrumental and visual (!) recording in most cases. The above definition of chirality is, as before, its only reliable formal diagnostic criterion; however, it is very difficult to find an algorithm for such a criterion. So far the qualitative estimation of chirality has been reduced to the determination of the sign. As to its quantitative estimation (Ruch, 1975; Richter *et al.*, 1973; Damhus & Schäffer, 1983; Kuz'min & Stel'makh, 1987*a*,*b*, 1989; Kuz'min *et al.*, 1990; Kutulya *et al.*, 1990, 1992; Zabrodsky *et al.*, 1992, 1993, 1995*a*,*b*; Moreau, 1997; Maruani *et al.*, 1994; Thomas *et al.*, 1990), no common approach has been developed as yet. The most sophisticated and universal methods (Kuz'min & Stel'makh, 1987*a*,*b*, 1989; Kuz'min *et al.*, 1990; Kutulya *et al.*, 1990, 1992; Zabrodsky *et al.*, 1992, 1993, 1995*a*,*b*; Moreau, 1997) do not give unambiguous results, whereas the methods producing unambiguous results (Ruch, 1975; Richter *et al.*, 1973; Damhus & Schäffer, 1983; Maruani *et al.*, 1994; Thomas *et al.*, 1990) lack universalism. We believe that such a state of the art is to a large extent due to the traditionally *negative* approach to chirality (Nogradi, 1984; Sokolov, 1979) through the *absence* of mirror planes, rotation–reflection axes and a center of inversion. The inefficiency of this approach has already been noted in the literature (Nikanorov, 1987). At the same time, even Pasteur (1922) oriented the researchers to a *positive* approach to chirality, *i.e.* to search for such factors for which *the presence but not the absence* of this phenomenon is due.

In this work, we reveal and analyze only those factors that are inherent in any object of any nature, no matter whether it is chiral or achiral and symmetric or asymmetric. We will show that this is quite sufficient for both the formal diagnosis of chirality and its qualitative and quantitative estimation.

2. Basic attributes of a figure and protosymmetry

Let us be given an arbitrary object which will be called a *figure*. A figure of *topological* dimensionality 3, 2, 1 or 0 will be called a *solid*, a *surface*, a *curvilinear* or a *scattered* figure, respectively. Let us denote coordinates of a point belonging to a solid, a surface or a curvilinear figure and its radius vector as z_i (where $1 \le i \le 3$) and $\mathbf{r} = \{z_1; z_2; z_3\}$, respectively. Let us denote coordinates of a point belonging to a scattered figure and its radius vector as z_{ki} (where k is the point number) and $\mathbf{r}_k = \{z_{k1}; z_{k2}; z_{k3}\}$, respectively.

Let us be given a scalar variable f, which will be called the *inertial function* of the figure. Let us assign to each point of the figure a certain value f, which will be denoted as $f(\mathbf{r})$; for a scattered figure, it will be denoted as f_k. The role of f can be, for example, the mass- or charge-distribution density at a point (the mass or charge of each point for a scattered figure). In the case of purely geometric considerations, the f parameter is dimensionless and has the same value for all points (for simplicity and without losing generality we suppose it to be equal to unity).

Let us consider the integral inertial parameters of solid (a), surface (b), curvilinear (c) and scattered (d) figures:

1. Parameter U, which is independent of the choice of the coordinate system; hereafter, it will be called the *independent parameter*,

$$U = \int_V f(\mathbf{r})\,\mathrm{d}v \tag{1a}$$

$$U = \int_S f(\mathbf{r})\,\mathrm{d}s \tag{1b}$$

$$U = \int_L f(\mathbf{r})\,\mathrm{d}l \tag{1c}$$

$$U = \sum_k f_k. \tag{1d}$$

2. Static moments M_i,

$$M_i = \int_V f(\mathbf{r}) z_i \, \mathrm{d}v \tag{2a}$$

$$M_i = \int_S f(\mathbf{r}) z_i \, \mathrm{d}s \tag{2b}$$

$$M_i = \int_L f(\mathbf{r}) z_i \, \mathrm{d}l \tag{2c}$$

$$M_i = \sum_k f_k z_k. \tag{2d}$$

3. Moments of inertia W_{ij},

$$W_{ij} = \int_V f(\mathbf{r}) z_i z_j \, \mathrm{d}v \tag{3a}$$

$$W_{ij} = \int_S f(\mathbf{r}) z_i z_j \, \mathrm{d}s \tag{3b}$$

$$W_{ij} = \int_L f(\mathbf{r}) z_i z_j \, \mathrm{d}l \tag{3c}$$

$$W_{ij} = \sum_k f_k z_{ki} z_{kj}. \tag{3d}$$

Obviously, in the general case a figure can be any combination of solid, surface, curvilinear and scattered parts. We will not discuss this circumstance further since it has no fundamental importance. It is as well to keep in mind that in such a case integration of inertial functions for each part of the figure should be performed according to corresponding rules (*a*)–(*d*).

By definition, the moments of inertia W_{ij} (3) are summands of the *positively defined quadratic form* of coordinates. In turn, the moments M_i (2) are summands of the *linear form* of coordinates. At the same time, the definition of the independent parameter U (1) contains no coordinates as factors, or, equivalently, it contains the *zeroth* powers of coordinates as factors, *i.e.* U is the *zeroth form* of coordinates. Thus, the integral inertial parameters 1–3 comprise all stages (including the initial one) of the reduction of positively defined quadratic forms to lower powers. These forms 'are a knot where theory of numbers, algebra, geometry, and crystallography are interlaced' (Galiulin, 1984), *i.e.* the disciplines for which symmetry is one of the most important systemic concepts. Hence, the most important part in our derivations is assigned to the integral inertial parameters.

For a given inertial function, the zeroth, linear and positively defined quadratic forms of the figure coordinates define unambiguously the set of its *basic attributes*. The *first* among them is the zeroth form, *i.e.* the independent parameter U (1).

Together with the terms of the linear form, *i.e.* static moments M_i (2), U defines the *second* basic attribute of a figure, the center of gravity with coordinates

$$c_i = M_i / U. \tag{4}$$

We will also call it the *natural origin* of the figure.

Terms of a positively defined quadratic form, *i.e.* moments of inertia W_{ij} (3), form the tensor of inertia of the figure (Voronkov, 1955)

$$\|W_{ij}\| = \begin{Vmatrix} (W_{22}+W_{33}) & -W_{12} & -W_{13} \\ -W_{21} & (W_{11}+W_{33}) & -W_{23} \\ -W_{31} & -W_{32} & (W_{11}+W_{22}) \end{Vmatrix}. \tag{5}$$

If we bring the center of gravity of the figure into coincidence with the origin, then the eigenvectors $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ of the tensor of inertia (5) will define the directions of the axes known as the *principal central, free or natural axes of inertia*. As is known from the theory of moments of inertia (Voronkov, 1955), any figure for a given inertial function has three mutually perpendicular natural axes of inertia passing through its center of gravity (Fig. 1).

For a particular inertial function, the figure can also have more than three natural axes (*e.g.* in the case of a multiple-thread screw). This circumstance in no way deteriorates the problem being faced. The choice of three natural axes for further derivations (irrespective of the fact whether there is only one set of axes or not) is determined only by the solution of

$$\begin{vmatrix} (W_{22}+W_{33}-\lambda) & -W_{12} & -W_{13} \\ -W_{21} & (W_{11}+W_{33}-\lambda) & -W_{23} \\ -W_{31} & -W_{32} & (W_{11}+W_{22}-\lambda) \end{vmatrix} = 0$$

with respect to λ, which also defines the crystallographic rules of the positioning of the polyhedron.

The unit vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ of vectors $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3$ defined as

$$\mathbf{e}_i = \mathbf{v}_i / |\mathbf{v}_i| \tag{6}$$

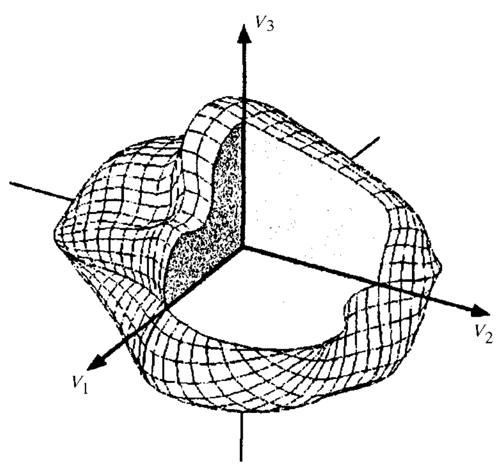

Fig. 1. Natural axes V_1, V_2 and V_3 of an arbitrary figure. Nondiagonal components of the tensor of inertia (5) are equal to zero.

form an orthonormal basis set. This basis set is the *third* basic attribute of the figure. We will call it and vectors $\mathbf{e}_i$ the *natural basis* of the figure and the *natural basis unit vectors*, respectively.

The nonreduced quadratic form of coordinates also defines the *fourth* basic attribute of the figure, *the central ellipsoid of inertia* (Voronkov, 1955). The principal axes a_1, a_2 and a_3 of this ellipsoid are related to the eigenvalues λ_1, λ_2 and λ_3 of tensor of inertia (5) by formula $a_i = \lambda_i^{-1/2}$.

Let us formulate the three basic theorems (Voronkov, 1955; Smirnov, Evtushenko & Lebedev, 1997). We shall not give their proofs (Smirnov, Evtushenko & Lebedev, 1997) here.

Theorem 1. If a figure has a center of inversion, then it coincides with the center of gravity of the given figure.

It follows from this theorem that no point other than the center of gravity (the natural origin) of the figure can be its center of inversion. Therefore the center of gravity of the figure is its unambiguously defined prototype of the center of inversion.

Theorem 2. If a figure has a rotation (including rotation–reflection) axis of symmetry, then its axis coincides with one of the natural axes of the given figure.

It follows from this theorem that no lines other than the natural axes of the figure can be its rotation (including rotation–reflection) axes of symmetry. Therefore, the natural axes of inertia of the figure are its unambiguously defined prototype of rotation (including rotation–reflection) axes of symmetry.

Theorem 3. If a figure has a mirror plane, then this plane coincides with one of the planes made by the natural axes of inertia of the given figure.

It follows from this theorem that no planes other than planes made by natural axes of the figure can be its mirror planes. Therefore, planes made by the natural axes of the figure are its unambiguously defined prototypes of mirror planes.

Let us formulate general conclusions from Theorems 1–3:

In the absence of a center of inversion, rotation (including rotation–reflection) axes of symmetry and mirror planes, the symmetry of the figure is far from being reduced to the identity transformation. All the symmetry elements mentioned above are conserved as their prototypes. These prototypes are the center of gravity, natural axes of inertia and planes made by these axes.

We will call the prototypes of symmetry elements the elements of *protosymmetry*.

Figuratively speaking, protosymmetry is a frontier that symmetry never surrenders under any circumstances and starting from this frontier it continues up to the $\infty\infty m$ group (the symmetry of a fixed sphere).

Revealing the protosymmetry elements opens the possibility of a successive positive approach to chirality. In our work, a comparative analysis of the parts of a figure, which are situated on the opposite sides of its prototypes (the mirror planes), serves as a basis for this approach.

3. Key indicators of chirality and classification of chirality in accordance with its formal nature

Let us bring the center of gravity of the figure into coincidence with the origin and its natural basis into coincidence with the coordinate basis. Then the planes made by natural axes of inertia will coincide with the coordinate planes and we will call them the *natural coordinate planes* (Smirnov, Lebedev & Evtushenko, 1997*a*). It is evident that any natural coordinate plane P_i, perpendicular to the natural unit vector $\mathbf{e}_i$ (6), divides the figure into two parts. We will call them *natural semifigures* and denote them as $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}_{i2}$. The second index is assigned to a natural semifigure according to the following rules:

$$\text{for } \boldsymbol{\Phi}_{i1},\ \text{all } z_i \geq 0; \quad \text{for } \boldsymbol{\Phi}_{i2},\ \text{all } z_i \leq 0,$$

where z_i is the ith coordinate of a point belonging to the semifigure. Evidently, each P_i defines its own pair $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}_{i2}$ (Fig. 2). It should be emphasized that the term semifigure by no means implies the equality of these parts, though it does not exclude it. We will call $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}_{i2}$ *fixed natural semifigures*. In addition to $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}_{i2}$, the mirror reflection of $\boldsymbol{\Phi}_{i2}$ in P_i ($\boldsymbol{\Phi}'_{i2}$) is required, which will be called the *reflected natural semifigure*.

We turn now to the crucial stage of our constructions, namely, determination of those formal features of $\boldsymbol{\Phi}_{i1}$, $\boldsymbol{\Phi}_{i2}$, and $\boldsymbol{\Phi}'_{i2}$ by which the chirality of the original figure must be determined. We will call these features the *key indicators* of chirality (Smirnov, Lebedev & Evtushenko, 1997*a*).

Let us consider $\boldsymbol{\Phi}_{i1}$, $\boldsymbol{\Phi}_{i2}$ and $\boldsymbol{\Phi}'_{i2}$ to be *independent figures* for each i and to have their *own* sets of basic attributes consisting of independent parameter, center of gravity, natural basis and central ellipsoid of inertia. If P_i is a mirror plane of the original figure, then $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}'_{i2}$ completely coincide. In this case, their uniform basic attributes (independent parameters $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}'_{i2}$, centers of gravity $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}'_{i2}$, natural bases $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}'_{i2}$, and central ellipsoids of inertia $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}'_{i2}$) also completely coincide. If $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}'_{i2}$ do not coincide (even in part), then at least a partial noncoincidence of their uniform basic attributes will necessarily occur. Therefore, the basic attributes of fixed and reflected natural semifigures are key indicators of chirality for the original figure. Since basic attributes of any natural semifigure and those of the original figure comprise all steps of reduction of the positively defined quadratic form of its coordinates to lower powers, the given set of indicators is *complete.*

The natural semifigures are unambiguously defined by basic attributes of the original figure. In turn, the key indicators of chirality are basic attributes of natural semifigures. Therefore, the key indicators of chirality are also basic attributes for the original figure and we will also call them *basic attributes of the second order*.

Since the key indicators of chirality of different kinds (basic attributes of the second order) are not reducible to one another, the formal genesis of chirality is *not uniform*. Therefore, the determination of formal genesis rather than that of the sign (as was accepted until now) should be considered as the qualitative determination of chirality. The genesis is defined by combination of noncoincidences of uniform key indicators. We will call the noncoincidence between the independent parameter of $\mathbf{\Phi}_{i1}$ and the independent parameter of $\mathbf{\Phi}'_{i2}$ the *noncoincidence of the first kind*, the noncoincidence between the center of gravity of $\mathbf{\Phi}_{i1}$ and the center of gravity of $\mathbf{\Phi}'_{i2}$ the *noncoincidence of the second kind*, the noncoincidence between the natural basis of $\mathbf{\Phi}_{i1}$ and the natural basis of $\mathbf{\Phi}'_{i2}$ the *noncoincidence of the third kind* and the noncoincidence between the central ellipsoid of inertia of $\mathbf{\Phi}_{i1}$ and the central ellipsoid of inertia of $\mathbf{\Phi}'_{i2}$ the *noncoincidence of the fourth kind.* All possible combinations of these noncoincidences are listed in Table 1.

The zeroth combination of noncoincidences means achirality of the figure. We will call the chirality due to

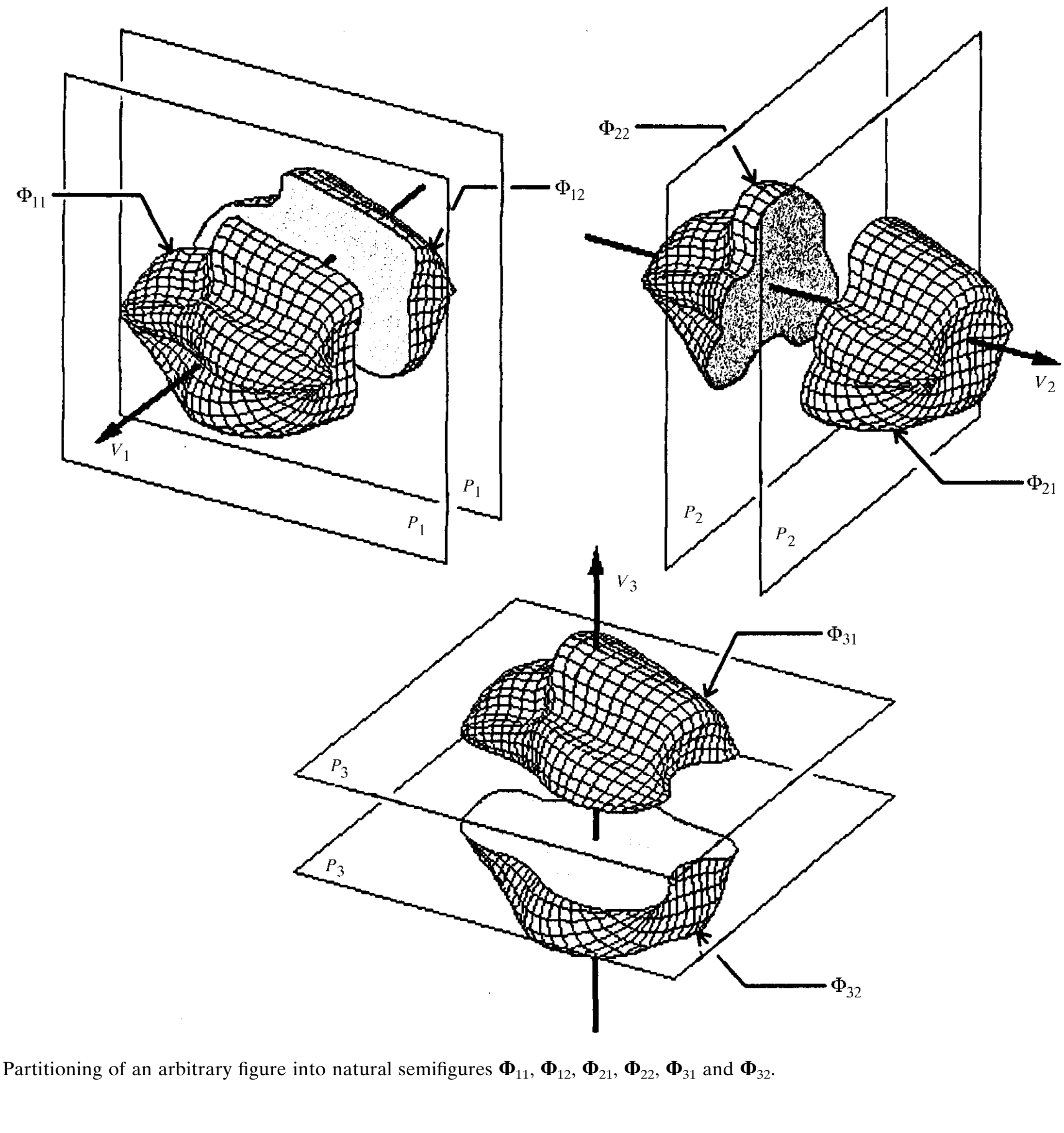

Fig. 2. Partitioning of an arbitrary figure into natural semifigures $\mathbf{\Phi}_{11}$, $\mathbf{\Phi}_{12}$, $\mathbf{\Phi}_{21}$, $\mathbf{\Phi}_{22}$, $\mathbf{\Phi}_{31}$ and $\mathbf{\Phi}_{32}$.

Table 1. *Possible combinations of noncoincidences between uniform key indicators of chirality*

No.	Kinds of non-coincidences	No.	Kinds of non-coincidences	No.	Kinds of non-coincidences	No.	Kinds of non-coincidences	No.	Kinds of non-coincidences
0	Absence of non-coincidences	1	I	5	I, II	11	I, II, III	15	I, II, III, IV
		2	II	6	I, III	12	I, II, IV		
		3	III	7	I, IV	13	I, III, IV		
		4	IV	8	II, III	14	II, III, IV		
				9	II, IV				
				10	III, IV				

only one of combinations 1–4 *homogeneous* chirality and the chirality due to any of the combinations 5–15 *heterogeneous* chirality.

The entire formal genesis of chirality is reduced to combinations 1–4. All possible *qualitative* differences between chiral objects (for the same inertial function) are reduced to combinations 1–15. Therefore, a quantitative estimation of chirality for any object in the framework of a given inertial function should be performed separately for each kind of noncoincidence.

We will call the chirality due to noncoincidences of the first kind *chirality of the first kind*, the chirality due to noncoincidences of the second kind *chirality of the second kind etc.*

It is evident that even if chirality of each kind is a scalar (*i.e.* a zeroth-rank tensor) and is described by a single number, then four (!) numbers rather than one (as previously: Kuz'min & Stel'makh, 1987*a*,*b*, 1989; Stel'makh & Kuz'min, 1987; Kuz'min *et al.*, 1990; Kutulya *et al.*, 1990, 1992; Zabrodsky *et al.*, 1992, 1993, 1995*a*,*b*; Thomas *et al.*, 1990) are required to completely describe the chirality in this (the simplest) case. We shall see later the actual ranks of tensors describing different kinds of chirality.

To this point, only a mirror plane was used as an achiralizing symmetry element. The use of a rotation–reflection axis will be discussed after solving basic problems related to the mirror plane. In this way, we will convince ourselves that such a sequence in considering the problem is reasonable. There will be no special discussion on the center of inversion since inversion is tantamount to a twofold rotation–reflection axis.

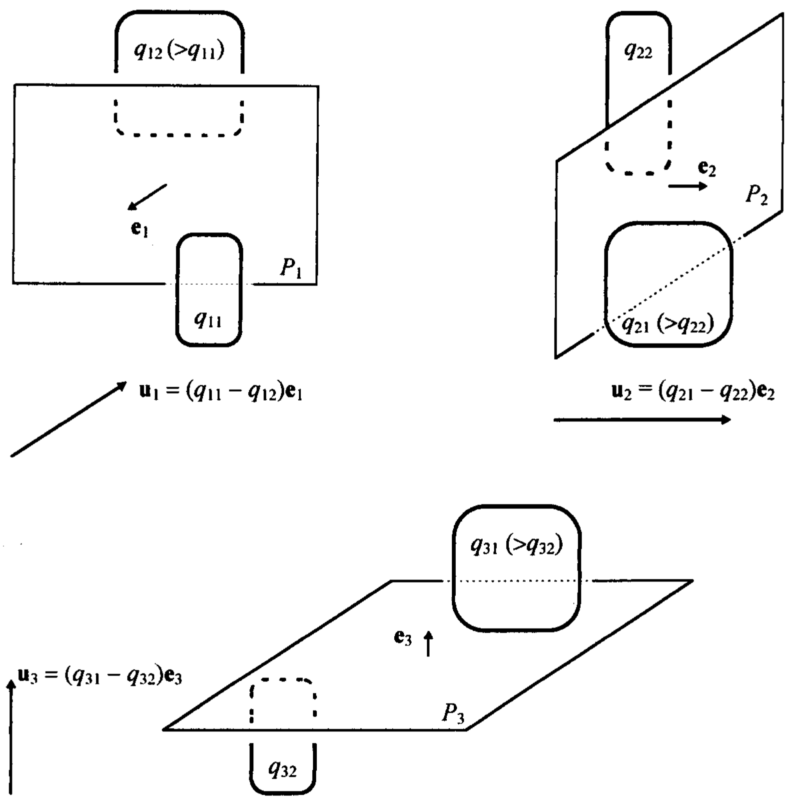

Fig. 3. The genesis of chirality in distribution. The $q_{i1,2}$ values are the values of an independent parameter for natural semifigures situtated on the opposite sides of the natural coordinate planes P_i.

4. Quantitative definition of chirality of the first kind

Let a figure having a given inertial function be divided into natural semifigures $\mathbf{\Phi}_{i1}$ and $\mathbf{\Phi}_{i2}$ by its natural coordinate plane (prototype of the mirror plane) P_i, perpendicular to the natural basis unit vector $\mathbf{e}_i$. Let the value of the independent parameter for the whole figure be U, while the values of the same parameter for $\mathbf{\Phi}_{i1}$ and $\mathbf{\Phi}_{i2}$ are q_{i1} and q_{i2}, respectively (Fig. 3). Obviously, the independent parameter has one (and the same) value for both $\mathbf{\Phi}_{i2}$ and $\mathbf{\Phi}'_{i2}$. Therefore, we will do without reflecting $\mathbf{\Phi}_{i2}$ in P_i. Let us define the vector $\mathbf{u}_i$ for each i:

$$\mathbf{u}_i = \Delta U_i \mathbf{e}_i, \tag{7}$$

where $\Delta U_i = q_{i1} - q_{i2}$, and call it the *inertial deviations for* P_i. By definition, the vectors $\mathbf{u}_i$ form an orthogonal basis. Therefore, the determinant

$$Q = \begin{vmatrix} u_{11} & 0 & 0 \\ 0 & u_{22} & 0 \\ 0 & 0 & u_{33} \end{vmatrix}, \tag{8}$$

where $u_{ii} = \Delta U_i$ is the ith coordinate of $\mathbf{u}_i$ [obviously, by virtue of definition (7) every $u_{ij\neq i} = 0$] and is equal to zero if and only if at least one of $\mathbf{u}_i$ equals zero. The latter is valid if and only if the figure is divided into two parts equivalent in a given independent parameter by at least one of P_i. It is apparent that it always occurs when P_i is a mirror plane of the figure and, thus, the figure is achiral. If no one P_i divides the figure into parts equivalent in the given parameter, then $Q \neq 0$ and this is a *diagnostic criterion* for reflection–asymmetric (chiral) distribution of the given parameter over the figure considered.

Let us use the determinant Q of equation (8) as the basis for a quantitative estimation of chirality of the first kind. We will also call this kind of chirality the *distributive chirality* or the *chirality in distribution* and will use the symbol $\boldsymbol{\chi}$; with the upper right index d.

Next, it is natural to specify the quantitative characteristic of chirality in such a way that it would be dimensionless and the same for any two similar figures. To this end, it is sufficient to use the Q' value defined as

$$Q' = \begin{vmatrix} u_{11} & 0 & 0 \\ 0 & u_{22} & 0 \\ 0 & 0 & u_{33} \end{vmatrix} U^{-3} = Q/U^3 \tag{9}$$

rather than the determinant Q. It is evident that Q' is dimensionless, has the same value for any two similar figures and $-1 \leq Q' \leq 1$.

Let us return to expression (8) and reduce it to the two-dimensional case. Then (8) takes the form

$$Q = \begin{vmatrix} u_{11} & 0 \\ 0 & u_{22} \end{vmatrix}.$$

It can easily be seen that in this case Q is the coordinate of the vector product

$$[\mathbf{u}_1 \times \mathbf{u}_2] = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ u_{11} & 0 & 0 \\ 0 & u_{22} & 0 \end{vmatrix} = \{0; 0; Q\} = Q\mathbf{e}_3. \tag{10}$$

Thus, the distributive chirality of a two-dimensional figure is a vector directed along an axis perpendicular to the plane of the given figure, *i.e.* lying in the *third* dimension.

Extending (10) to the three-dimensional case and taking into account condition (9), we finally define the distributive chirality as the vector

$$\boldsymbol{\chi}^d = \overrightarrow{\chi}^d = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 & \mathbf{e}_4 \\ u_{11} & 0 & 0 & 0 \\ 0 & u_{22} & 0 & 0 \\ 0 & 0 & u_{33} & 0 \end{vmatrix} U^{-3}$$
$$= \{0; 0; 0; Q'\} = Q'\mathbf{e}_4. \tag{11}$$

By definition (11), the vector $\boldsymbol{\chi}^d$ is dimensionless, its absolute value does not exceed unity and in the case of a k-dimensional chiral-in-distribution figure it lies completely in the $(k+1)$th dimension. For the two- and one-dimensional cases, (11) takes the forms

$$\boldsymbol{\chi}^d = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ u_{11} & 0 & 0 \\ 0 & u_{22} & 0 \end{vmatrix} U^{-2} = \{0; 0; Q'\} = Q'\mathbf{e}_3$$

and

$$\boldsymbol{\chi}^d = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 \\ u_{11} & 0 \end{vmatrix} U^{-1} = \{0; Q'\} = Q'\mathbf{e}_2,$$

respectively.

For an arbitrary k-dimensional case, the distributive chirality is defined as

$$\boldsymbol{\chi}^d = \overrightarrow{\chi}^d = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \dots & \mathbf{e}_k & \mathbf{e}_{k+1} \\ u_{11} & 0 & \dots & 0 & 0 \\ 0 & u_{22} & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & u_{kk} & 0 \end{vmatrix} U^{-k}$$
$$= \{0; 0; \dots; 0; Q'\} = Q'\mathbf{e}_{k+1}. \tag{12}$$

Thus, even for the simplest case of scalar key indicators, chirality appears to be a *vector* (*i.e.* a first-rank tensor) *but not a scalar*. Nevertheless, since for any number of dimensions (k), $\boldsymbol{\chi}^d$ (12) can have only one nonzero coordinate, namely the $(k+1)$th, it is possible to apply not only relations ‘equal’ and ‘not equal’ but also relations ‘more’ and ‘less’ to corresponding vectors $\boldsymbol{\chi}^d$ when comparing any two k-dimensional figures in distributive chirality.

5. Quantitative definition of chirality of the second kind

Let the natural coordinate plane $P_i \perp \mathbf{e}_i$ divide the figure into natural semifigures $\mathbf{\Phi}_{i1}$ and $\mathbf{\Phi}_{i2}$. Let us denote the radius vectors of their centers of gravity as $\mathbf{r}_{i1}$ and $\mathbf{r}_{i2}$, respectively, and the radius vector of the center of gravity of reflected natural semifigure $\mathbf{\Phi}'_{i2}$ as $\mathbf{r}'_{i2}$ (Fig. 4). Let us define vector $\mathbf{g}_i$ for each i, which will be called the *deviation of the centers of gravity for* P_i (Smirnov, Lebedev & Evtushenko, 1997*b*):

$$\mathbf{g}_i = \mathbf{r}'_{i2} - \mathbf{r}_{i1}. \tag{13}$$

Let us use the determinant G of a matrix formed by the components g_{ij} of vectors $\mathbf{g}_i$ (13) as the basis for a quantitative estimation of chirality of the second kind:

$$G = \begin{vmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{vmatrix}. \tag{14}$$

It is evident that $G \neq 0$ if and only if the $\mathbf{g}_i$ are linearly independent. Otherwise, no chirality of the second kind occurs. However, it is impossible to be sure of it by inspecting any one of vectors $\mathbf{g}_i$ (except for cases when at least one of them equals zero). That is why the G value (14) characterizing the totality of $\mathbf{g}_i$ rather than just one of them should be used for quantitative estimation of chirality of the second kind.

As in the case of chirality of the first kind, it is natural to aim at using a dimensionless quantitative measure of chirality with the same values for any two similar figures. To this end, we will use a dimensionless quantity G' instead of G:

$$G' = G/g_1g_2g_3, \tag{15}$$

where $g_i = |\mathbf{g}_i|$. Note that the denominator in (15) is equal to the volume of a *rectangular* parallelepiped with edges equal to g_i, whereas G (14) is the volume of a parallelepiped constructed on the edges of vectors $\mathbf{g}_i$ taking into account their directions and can be either

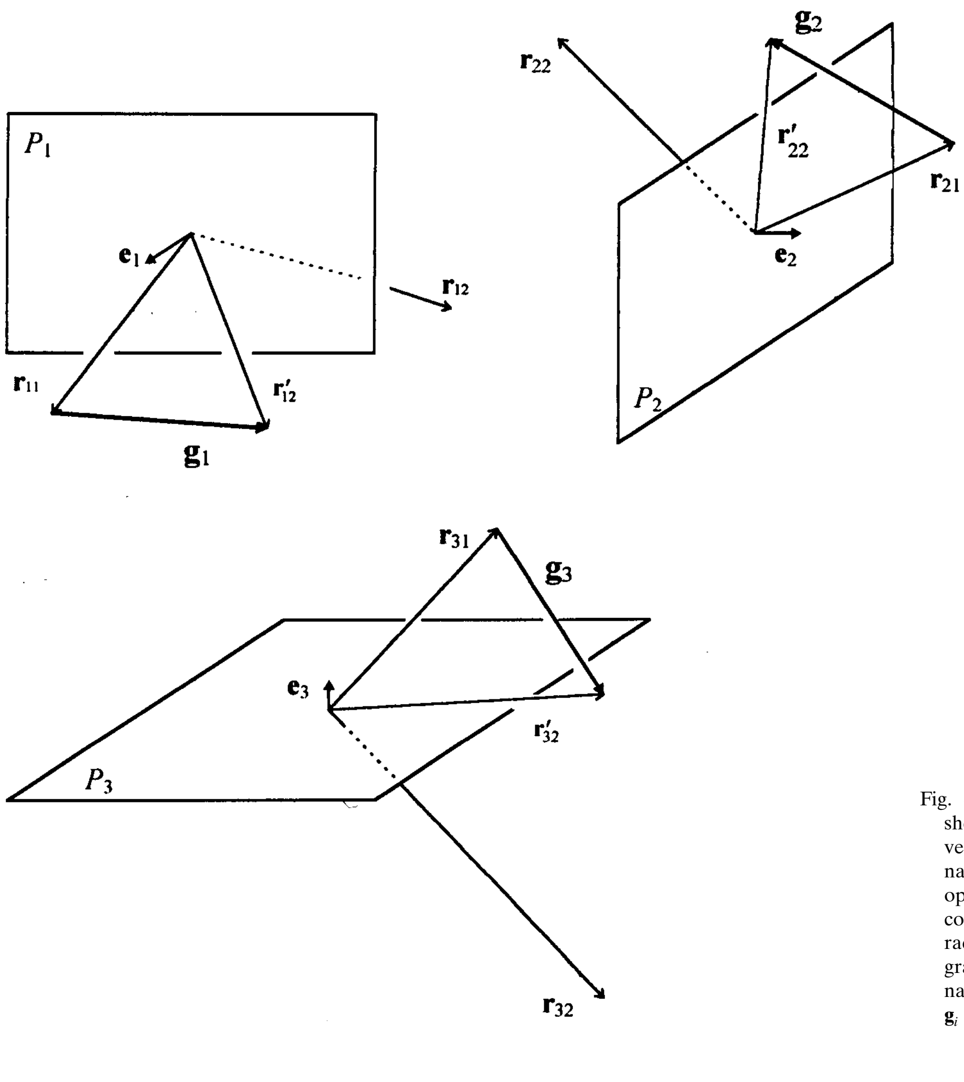

Fig. 4. The genesis of chirality in shear: $\mathbf{r}_{i1}$ and $\mathbf{r}_{i2}$ are the radius vectors of the centers of gravity of natural semifigures situated on the opposite sides of the natural coordinate planes P_i, $\mathbf{r}'_{i2}$ are the radius vectors of the centers of gravity of the corresponding natural reflected semifigures and $\mathbf{g}_i = \mathbf{r}'_{i2} - \mathbf{r}_{i1}$.

positive or negative. Thus, G' is the ratio of the volume of the second parallelepiped to the volume of the first one (*i.e.* the *Staudt sine* of a three-hedral angle based on vectors $\mathbf{g}_i$) and, hence, $-1 \le G' \le 1$. By virtue of the definition of G [equation (14)], $|G'| = 1$ if and only if vectors $\mathbf{g}_i$ [equation (13)] form an orthogonal basis.

Let us draw attention to the fact that any of the parallelepipeds mentioned above is derived from another by shear deformation. Therefore, we will also call the chirality of the second kind the *shear chirality* or the *chirality in shear* and will use the symbol $\boldsymbol{\chi}$ with the upper right index s.

Let us return again to expression (14). We draw attention to the fact that the matrix in this expression only differs from those in (8) and (9) in (generally) nonzero off-diagonal components, whereas they are always equal to zero in (8) and (9). Hence, it is possible to exactly apply all arguments and mathematics concerning the distributive chirality, which follow expression (9), to the shear chirality and restrict ourselves here to the general formula of shear chirality for an arbitrary k-dimensional case:

$$\boldsymbol{\chi}^s = \overrightarrow{\chi}^s = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \cdots & \mathbf{e}_k & \mathbf{e}_{k+1} \\ g_{11} & g_{12} & \cdots & g_{1k} & 0 \\ g_{21} & g_{22} & \cdots & g_{2k} & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ g_{k1} & g_{k2} & \cdots & g_{kk} & 0 \end{vmatrix} (g_1 g_2 \cdots g_k)^{-1}$$
$$= \{0; 0; \ldots; 0; G'\} = G'\mathbf{e}_{k+1}. \quad (16)$$

6. Chiral size and chiral gap

Let us draw attention to the fact that, by virtue of definitions (12) and (16), vectors $\boldsymbol{\chi}^d$ and $\boldsymbol{\chi}^s$ are not only directed along the same coordinate axis but have the same dimensionalities (both of them are dimensionless). For this reason, both the congruence and the addition and subtraction operations are defined for these vectors.

In this connection, let us consider the coordinate Q' of vector $\boldsymbol{\chi}^d$ and coordinate G' of vector $\boldsymbol{\chi}^s$. We will call the greater of them the *upper chiral level* and the lesser one the *lower chiral level* and denote them as $B^{\chi}_{\max}$ and $B^{\chi}_{\min}$, respectively. We will call the difference

$$D^{\chi} = B^{\chi}_{\max} - B^{\chi}_{\min} \quad (17)$$

the *chiral size* of the figure. It is evident that $D^{\chi} = 0$ if and only if $\boldsymbol{\chi}^d = \boldsymbol{\chi}^s$. We will call such figures *chirally planar figures*. If $\boldsymbol{\chi}^d \neq \boldsymbol{\chi}^s$, they will be called *chirally nonplanar figures*. Obviously, a chirally planar figure is achiral in both distribution and shear if and only if $\boldsymbol{\chi}^d = \boldsymbol{\chi}^s = 0$.

We will call parallel planes perpendicular to the $(k+1)$th coordinate axis and defined by normal equations

$$\begin{cases} \mathbf{r} \cdot \boldsymbol{\chi}^d = Q'^2 \\ \mathbf{r} \cdot \boldsymbol{\chi}^s = G'^2 \end{cases} \quad (18)$$

the *chiral boundaries* of the figure. We will call chiral boundaries (18) corresponding to $B^{\chi}_{\max}$ and $B^{\chi}_{\min}$ the *upper and lower chiral boundary*, respectively. We will call the span between the chiral boundaries of a figure the *chiral gap* of the figure. It is apparent that the width of the chiral gap for any figure is equal to its chiral size (17) and at $\boldsymbol{\chi}^d = \boldsymbol{\chi}^s$ the chiral boundaries of the figure coincide.

Thus, the extension of any k-dimensional object in the $(k+1)$th dimension is equal to its chiral size. In this case, any point of the object is either inside its chiral gap or on one of its chiral boundaries (Fig. 5). In the case of arbitrary k-dimensional movement of a fixed k-dimensional object, the trajectory of any of its points in the $(k+1)$-dimensional space is either parallel to its chiral boundaries or entirely lies on one of the latter.

It should be added that our conclusions that the distributive and shear chiralities of k-dimensional objects have the $(k+1)$-dimensional nature are partly in line with the results obtained by Heesch (1930) in the field of color symmetry.

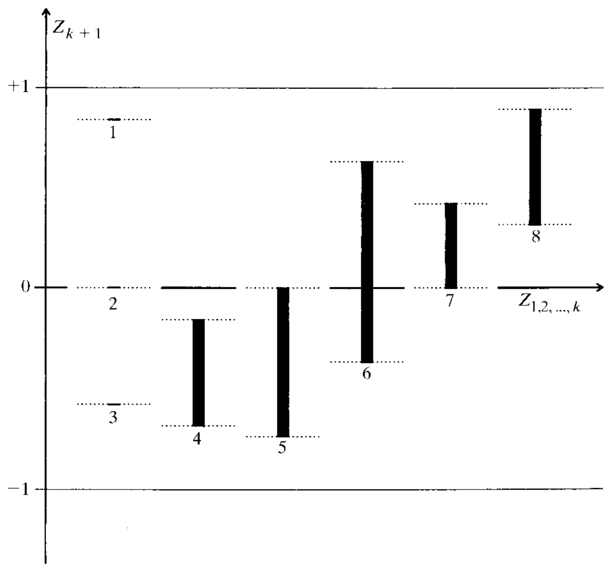

Fig. 5. Possibilities of arranging k-dimensional objects in the $(k+1)$th-dimensional space. The direction of incidence is perpendicular to the $(k+1)$th coordinate axis and is parallel to the plane made by the first k coordinate axes. The chiral boundaries of each object are shown by dotted lines. 1–3: chirally planar objects; 4–8: chirally nonplanar objects.

7. Quantitative definition of chirality of the third kind

Let a natural coordinate plane $P_i \perp \mathbf{e}_i$ divide a figure into natural semifigures $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}_{i2}$. As in the case of chirality of the second kind, let us compare $\boldsymbol{\Phi}_{i1}$ and the reflected natural semifigure $\boldsymbol{\Phi}'_{i2}$. Let us denote the natural basis unit vectors for $\boldsymbol{\Phi}_{i1}$ as $\mathbf{o}_{i1}$, $\mathbf{o}_{i2}$ and $\mathbf{o}_{i3}$ and those for $\boldsymbol{\Phi}'_{i2}$ as $\mathbf{o}'_{i1}$, $\mathbf{o}'_{i2}$ and $\mathbf{o}'_{i3}$. Let us bring the origins of these bases into coincidence by translation (Smirnov, Lebedev & Evtushenko, 1997*c*). Each vector $\mathbf{o}'_{ik}$ makes an angle with each of the vectors $\mathbf{o}_{ij}$ (Fig. 6). As a whole, three vectors $\mathbf{o}'_{ik}$ make nine angles with three vectors $\mathbf{o}_{ij}$. Let us use the operator

$$\mathbf{X}_i^r = \begin{pmatrix} \chi^r_{i11} & \chi^r_{i12} & \chi^r_{i13} \\ \chi^r_{i21} & \chi^r_{i22} & \chi^r_{i23} \\ \chi^r_{i31} & \chi^r_{i32} & \chi^r_{i33} \end{pmatrix}, \tag{19}$$

where $\chi^r_{ijk} = (\mathbf{o}'_{ik} \cdot \mathbf{o}_{ij})$ is the cosine of an angle between $\mathbf{o}'_{ik}$ and $\mathbf{o}_{ij}$, as the basis for a quantitative estimation of chirality of the third kind. Operator (19) along with analogous operators for two other prototypes of mirror planes forms a third-rank tensor

$$\|\chi^r_{ijk}\| = \begin{Vmatrix} \chi^r_{111} & \chi^r_{112} & \chi^r_{113} & \chi^r_{211} & \chi^r_{212} & \chi^r_{213} & \chi^r_{311} & \chi^r_{312} & \chi^r_{313} \\ \chi^r_{121} & \chi^r_{122} & \chi^r_{123} & \chi^r_{221} & \chi^r_{222} & \chi^r_{223} & \chi^r_{321} & \chi^r_{322} & \chi^r_{323} \\ \chi^r_{131} & \chi^r_{132} & \chi^r_{133} & \chi^r_{231} & \chi^r_{232} & \chi^r_{233} & \chi^r_{331} & \chi^r_{332} & \chi^r_{333} \end{Vmatrix}. \tag{20}$$

It is obvious that operator (19) is nothing but an operator of rotation. That is why the upper right index r was used for denoting operator (19), tensor (20) and their components. We will also call the chirality of the third kind the *rotation chirality*, or *chirality in rotation*.

If P_i is the mirror plane of the figure, then natural bases $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}'_{i2}$ coincide. Then, operator (19) has a *degenerate* form

$$\mathbf{X}_i^r = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{21}$$

The presence of at least one block of type (21) in tensor (20) is a diagnostic criterion for achirality of the figure in rotation.

8. Quantitative definition of chirality of the fourth kind

Let a natural coordinate plane $P_i \perp \mathbf{e}_i$ divide a figure into natural semifigures $\boldsymbol{\Phi}_{i1}$ and $\boldsymbol{\Phi}_{i2}$. Let us compare the

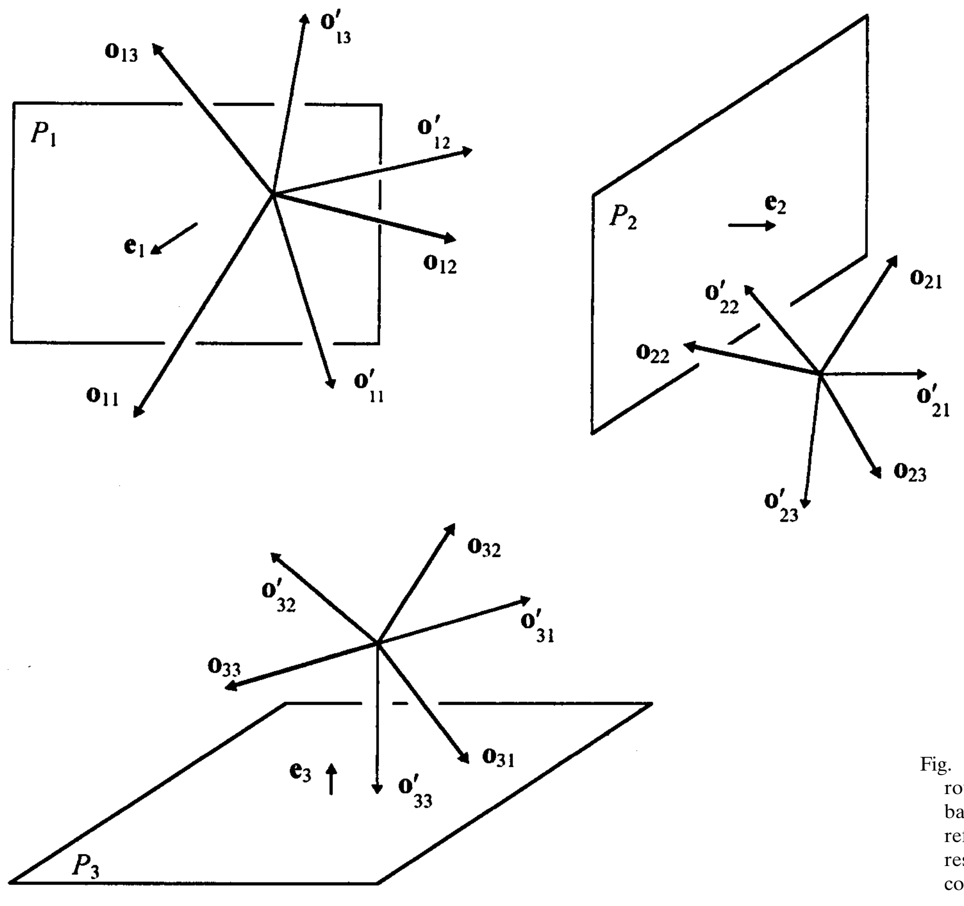

Fig. 6. The genesis of chirality in rotation: $\mathbf{o}_{ij}$ and $\mathbf{o}'_{ik}$ are natural basis unit vectors of a fixed and reflected natural semifigure, respectively, defined by natural coordinate planes P_i.

central ellipsoids of inertia $\mathbf{\Phi}_{i1}$ and $\mathbf{\Phi}'_{i2}$ (Fig. 7). It will be recalled that the inverse square of the principal axis a_i of such an ellipsoid is the corresponding eigenvalue λ_i of the tensor of inertia of the corresponding figure (in this case of the natural semifigure). Here we will use the eigenvalues of tensors of inertia (Smirnov, Lebedev & Evtushenko, 1997*d*). Let them be λ_{I1}, λ_{i2} and λ_{i3} for $\mathbf{\Phi}_{i1}$ and λ'_{I1}, λ'_{I2} and λ'_{I3} for $\mathbf{\Phi}'_{i2}$.

Any ellipsoid is transformed into any other ellipsoid by tension compression along the principal axes (so-called normal deformations). Therefore, we will also call the chirality of the fourth kind *normal chirality* or the *chirality in tension compression* and will use the index n for its notation. Let us use the operator

$$\mathbf{X}_i^n = \begin{pmatrix} \chi_{i11}^n & 0 & 0 \\ 0 & \chi_{i22}^n & 0 \\ 0 & 0 & \chi_{i33}^n \end{pmatrix}, \quad (22)$$

where

$$\chi_{ijj}^n = \tanh\{[\lg(\lambda_{ij}/\lambda'_{ij})]/2\} \quad (23)$$

as the basis for its quantitative estimation. Formula (23) is suggested for determination of the diagonal components of operator (22) from considerations of:

1. monotonicity: if $x_1 > x_2$, then $\tanh(\lg x_1) > \tanh(\lg x_2)$;
2. oddness: $\tanh(-x) = -\tanh x$, $\lg(x_2/x_1) = -\lg(x_1/x_2)$;
3. boundedness in the absolute value: $-1 < \tanh x < 1$.

In special cases (points of discontinuity), χ'_{ijj} is defined as follows:

1. if $\lambda_{ij} = 0 = \lambda'_{ij}$, then $\chi_{ijj}^n = 0$;
2. if $\lambda_{ij} = 0 \neq \lambda'_{ij}$, then $\chi_{ijj}^n = -1$;
3. if $\lambda_{ij} \neq 0 = \lambda'_{ij}$, then $\chi_{ijj}^n = 1$.

Operator (22) together with analogous operators for two other prototypes of mirror planes forms a third-rank tensor

$$\|\chi_{ijk}^n\| = \left\| \begin{matrix} \chi_{111}^n & 0 & 0 & \chi_{211}^n & 0 & 0 & \chi_{311}^n & 0 & 0 \\ 0 & \chi_{122}^n & 0 & 0 & \chi_{222}^n & 0 & 0 & \chi_{322}^n & 0 \\ 0 & 0 & \chi_{133}^n & 0 & 0 & \chi_{233}^n & 0 & 0 & \chi_{333}^n \end{matrix} \right\|. \quad (24)$$

If P_i is a mirror plane of the figure, then operator (22) takes the degenerate form

$$\mathbf{X}_i^n = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (25)$$

The presence of at least one block of type (25) in tensor (24) is a diagnostic criterion for achirality of the figure in tension compression.

9. The rotation–reflection axis as achiralizing symmetry element

Now we will consider a natural axis of inertia as a prototype of a rotation–reflection symmetry axis.

Let a figure have a rotation–reflection axis of order $2n$ (n is an integer) defined by the natural basis unit vector $\mathbf{e}_i$. Then, a fixed natural semifigure $\mathbf{\Phi}_{i2}$ is the mirror reflection of the fixed natural semifigure $\mathbf{\Phi}_{i1}$ in the natural coordinate plane $P_i \perp \mathbf{e}_i$ rotated about $\mathbf{e}_i$ by an angle $\theta = 2\pi/2n = \pi/n$. It is easy to check that in this case $\boldsymbol{\chi}^d = \boldsymbol{\chi}^s = 0$, the operator of normal chirality $\mathbf{X}_i^n$ (22) has the degenerate form (25), and the operator of rotation chirality $\mathbf{X}_i^r$ (19) has one of partially degenerate form:

$$\mathbf{X}_1^r = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{pmatrix},$$
$$\mathbf{X}_2^r = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}, \quad (26)$$
$$\mathbf{X}_3^r = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus, the rotation–reflection axis acting as an achiralizing symmetry element adds to our results only partially degenerate forms (26) of operators $\mathbf{X}_i^r$ as additional diagnostic criteria for achirality.

Eventually, it can be said that the chirality of any fixed object is exhaustively described by the operators of distributive, shear, rotation and normal chiralities suggested above. The components of these operators (a total of 62 in the three-dimensional case including 24

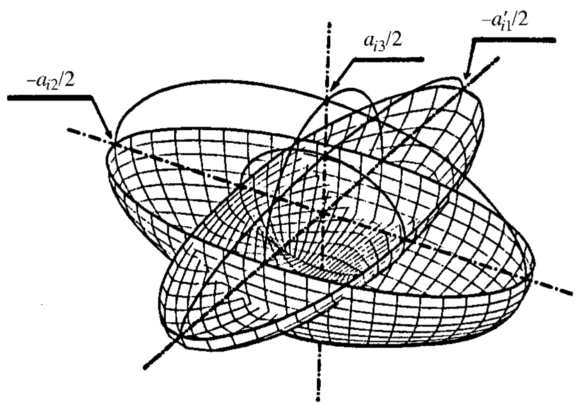

Fig. 7. The genesis of normal chirality: $a_{i1,2,3} = (\lambda_{i1,2,3})^{-1/2}$ and $a'_{i1,2,3} = (\lambda'_{i1,2,3})^{-1/2}$ are the principal axes of the central ellipsoids of inertia (shown in section) of fixed and reflected natural semifigures, respectively, defined by natural coordinate planes P_i. Only visible vertices of the central ellipsoids of inertia are shown.

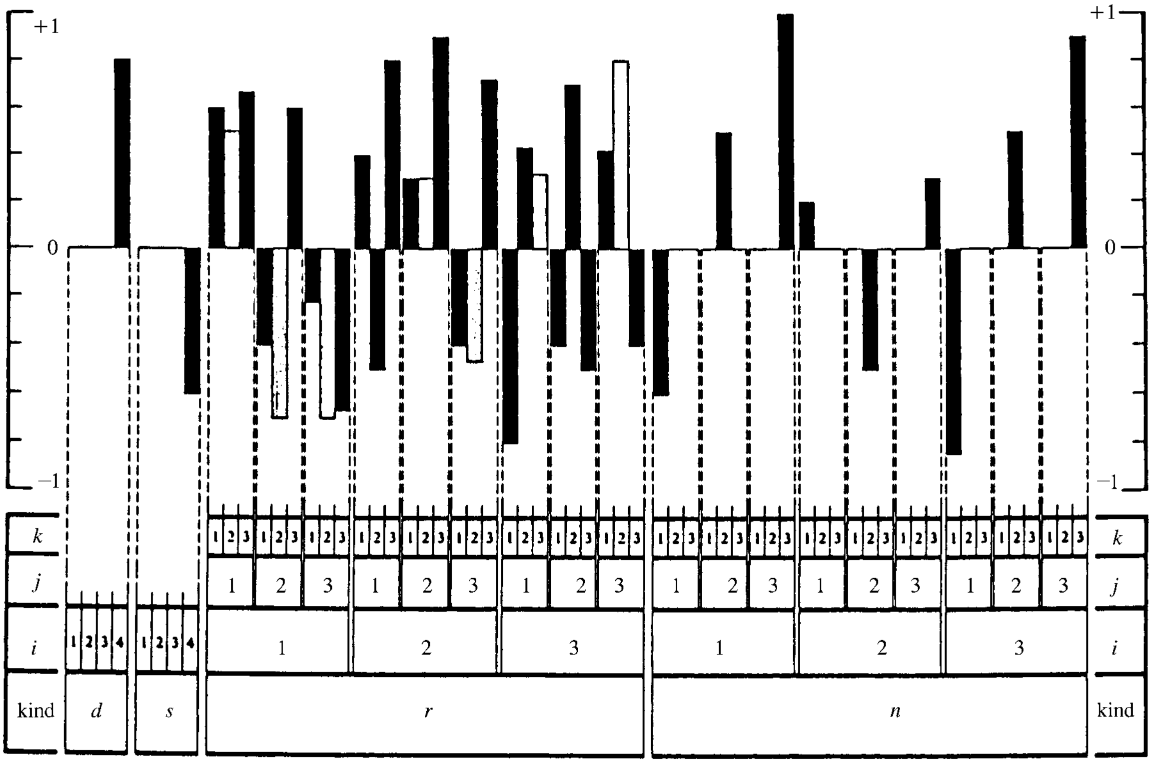

Fig. 8. Spectrum of conventional components of tensors of distributive (d), shear (s), rotational (r) and normal (n) chirality for a conventional object for a conventional inertial function; i, j, k are the component subscripts.

zero components in operators of distributive, shear and normal chiralities) form the complete spectrum of basic chirality constants of a given object for a given inertial function, which is schematically shown in Fig. 8.

10. Chirality as a symmetry phenomenon

So far we used the term operator only with regard to the rotation and normal chiralities. However, this term is equally appropriate when applied to the distributive and shear chiralities. In fact, in the case of a k-dimensional object, vectors $\boldsymbol{\chi}^d$ (12) and $\boldsymbol{\chi}^s$ (16) differ from operators of translation, characteristic of symmetry space groups, only in that the latter operate entirely in the space of dimensions of the object while the former operate along only the $(k+1)$th coordinate axis.

It is obvious that $\boldsymbol{\chi}^d$ and $\boldsymbol{\chi}^s$ as operators of translation and $\mathbf{X}_i^r$ (19) as operators of rotation perform a mutual one-to-one mapping of the space (and of everything associated with this space) onto themselves without changing distances between points (Konovalov & Galiulin, 1989). Hence, by virtue of the definition of symmetry transformations (Konovalov & Galiulin, 1989), the operators of distributive, shear and rotation chiralities are nothing but symmetry operators.

At first glance, the operators of normal chirality $\mathbf{X}_i^n$ (22) are not symmetry operators since, in the general case, tension compression of the space changes distances between points. On the other hand, these operators are formed by finite real numbers (23). Therefore, by virtue of Maschke's theorem (Van der Waerden, 1970),† for any X_i^n, there exists such a coordinate system where a given operator is a symmetry operator.

Thus, we come to the following definition:

Definition 1. The chirality of an object for a given inertial function is the totality of symmetry transformations relating its uniform basic attributes of the second order.

It will be recalled that the statement of the problems for determination of chirality of any finite or infinite object (and, in the general case, the statement of any problems associated with its symmetry) has a sense if and only if an inertial function is given on the object.

The *sufficient condition* of equivalent chirality and, in general, of symmetry of the same object for any two inertial functions is similarity of these functions on the

† For our purposes, the most convenient formulation of this theorem was given by Dr R. V. Galiulin (1984).

object regardless of physical dimensionality of the similarity coefficient.

It should be emphasized that, if one or other kind of deformation or motion (shear, rotation or tension–compression) is specified in the name of chirality, then on no account is deformation or motion of the object in question concerned. Deformation or motion of an abstract figure conjugated with objects is implied: a parallelepiped built on vectors – deviations of the centers of gravity of fixed and reflected natural semifigures, natural bases or central ellipsoids of inertia of natural semifigures.

11. On the types of variables forming symmetry operators

We have established that operators of chirality are nothing but symmetry operators. It is reasonable to discuss in detail differences between their general [equations (11), (16), (19), (22)] and degenerate [$\chi^d = \chi^s = 0$ and equations (21), (25), (26)] forms.

It is easily seen that nonzero components of these operators in their general forms take on *any* values from the segment $[-1; 1]$, whereas in degenerate forms they take on only values of the type

$$\pm\cos(\pi/m) \quad \text{or} \quad \pm\sin(\pi/m), \tag{27}$$

where m is any positive integer including such m as turn these values into either zero or ± 1.

The range of admissible values for the components of achiralizing symmetry operators (mirror reflection, mirror rotation and inversion) is also exhausted by these numbers (27). The components of operators of rotation about a symmetry axis of any rational order p/q, where p and q are any natural numbers, belong to the same type of variables. These components are the real and imaginary parts, respectively, of the roots of equations of the type

$$x^{p/q} = 1. \tag{28}$$

This means that the components of degenerate chirality operators as well as those of achiralizing symmetry operators and of operators of rotation about rational-order symmetry axes are *algebraic* numbers and form an *infinite denumerable* set, whereas the components of chirality operators in nondegenerate (general) forms are *any real* numbers from the segment $[-1; 1]$ and form *a continuum*.

Thus, chirality as nonsuperposability of an object with its mirror reflection exists or does not exist depending on the type of variables forming its operators. It is natural to expect that this is not the only symmetry phenomenon for which this is a defining condition. Therefore, it is reasonable to reflect this condition in terminology. We suggest the symmetry operators formed by real and imaginary parts of numbers x of the type (28) be called the operators of *algebraic* symmetry and symmetry operators formed by any real numbers the operators of *analytical* symmetry (based on the fact that real numbers, continuum and other sets whose power is equal or higher than that of a continuum are objects of mathematical analysis).†

In this connection, it is natural to assume that terms asymmetry and dissymmetry are only traditional notations for all nondegenerate forms of analytical symmetry and the problem of qualitative and quantitative descriptions of the phenomena of such a type using symmetry terms and symmetry operators are reduced to a correct revealing of relevant key indicators.

Eventually, let us note that the degeneration of operators of analytical symmetry and the associated generation of achiralizing symmetry elements is nothing but reduction of the range of admissible values of the components of symmetry operators from a continuum to an infinite denumerable set. In this connection, it is logical to pose a question on the possibility of further reduction of a given set to a finite one.

A positive answer to this question existed long before it had been asked. In fact, in the case of color symmetry (including antisymmetry), there are operators of the type of sign change, recoloration, and similar operators whose components have a trigger character and form *finite* sets (consisting, in the case of antisymmetry, of only two elements). The variables of such a type and the operations performed are the subject of mathematical logic. From this viewpoint, it is reasonable to call the color symmetry (including antisymmetry) the *logical symmetry* and use the laws of mathematical logic when performing corresponding operations.

It should be added that all steps of reduction of a continuum to a finite set are exhausted by the sequence analytical symmetry → algebraic symmetry → logical symmetry that only can be enhanced to the sets whose power is higher than that of continuum and to variables of relevant types.

12. Conclusions

Let us sum up all the work performed without dwelling on particular results.

(*a*) A consecutive positive approach to chirality has been realized based on analysis of those, and only those, factors that are always inherent in any object.

(*b*) Concepts of the minimum level of symmetry have been revised. It has been established that elements of protosymmetry given by inertial parameters of an object are always inherent in any object.

† In our preceding communication (Smirnov, Lebedev & Evtushenko, 1997*d*), we have interpreted analytical symmetry as a generalization of 'traditional' (algebraic) symmetry. Later, Dr R.V. Galiulin called our attention to the fact that nonalgebraic components of symmetry operators do *not* lead to generalization of the symmetry concept (Konovalov & Galiulin, 1989) itself.

(*c*) The inhomogeneity of formal genesis of chirality has been established and all formal factors specifying its presence or absence have been revealed.

(*d*) Rigorous and universal rules for qualitative and quantitative estimations of chirality have been developed.

(*e*) A constructive definition of chirality as a totality of symmetry transformations has been given for the first time and scalar parameters and geometric images related by these transformations have been determined.

(*f*) The existence of symmetry phenomena dependent not only on the structure of corresponding symmetry operators but also on the type of variables forming these operators has been revealed.

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