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ISOSYMMETRIC MANIFOLDS IN FORM SPACES AND THE NORMAL DEFORMATIONS OF POLYGONAL FORMS

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Abstract—Form variations are described in an appropriately constructed form space $\mathbb{F}$ (typically an $\mathbb{R}^n$), where every point of $\mathbb{F}$ represents a different form. Regarding the symmetries of the forms, $\mathbb{F}$ can be divided into disjunct isosymmetric manifolds, i.e., points, lines, surfaces, and volumes whose points correspond to forms with equal symmetries. These manifolds are derived from a symmetry analysis of possible deformations of the forms. This analysis is comparable to the construction of symmetry coordinates in a normal coordinate analysis of molecules and results in normal modes of deformation ("normal deformations") of these forms. From the symmetry species of a normal deformation, the symmetry of the resulting form can be inferred. Transformation of the form space coordinates into normal coordinates (the differentials of which are the normal deformations) facilitates the description of the high-dimensional form spaces and can be made the basis of an easy symmetry diagnosis of forms. Furthermore, the problem of an ascent in symmetry by deformation is discussed.

1. INTRODUCTION

For a biologist, the idea of a variation or evolution of forms of living beings is common. During such a change of form, there will normally also be a change of symmetry of the form. In general, there is a great wealth of possibilities for continuous deformations of a given form, which will either preserve the symmetry (symmetry group) of the original form or lower it to a subgroup of this symmetry (in the extreme case to total asymmetry), or in some rare instances, enhance it to a supergroup of the original symmetry. There is a need for a systematic treatment of the interdependence of the deformation of a form and the corresponding change in its symmetry. This will be done here for two-dimensional polygonal forms by applying to them a method analogous to the construction of symmetry coordinates within the normal coordinate analysis of vibrating molecules and performing a symmetry analysis and classification of the possible deformations of a form.

The variation of a given form by a set of allowed continuous deformations will be treated within a *form space* $\mathbb{F}$ spanned by suitably chosen coordinates. In such a form space, every point represents a different form. Thus, the existence of a continuous symmetry-preserving deformation will give rise to a line of constant symmetry in the form space. A systematic look into such relations will reveal isolated points, lines, surfaces, and volumes—in general: *manifolds*—of constant symmetry within the form space. They will be termed "*isosymmetric manifolds.*"

2. FORM VARIATIONS AND FORM SPACES

In this paper, form variations will be treated as variations of certain continuous parameters x_i (e.g., coordinates). If there are N such parameters, they will span an N-dimensional space $\mathbb{F}$ (see footnote[1]). If every N-tuple of parameter values corresponds to a different form, we have a one-to-one mapping of the possible forms to the points of $\mathbb{F}$ so that $\mathbb{F}$ can be regarded as a *form*

I am deeply indebted to cand. phys. Thomas Köhler for preparing the figures for this paper.
[1]Normally, $\mathbb{F}$ is an $\mathbb{R}^N$ so that $\mathbb{F} = \{\vec{r} = (x_1, \ldots, x_N)^\top \in \mathbb{R}^N\}$.

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space. Each form $\mathfrak{F}$ which is possible under the set of allowed deformations[2] corresponds to a point $P(x_1,\ldots,x_N)$ or vector $\vec{r}=(x_1,\ldots,x_N)^{\mathsf{T}}$ in $\mathbb{F}$, and a form variation $\delta\mathfrak{F}$ can be described as a parameter or coordinate variation $\delta\vec{r}=(\delta x_1,\ldots,\delta x_N)^{\mathsf{T}}$ in $\mathbb{F}$. A form transition $\mathfrak{F}_1\to\mathfrak{F}_2$ is then represented by a trajectory within $\mathbb{F}$.

Some examples of form variations will be sketched now:

(i) In a recent paper [1], I proposed a characterisation of two-dimensional forms by the Fourier coefficients a_k and b_k of their form functions $R(\varphi)$:

$$R(\varphi)=\sum_{k=0}^{K}(a_k\cdot\cos k\varphi+b_k\cdot\sin k\varphi) \tag{1}$$

(R: radius, φ: angle). Here, the a_k's and b_k's span a $(2K+2)$-dimensional real space $\mathbb{F}=\mathbb{R}^{2K+2}$, with K being the maximum number of terms taken in the Fourier series [1]. A continuous form variation can be carried out by varying the Fourier coefficients.

(ii) Another possible form variation described in [1] is a continuous form transition between two forms $\mathfrak{F}_1$ and $\mathfrak{F}_2$ through intermediate forms $\mathfrak{F}_X$ generated by weighted addition of the form functions of $\mathfrak{F}_1$ and $\mathfrak{F}_2$ according to

$$R_X(\varphi)=\beta_1\cdot R_1(\varphi)+\beta_2\cdot R_2(\varphi) \tag{2}$$

(β_1, β_2: weight factors) or by weighted addition of their respective Fourier coefficients ("*mixing* of forms"). In general, if M forms are to be mixed, we have

$$R_X(\varphi)=\sum_{m=1}^{M}\beta_m R_m(\varphi) \tag{3}$$

and, if only relative positive weights are meaningful,

$$\sum_m \beta_m=1. \tag{4}$$

Then, the appropriate form space for the mixing of M forms is the *simplex* $\mathbb{S}^M$ which is given by

$$\mathbb{S}^M=\{\vec{r}=(\beta_1,\ldots,\beta_M)^{\mathsf{T}}\in\mathbb{R}^M:\beta_m\geq 0,\ \sum_m\beta_m=1\} \tag{5}$$

(see Section 5.6).

(iii) A form variation by variation of coordinates may be illustrated by a triangle whose points A and B are fixed, whereas point C is freely movable in the plane (Figure 1a). Each resulting triangle will be characterised by the angles α and β which span the form space (restricted by the relation $\alpha+\beta+\gamma=\pi$). The highest possible symmetry is $\mathbb{D}_3^*$ (see footnote[3]), which is found at $\alpha=\beta=\gamma=\pi/3$. A $\mathbb{D}_1^*$ symmetry occurs along three lines which intersect in the $\mathbb{D}_3^*$ point. The "background" of the diagram in Figure 1b corresponds to triangles with $\mathbb{C}_1^*$ symmetry.

(iv) The same form variation can be described in another way, *viz.* by taking the Cartesian coordinates of point C as coordinates of the form space ($\mathbb{F}=\mathbb{R}^2$). This example can be generalised by allowing all three points to move freely within the plane. Then one has $\mathbb{F}=\mathbb{R}^6$ (see Section 5.3).

(v) A form variation can also be managed by a *superposition* of some forms whose orientation in space is variable. Consider, for instance, two ellipses who have one focus in common and can rotate freely around it. The superposition of the two forms can be done by adding the two respective form functions or their Fourier coefficients. Then, the rotation angles α_1, α_2 can be taken as coordinates for the form space $\mathbb{F}$. This case will be described in Section 5.1.

[2] This set comprises all deformations which can be set up from variations of the parameters considered.

[3] There are only two types of two-dimensional point groups: $\mathbb{C}_n^*$ and $\mathbb{D}_n^*$. Here, $\mathbb{C}_n^*$ denotes a rotation group (cyclic group) having only an n-fold rotation point C_n; $\mathbb{D}_n^*$ denotes a dihedral group consisting of an n-fold rotation point and n mirror lines (σ). I use the Schoenfliess-Niggli nomenclature; the corresponding international (Hermann-Mauguin) symbols are: **n** for $\mathbb{C}_n^*$, **m** for $\mathbb{D}_1^*$, **mm** for $\mathbb{D}_2^*$, **nm** for $\mathbb{D}_n^*$ (n odd), and **nmm** for $\mathbb{D}_n^*$ (n even) [2]. In contrast to three-dimensional symmetry groups, two-dimensional groups will be marked with an asterisk. Symmetry elements and symmetry operations as such will be typed in standard or Greek letters (E, C_n, σ); for their operators and transformation matrices, I will use a caret ($\hat{\mathrm{C}}_n$) and square brackets ($[\mathrm{C}_n]$), respectively.

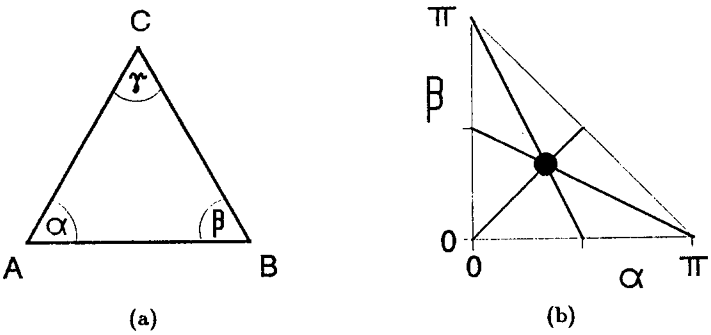

Figure 1. Symmetry diagram (b) for the form variation of a triangle (a) by changing the angles α and β, respectively (γ is given by the relation $\alpha+\beta+\gamma=\pi$). Occurring symmetries are: $\mathbb{D}_3^*$ (•), $\mathbb{D}_1^*$ (bold lines), and $\mathbb{C}_1^*$ ("background," i.e., all other points).

3. NORMAL DEFORMATIONS OF POLYGONAL FORMS

Plane K-vertex polygons can be characterised by the $2K$ Cartesian coordinates of their vertices.[4] Therefore, the appropriate form space is $\mathbb{F}=\mathbb{R}^{2K}$, and every point $P(x_1, y_1, \ldots, x_K, y_K)$ or $P(x_1, \ldots, x_N)$ (see footnote[5]) in $\mathbb{F}$ corresponds to a different (but maybe equivalent) form. A deformation of the polygon can be achieved by displacements of the vertices. To describe such displacements, we attach separate local Cartesian coordinate systems to each vertex of the polygon with the vertices in the origins and all x and y axes pointing into parallel directions, respectively. Then, a general deformation of the polygon will be expressed as a linear combination of the Cartesian displacements of the vertices:

$$dr_j = \sum_{i=1}^{N} c_{ji} \cdot dx_i \quad \text{or} \quad dr_j = \sum_{k=1}^{K} (a_{jk} \cdot dx_k + b_{jk} \cdot dy_k) \tag{6}$$

with a_{jk}, b_{jk}, c_{jk} real and $N = 2K$. This way, all $2K$ degrees of motional freedom of the K polygon vertices are resolved into Cartesian displacements.

These displacements can be made the basis of a matrix representation of the symmetry group $\mathbb{G}$ of the polygon. This representation comprises the transformation matrices $[\mathrm{G}_j]$ for all symmetry operations G_j of $\mathbb{G}$ ($j = 1, \ldots, g$ with g: order of $\mathbb{G}$). It will normally be reducible, i.e., after a similarity transformation, the matrices will have a block diagonal form so that the system of transformation equations will become partly or completely decoupled. The new basis then defines the normal modes of deformation ("*normal deformations*") of the polygon [3–6]. It must be stressed that the term "normal deformation" is a shorthand for "normal mode of deformation" analogous to "normal vibrations," and should not be confused with deformations in normal directions in elasticity theory.

As an example, let us analyse the deformations of a square which will be represented by its four vertex points $P_1 \ldots P_4$ (Figure 2a). The Cartesian coordinates x_k, y_k ($k = 1, \ldots, 4$) of these points constitute the form space $\mathbb{F} = \mathbb{R}^8$. A general deformation of the square can then be described by a linear combination of the 8 Cartesian displacements dx_k and dy_k for every vertex according to equation 6.

We choose the 8 Cartesian displacements of the vertices as basis for a matrix representation of the symmetry group of the square, $\mathbb{D}_4^*$. To get this representation, we have first to set up the transformation matrices transforming the coordinate displacements under the symmetry operations of $\mathbb{D}_4^*$:

$$d\vec{r}\,' = [\mathrm{G}_j] d\vec{r} \tag{7}$$

[4] In this regard, the K-vertex polygons correspond to molecules consisting of K atoms, whose deformations (leading to vibrations) are described in the same way. The application of the methods described below to *three-dimensional* polyhedral forms is straightforward.

[5] For general considerations and matrix equations, coordinates will be described by $\vec{r} = (x_1, \ldots, x_i, \ldots, x_N)^{\mathrm{T}}$, whereas Cartesian coordinates for particular K-vertex polygons will be written as $\vec{r} = (x_1, y_1, \ldots, x_k, y_k, \ldots, x_K, y_K)^{\mathrm{T}}$.

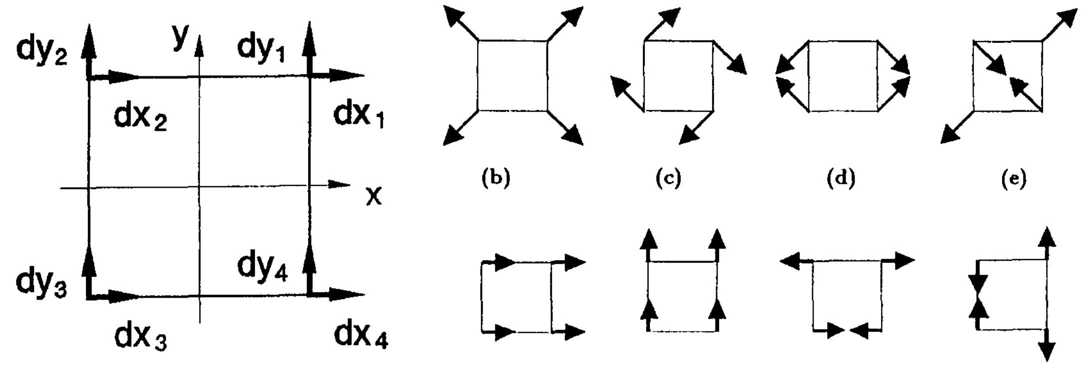

Figure 2. Cartesian basis displacements (a) and normal deformations corresponding to A_1 (b), A_2 (c), B_1 (d), B_2 (e), and E (f and g) for a square.

([G_j]: transformation matrix for the symmetry operation G_j; $d\vec{r}$: vector of coordinate displacements; $d\vec{r}'$: vector of the resulting displacements). The trace tr [G_j] of each matrix gives the so-called *character* χ (G_j) for the corresponding symmetry operation G_j [4, p. 55; 5, p. 95]. This way we get the following character set for $\mathbb{D}_4^*$:

Class of symmetry operations (C):	E	$2C_4$	C_2	$2\sigma_x$	$2\ \sigma_y$
Character $\chi(C)$	8	0	0	0	0

This set has to be compared to the character table of the $\mathbb{D}_4^*$ group. Since the symmetry elements of $\mathbb{D}_4^*$ are identical with the ones of the three-dimensional group $\mathbb{C}_{4v}$, we may use the character table of $\mathbb{C}_{4v}$ given in the literature [4, Appendix; 6, p. 421 ff]. Since there is no 8-dimensional (i.e., χ (E) = 8) character set in this table, thus, our set must be reducible. The reduction can be done with the help of the reduction formula [4, p. 69; 5, p. 96; 7, p. 192]

$$a(\Gamma_k) = \frac{1}{g} \cdot \sum_{j=1}^{g} \chi(\mathrm{G}_j, \Gamma_k) \cdot \chi(\mathrm{G}_j, \Gamma), \tag{8a}$$

$$a(\Gamma_k) = \frac{1}{g} \cdot \sum_{C} n_C \cdot \chi(C, \Gamma_k) \cdot \chi(C, \Gamma) \tag{8b}$$

($a(\Gamma_k)$: multiplicity of Γ_k in Γ; g: order of $\mathbb{G}$; $\chi(C, \Gamma_k)$, $\chi(C, \Gamma)$: characters for class C of symmetry elements in the irreducible representation Γ_k and in the reducible representation Γ, respectively; n_C: number of elements in class C). Reduction of our character set results in the sum

$$\Gamma = A_1 + A_2 + B_1 + B_2 + 2E, \tag{9}$$

i.e., the reducible representation decomposes into 1 two-dimensional and 4 one-dimensional irreducible representations (or "*symmetry species*"). This means that we must be able to transform our set of Cartesian displacements into a new set (symmetry-adapted or normal deformations) whose members will belong to the very symmetry species listed in equation (9). Since the totally symmetric representation A_1 is contained in the sum equation (9), there must exist a symmetry-preserving deformation among the 8 normal deformations (*vide infra*). Moreover, among the deformations, the rotation R_z (see footnote[6]) around the centre of the square and the translations T_x and T_y will also be present. R_z belongs to the symmetry species A_2, whereas T_x and T_y jointly belong to E. Subtracting the symmetry species of these three symmetry transformations from our representation, we end up with the representation for the *genuine deformations*:

$$\Gamma_{\text{def}} = A_1 + B_1 + B_2 + E. \tag{10}$$

[6] In three dimensions, it corresponds to a rotation around the z axis; the nomenclature has been taken over here also for two dimensions to facilitate the comparison with character tables.

To get explicit expressions for the symmetry-adapted normal deformations, it is convenient to utilize the method of the *projection operator* $\hat{P}(\Gamma_k)$ [5, p. 111 ff; 7, p. 196]. This operator projects the vectors taken as a basis of the representation along new symmetry-adapted directions giving the vectors of the normal deformations. The projection operator $\hat{P}(\Gamma_k)$ belonging to the representation Γ_k is defined either as a "*character projection operator*" [5, p. 117; 7, p. 196] by

$$\hat{P}(\Gamma_k) \equiv \frac{1}{g} \cdot \sum_{j=1}^{g} \chi(\mathrm{G}_j, \Gamma_k) \cdot \hat{\mathrm{G}}_j \tag{11}$$

($\hat{\mathrm{G}}_j$: operator of the symmetry operation G_j) or as "*matrix-element projection operator*" [5, p. 118] by

$$\hat{P}_{ij}(\Gamma_k) \equiv \frac{d_k}{g} \cdot \sum_{l=1}^{g} \mathrm{G}_{ij(l)}^{(k)} \cdot \hat{\mathrm{G}}_j \tag{12}$$

($\mathrm{G}_{ij(l)}^{(k)}$: matrix element ij of the transformation matrix $[\mathrm{G}_l]$ for symmetry operation G_l in the irreducible representation Γ_k; d_k: dimension of Γ_k). Whereas the first operator is easier to use, it may lead to ambiguities for degenerate representations so that in these cases, the second formula should be used [5, p. 111 ff].

Taking a certain displacement (say, dx_1) as a basis, it must be transformed by all symmetry operations of the group. If the set of transformed displacements dx'_1 does not exhaust the basis set $\{dx_i\}$ of displacements, another basis must be treated in the same way. With dx_1 as a basis, we get[7]

G:	E	C_4	C_4^3	C_2	σ'_v	σ''_v	σ'_d	σ''_d
$\hat{\mathrm{G}} \cdot dx_1$:	dx_1	dy_2	$-dy_4$	$-dx_3$	dx_4	$-dx_2$	dy_1	$-dy_3$
$\chi(A_2)$:	1	1	1	1	−1	−1	−1	−1

(here, also the characters for symmetry species A_2 are given). Then, the projection operator must be applied to all bases. This gives for A_2, using the definition of equation 11:

$$\begin{aligned} \hat{P}(A_2) \cdot dx_1 &= \frac{1}{8} \cdot [\chi(\mathrm{E}, A_2) \cdot \hat{\mathrm{E}} \cdot dx_1 + \chi(\mathrm{C}_4, A_2) \cdot \hat{\mathrm{C}}_4 \cdot dx_1 \\ &\quad + \chi(\mathrm{C}_4^3, A_2) \cdot \hat{\mathrm{C}}_4^3 \cdot dx_1 + \chi(\mathrm{C}_2, A_2) \cdot \hat{\mathrm{C}}_2 \cdot dx_1 + \ldots]. \end{aligned} \tag{13}$$

The resulting normal deformations are:[8]

$$\begin{array}{rll} A_1: & dn_1 = dx_1 + dy_1 - dx_2 + dy_2 - dx_3 - dy_3 + dx_4 - dy_4, & \\ A_2: & dn_2 = dx_1 - dy_1 + dx_2 + dy_2 - dx_3 + dy_3 - dx_4 - dy_4, & (R_z), \\ B_1: & dn_3 = dx_1 - dy_1 - dx_2 - dy_2 - dx_3 + dy_3 + dx_4 + dy_4, & \\ B_2: & dn_4 = dx_1 + dy_1 + dx_2 - dy_2 - dx_3 - dy_3 - dx_4 + dy_4, & \\ E: & dn_5 = dx_1 + dx_2 + dx_3 + dx_4, & (T_x), \\ & dn_6 = dy_1 + dy_2 + dy_3 + dy_4, & (T_y), \\ E: & dn_7 = dx_1 - dx_2 + dx_3 - dx_4, & \\ & dn_8 = dy_1 - dy_2 + dy_3 - dy_4. & \end{array} \tag{14}$$

They are depicted in Figures 2b–g.

The next problem is: what kind of symmetry will result after the deformation of a form by a certain normal deformation dn? This can be judged from the character set of the respective irreducible representation to which dn belongs:

[7]The nomenclature of the mirror lines in the table follows the convention used in the character tables. Confer, however, Footnote 12.

[8]Normalising factors like $(1/g)$ resulting from the projection operator scheme have been omitted throughout this paper since they have no meaning for normal deformations.

(i) A symmetry element G will be preserved in a deformation dn belonging to the one-dimensional representation Γ_k, if $\chi(\mathrm{G}, \Gamma_k) = +1$. The reason for this can be seen as follows: a certain normal deformation dn will be transformed by the symmetry operation G as

$$dn' = [\mathrm{G}] \cdot dn = [\pm 1] \cdot dn, \tag{15}$$

the character (trace) of the transformation matrix $[\pm 1]$ being ± 1. If the character is $+1$, dn is transferred into itself by the symmetry operation G, i.e., it is invariant under G. This means, on the other hand, that dn preserves the symmetry element G. The deformation $d\mathfrak{F}$ corresponding to dn will then lead to a form $\mathfrak{F}'$ which also displays this symmetry element. If the character is -1, then dn is incompatible with G, which therefore will not be preserved under dn. Thus, the symmetry group resulting after a deformation dn belonging to the irreducible representation Γ_k comprises all symmetry elements G_j whose character $\chi(\mathrm{G}_j, \Gamma_k)$ is $+1$. This means especially that the totally symmetric representation always preserves the full symmetry of the form. Strictly speaking, the above rule is valid only for genuine deformations. The rotation R_z, and likewise the translations T_x and T_y which do not belong to the totally symmetric representation, nevertheless (by definition) preserve the full symmetry of the form. The representations to which R_z, T_x, and T_y belong can be seen in the respective character table. If these representations appear in the sum after the reduction of Γ, it has to be found out whether they belong to the rotations/translations or constitute genuine deformations.

(ii) If the representation is degenerate, the specific transformation matrix [G] has to be considered. A certain symmetry element G will be preserved under a deformation dn only if the transformation matrix [G] has a block diagonal form and if the matrix element transforming dn equals $+1$. To give an example: in the case of an E representation

$$\begin{pmatrix} dn'_1 \\ dn'_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} dn_1 \\ dn_2 \end{pmatrix}, \tag{16}$$

the symmetry element G corresponding to the 2×2 matrix [G] is preserved only by dn_1 but not by dn_2. A linear combination of the degenerate normal deformations may result in a new set of normal deformations which preserve other symmetry elements and thus lead to forms with other symmetries. For examples, see Sections 5.2 to 5.4.

4. NORMAL COORDINATES OF THE FORM SPACE

Having developed the normal deformations for a particular problem, the coordinates of the form space may be transformed into symmetry-adapted normal coordinates by simply taking the linear combinations of Cartesian coordinates corresponding to the individual normal deformations as the appropriate normal coordinates. Thus, since the normal deformations are given by

$$dn_j = \sum_i e_{ji} \cdot dx_i \tag{17}$$

(e_{ji} real), the corresponding linear combinations

$$n_j = \sum_i e_{ji} \cdot x_i \tag{18}$$

will form the corresponding set of symmetry-adapted normal coordinates for the form space.

These normal coordinates have important advantages over Cartesian coordinates for the form space:

(i) A normal deformation dn_i of a form can be easily achieved by changing the corresponding normal coordinate n_i. In this way, also the translation or rotation of a form is possible.
(ii) It is possible to determine the symmetry of a form from the values of normal coordinates in a simple manner. This will be shown in Section 6.3.

5. EXAMPLES

5.1. *Two Points on a Circle (Two Confocal Ellipses)*

First, the superposition of objects of the same kind will be treated, *viz.*, two ellipses which have one of their foci in common and can rotate around this point. To simplify the analysis, each ellipse will be replaced by two points (e.g., the foci), since both an ellipse and two points on a line have the symmetry $\mathbb{D}_2^*$ (two points with fixed distance represent a minimal point set which is symmetry-equivalent to an ellipse). To model two confocal ellipses, let one point of each pair coincide so that the other can move on a circle (Figure 3a). The rotation angles α_1 and α_2 constitute the coordinates of the form space $\mathbb{F}$. The angular displacements $d\alpha_1$ and $d\alpha_2$ are the basis set for the construction of normal deformations of this system. Special configurations have $\mathbb{D}_2^*$ and $\mathbb{D}_1^*$ symmetry, respectively (Figures 3b and 3c).

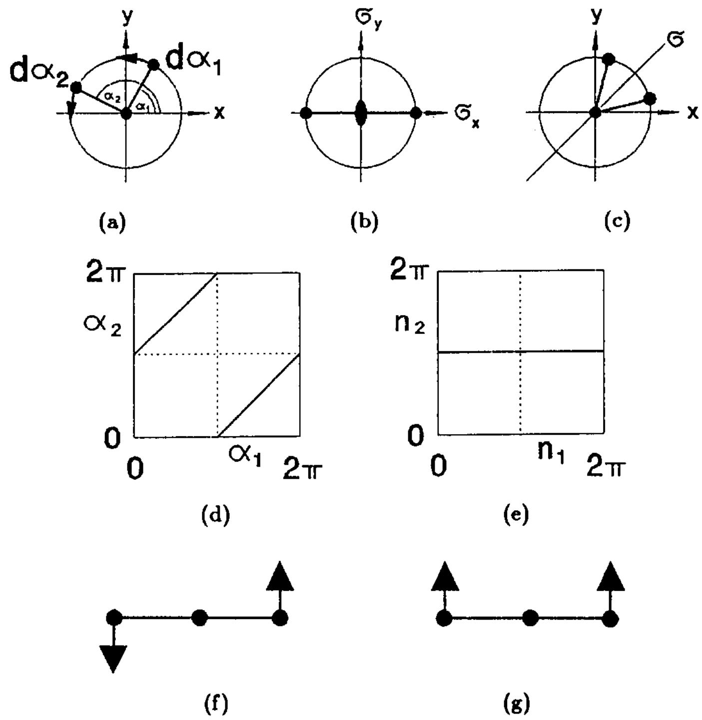

Figure 3. Two points on a circle: coordinates and basis displacements (a), characteristic configurations with symmetries $\mathbb{D}_2^*$ (b) and $\mathbb{D}_1^*$ (c), and symmetry diagram for α_2 vs. α_1 (d) and n_2 vs. n_1 (e) with symmetries $\mathbb{D}_2^*$ (bold lines) and $\mathbb{D}_1^*$ ("background"), and normal deformations of a $\mathbb{D}_2^*$ configuration for $A_2 = R_z$ (f) and B_2 (g).

Starting with the $\mathbb{D}_2^*$ configuration of Figure 3b, we get[9] a reducible character set $\chi(\Gamma) = \{2, 0, -2, 0\}$ whose reduction ends up with the decomposition $\Gamma = A_2 + B_2$. The corresponding normal deformations are:

$$\begin{aligned} A_2 &: \quad dn_1 = d\alpha_1 + d\alpha_2 \quad R_z, \\ B_2 &: \quad dn_2 = d\alpha_1 - d\alpha_2 \quad \text{deformation to } \mathbb{D}_1^* \end{aligned} \tag{19}$$

(see Figures 3f and 3g). An analogous analysis for an arbitrary $\mathbb{D}_1^*$ configuration gives $\Gamma = A_1 + A_2$, and the normal deformations are

$$\begin{aligned} A_2 &: \quad dn_1 = d\alpha_1 + d\alpha_2 \quad R_z, \\ A_1 &: \quad dn_2 = d\alpha_1 - d\alpha_2 \quad \text{totally symmetric deformation.} \end{aligned} \tag{20}$$

[9]For $\mathbb{D}_n^*$ groups, I use the character tables for the three-dimensional $\mathbb{C}_{nv}$ groups as indicated above, whereas for $\mathbb{C}_n^*$ groups, the character tables for $\mathbb{C}_n$ have to be considered.

To characterise the symmetries within the form space, I propose a *symmetry diagram* (Figure 3d) where points which represent forms with equal symmetries are depicted in the same way. It can be seen that there is a line of constant ($\mathbb{D}_2^*$) symmetry corresponding to the rotation R_z. From equation 19 and the data for the configuration in Figure 3b ($\alpha_1 = 0$, $\alpha_2 = \pi$), there follows for this isosymmetric line

$$d\alpha_2 = d\alpha_1 \quad \text{and} \quad \alpha_2 = \alpha_1 + \pi \quad \text{or} \quad \alpha_2 = \alpha_1 - \pi; \tag{21}$$

these are the two isosymmetric lines seen in Figure 3d. Deformation of a $\mathbb{D}_2^*$ configuration along dn_2 (in the diagram of Figure 3d: perpendicularly to the isosymmetric line) destroys the $\mathbb{D}_2^*$ symmetry and leads to a form with $\mathbb{D}_1^*$ symmetry.

Since the rotation of a form is not a genuine deformation, this redundancy can be omitted by taking $(\alpha_2 - \alpha_1)$ as a coordinate for the form space. Then we end up in a one-dimensional form space consisting of $\mathbb{D}_1^*$ isosymmetric lines meeting in an isolated $\mathbb{D}_2^*$ point at $\alpha_2 - \alpha_1 = \pi$. On the other hand, a transformation of the form space coordinates into normal coordinates according to

$$\begin{aligned} n_1 &= \alpha_1 + \alpha_2, \\ n_2 &= \alpha_1 - \alpha_2 \end{aligned} \tag{22}$$

results in a similar simplification of the structure of the form space (Figure 3e). The $\mathbb{D}_2^*$ isosymmetric line is now parallel to n_1 since dn_1 belongs to the totally symmetric representation and therefore does not change the symmetry of a $\mathbb{D}_2^*$ form.

The model system described so far may be extended to the superposition of two ellipses with their *centres* in common. This corresponds to two *pairs* of points laying on two diameters of the circle. The symmetry diagrams for these concentric ellipses correspond to the ones given in Figures 3d and 3e, but they have half the identity period (the point 2π of Figures 3d and 3e corresponds to π for this system) so that they are made up of 4 identical copies of the diagrams in Figures 3d and 3e. The symmetry $\mathbb{D}_2^*$ in Figures 3d and 3e has to be replaced by $\mathbb{D}_4^*$, and instead of $\mathbb{D}_1^*$, one gets $\mathbb{D}_2^*$. The normal deformations belong to the same irreducible representations and result in the same combinations of Cartesian displacements.

5.2. Three Points on a Circle (Three Confocal Ellipses)

This example deals with the superposition of three confocal rotatable ellipses which may be represented by three points on a circle taking account of the center of the circle (the focus which is common to all three ellipses). Coordinates of the form space are the three angles α_1, α_2, α_3; the corresponding displacements are $d\alpha_1$, $d\alpha_2$, and $d\alpha_3$ (Figure 4a).

Characteristic configurations of the system have $\mathbb{D}_3^*$ and $\mathbb{D}_1^*$ symmetries, respectively (Figures 4b and 4c). The three basis displacements give under $\mathbb{D}_3^*$ symmetry a reducible representation with $\chi(\Gamma) = \{3, 0, -1\}$, whose reduction leads to $\Gamma = A_2 + E$, and the corresponding normal deformations are (cf. Figures 4f–h):

$$\begin{aligned} A_2: &\quad dn_1 = d\alpha_1 + d\alpha_2 + d\alpha_3, && R_z(\text{preserves } \mathbb{D}_3^*), \\ E: &\quad dn_2 = 2d\alpha_1 - d\alpha_2 - d\alpha_3, && \text{deformation to } \mathbb{C}_1^*, \\ &\quad dn_3 = d\alpha_2 - d\alpha_3, && \text{deformation to } \mathbb{D}_1^*. \end{aligned} \tag{23}$$

These normal deformations can be derived by using the projection operator technique. Here, a simplification of the procedure may be introduced [6, pp. 176 f, 182; 7, p. 250]: since in E representations of $\mathbb{C}_{nv}$ groups, characters for mirror lines invariably vanish, the whole information is contained in the rotational subgroup $\mathbb{C}_n$. Therefore, only the character table for $\mathbb{C}_3$ has to be considered to find out the E normal deformations in our example. However, the complex characters have to be transformed into real ones by linear combination resulting in [6, p. 182; 7, p. 250]

$$\begin{array}{cc} & \begin{array}{ccc} \mathrm{E} & \mathrm{C}_3 & \mathrm{C}_3^2 \end{array} \\ E & \begin{pmatrix} 2 & -1 & -1 \\ 0 & 1 & -1 \end{pmatrix}. \end{array}$$

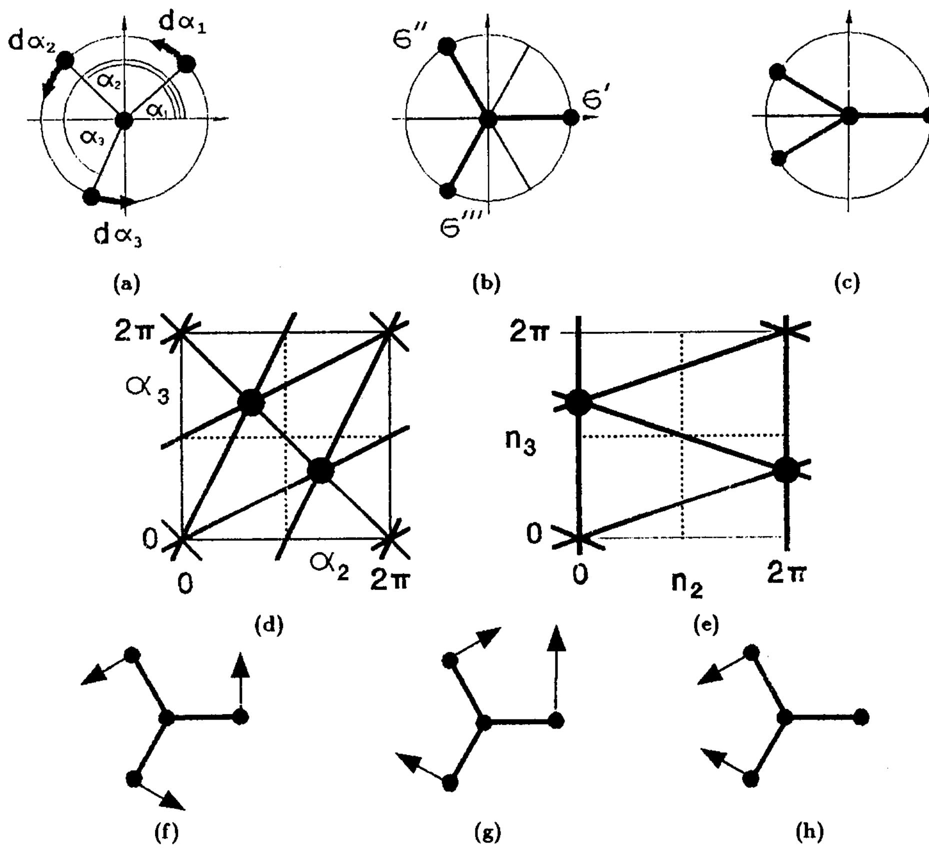

Figure 4. Three points on a circle: coordinates and basis displacements (a), characteristic configurations with symmetries $\mathbb{D}_3^*$ (b) and $\mathbb{D}_1^*$ (c), and symmetry diagram in the (α_2, α_3) plane for $\alpha_1 = 0$ (d) and in the (n_2, n_3) plane (e) with symmetries $\mathbb{D}_3^*$ (•), $\mathbb{D}_1^*$ (bold lines) and $\mathbb{C}_1^*$ ("background"), and normal deformations of a $\mathbb{D}_3^*$ configuration for A_2 (f) and E (g,h). The E deformations correspond to dn_2 and dn_3.

Application of the projection operator onto $d\alpha_1$ as a basis deformation then gives dn_2 and dn_3 (*vide supra*). The matrices for the E representation are:[10]

$$\begin{aligned}
&[\mathrm{E}] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad [\mathrm{C}_3] = \begin{pmatrix} -0.5 & 1.5 \\ -0.5 & -0.5 \end{pmatrix}, \quad [\mathrm{C}_3^2] = \begin{pmatrix} -0.5 & -1.5 \\ 0.5 & -0.5 \end{pmatrix}, \\
&[\sigma'] = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad [\sigma''] = \begin{pmatrix} 0.5 & 1.5 \\ 0.5 & -0.5 \end{pmatrix}, \quad [\sigma'''] = \begin{pmatrix} 0.5 & -1.5 \\ -0.5 & -0.5 \end{pmatrix}.
\end{aligned} \tag{24}$$

Contemplation of the rules given in Section 3 shows that dn_2 preserves only E and thus leads to $\mathbb{C}_1^*$, whereas dn_3 preserves E and σ' (but not σ'' or σ''') and hence transforms the configuration to $\mathbb{D}_1^*$ as specified above. The degeneracy of dn_2 and dn_3 has an additional effect: since both normal deformations belong to the same reducible representation, they can be combined linearly to give other sets of normal deformations. Among these, two sets are especially noteworthy:

$$\begin{aligned}
dn'_2 &= d\alpha_1 - 2d\alpha_2 + d\alpha_3 = \frac{1}{2} \cdot dn_2 - \frac{3}{2} \cdot dn_3, \\
dn''_3 &= d\alpha_1 - d\alpha_3 = \frac{1}{2} \cdot dn_2 + \frac{1}{2} \cdot dn_3,
\end{aligned} \tag{25a}$$

[10]The upper row of the matrices corresponds to dn_2, the lower row to dn_3. This is important for the discussion which follows.

and

$$dn''_2 = d\alpha_1 + d\alpha_2 - 2d\alpha_3 = \frac{1}{2} \cdot dn_2 + \frac{3}{2} \cdot dn_3,$$
$$dn''_3 = -d\alpha_1 + d\alpha_2 = -\frac{1}{2} \cdot dn_2 + \frac{1}{2} \cdot dn_3. \tag{25b}$$

From the transformation matrices for the mirror reflections,

for $\begin{pmatrix} dn'_2 \\ dn'_3 \end{pmatrix}$:

$$[\sigma'] = \begin{pmatrix} 0.5 & -1.5 \\ -0.5 & -0.5 \end{pmatrix}, \quad [\sigma''] = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad [\sigma'''] = \begin{pmatrix} 0.5 & 1.5 \\ 0.5 & -0.5 \end{pmatrix}, \tag{26a}$$

for $\begin{pmatrix} dn''_2 \\ dn''_3 \end{pmatrix}$:

$$[\sigma'] = \begin{pmatrix} 0.5 & 1.5 \\ 0.5 & -0.5 \end{pmatrix}, \quad [\sigma''] = \begin{pmatrix} 0.5 & -1.5 \\ -0.5 & -0.5 \end{pmatrix}, \quad [\sigma'''] = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{26b}$$

it can be seen that dn'_3 preserves σ'' whereas dn''_3 preserves σ'''. Other linear combinations of dn_2 and dn_3 will preserve none of the mirror lines. Thus, degeneracy of dn_2 and dn_3 means that different linear combinations of them will preserve different mirror lines of the same class (σ).

Reduction of the character set $\chi(\Gamma) = \{3, -1\}$ for $\mathbb{D}_1^*$ symmetry (Figure 4c) gives $\Gamma = A_1 + 2A_2$; the normal deformations are (if the symmetry line dissects point P_1):

$$\begin{array}{lll} A_2: & dn_1 = d\alpha_1 + d\alpha_2 + d\alpha_3, & R_z \text{ (preserves } \mathbb{D}_1^*), \\ A_2: & dn_2 = d\alpha_2 + d\alpha_3, & \text{deformation to } \mathbb{C}_1^*, \\ A_1: & dn_3 = d\alpha_2 - d\alpha_3, & \text{totally symmetric deformation.} \end{array} \tag{27}$$

Since dn_1 and dn_2 belong to the same symmetry species A_2, they may mix. This means especially that the linear combination

$$dn_2^* = 2dn_1 - 3dn_2 = 2d\alpha_1 - d\alpha_2 - d\alpha_3,$$

which is identical to dn_2 under $\mathbb{D}_3^*$ symmetry (equation (23)), also transforms according to A_2 so that $(2d\alpha_1 - d\alpha_2 - d\alpha_3)$ can be used as a form space normal coordinate both under $\mathbb{D}_3^*$ and $\mathbb{D}_1^*$ symmetries whereas $(d\alpha_2 + d\alpha_3)$ is a normal coordinate only under $\mathbb{D}_1^*$ symmetry but not under $\mathbb{D}_3^*$.

The symmetry diagram for the whole system is depicted in Figure 4d. The filled circles mark intersection points of $\mathbb{D}_1^*$ isosymmetric lines where the symmetry is $\mathbb{D}_3^*$. It must be stressed, however, that there are also intersection points of the same three $\mathbb{D}_1^*$ isosymmetric lines (points $P(0,0)$, $P(0,2\pi)$, and so on) where the symmetry is only $\mathbb{D}_1^*$. These two types of intersection points are to be discussed separately:

(i) $\mathbb{D}_3^*$ intersection point: there is a symmetry-preserving rotation (dn_1) giving rise to a $\mathbb{D}_3^*$ isosymmetric line which intersects the plane of the paper obliquely in the $\mathbb{D}_3^*$ intersection point. On the other hand, dn_3 deforms the $\mathbb{D}_3^*$ configuration to $\mathbb{D}_1^*$, whereas dn_2 leads to $\mathbb{C}_1^*$. But, as has been explained above, dn_3, dn'_3, and dn''_3 constitute three equivalent possibilities for breaking the $\mathbb{D}_3^*$ symmetry, by preserving σ', σ'', or σ''' separately to give three equivalent $\mathbb{D}_1^*$ configurations.

(ii) $\mathbb{D}_1^*$ intersection point: here, the three symmetry lines are *coincident*; therefore, the symmetry of the configuration is only $\mathbb{D}_1^*$. There are three ways to preserve this $\mathbb{D}_1^*$ symmetry under a deformation, *viz.*, by rotating a *pair* of lines by an angle $\pm d\alpha$ off the fixed third line: in the resulting configuration, the mirror line σ', σ'', or σ''' may be the bisector and will then be preserved. These three possibilities correspond to the three lines meeting in the $\mathbb{D}_1^*$ intersection point. Mathematically, there is an ambiguity in the assignment of the transformed basis deviations: since $d\alpha_1 = d\alpha_2 = d\alpha_3$ and $d\alpha'_1 = \sigma(d\alpha_1) = -d\alpha_1$, one may equally well take the assignments $d\alpha'_1 = -d\alpha_2$ or $d\alpha'_1 = -d\alpha_3$. These three assignments lead to the same three $\mathbb{D}_1^*$ lines intersecting in the $\mathbb{D}_1^*$ point.

The symmetry diagram may be reduced since only two non-trivial deformations are present. This reduction has already been performed in Figure 4d by setting $\alpha_1 = 0$ (another way would have been a plot of $(\alpha_3 - \alpha_1)$ vs. $(\alpha_2 - \alpha_1)$). Alternatively, the form space coordinates may be transformed into normal coordinates (Figure 4e). In this case, it is necessary to have the same normal deformations throughout the form space. Therefore, in the case of $\mathbb{D}_1^*$ symmetry, the normal deformation $dn_2^* = 2d\alpha_1 - d\alpha_2 - d\alpha_3$ was taken instead of $dn_2 = d\alpha_2 + d\alpha_3$ as has been explained above. After the transformation of the form space coordinates into normal coordinates, the structure of the form space is nicely simple but nevertheless topologically equivalent. Isosymmetric $\mathbb{D}_1^*$ lines in Figure 4e correspond to dn_3 (vertical lines), dn_3' (ascending lines), and dn_3'' (descending lines). They illustrate the degeneracy of the deformations dn_2 and dn_3 in accordance with the above discussion.

As in Section 5.1, we may extend the problem to the analysis of three *concentric* rotatable ellipses. This system corresponds to three *pairs* of points on a diameter each which can move on the circle. The symmetry diagram corresponds to a collage of four copies of the diagram in Figure 4d or 4e, since its identity period is half the size of the present diagram. Instead of $\mathbb{D}_3^*$ symmetry, we find $\mathbb{D}_6^*$, and instead of $\mathbb{D}_1^*$, we have $\mathbb{D}_2^*$, the "background" symmetry being $\mathbb{C}_2^*$. The deformations under $\mathbb{D}_6^*$ are:

$$\begin{aligned} A_2:&\quad dn_1 = d\alpha_1 + d\alpha_2 + d\alpha_3, && R_z, \\ E_2:&\quad dn_2 = 2d\alpha_1 - d\alpha_2 - d\alpha_3, && \text{deformation to } \mathbb{C}_2^*, \\ &\quad dn_3 = d\alpha_2 - d\alpha_3, && \text{deformation to } \mathbb{D}_2^*, \end{aligned} \tag{28}$$

in perfect analogy to the case of three confocal ellipses.

5.3. Three Points in a Plane (Arbitrary Triangles)

Symmetries of arbitrary triangles can be treated (as an extension of the problem sketched in Section 2) by allowing all three vertex points P_1, P_2, and P_3 of the triangle to move freely within the plane. Taking the coordinates x and y for each point as a basis (Figure 5a) gives a form space $\mathbb{F} = \mathbb{R}^6$. Of course, the system is redundant if rotation and translations are considered unimportant. In this case, besides a transformation of the form space coordinates into normal coordinates, also other ways to tackle the problem with a reduced coordinate set may be advantageous (*vide infra*).

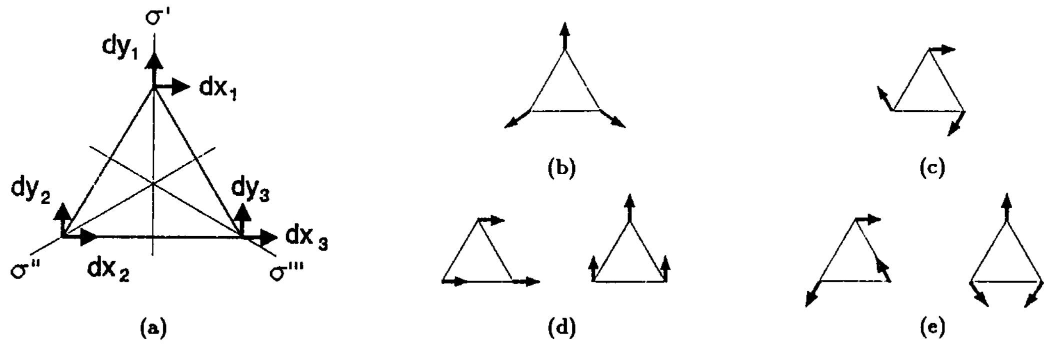

Figure 5. Cartesian basis displacements for an equilateral triangle (a) and the corresponding normal deformations: A_1 (b), A_2 (c), and E (d and e).

The highest symmetry in the system is $\mathbb{D}_3^*$ (if the special case of an incidence of *all* points giving $\mathbb{D}_\infty^*$ symmetry is not to be taken into account, though it corresponds to a point of our form space). Under $\mathbb{D}_3^*$ symmetry, the reducible character set for the displacements dx_k, dy_k $(k = 1, \ldots, 3)$ is $\chi(\Gamma) = \{6, 0, 0\}$ which can be reduced to $\Gamma = A_1 + A_2 + 2E$. The corresponding normal deformations are (with $a = 1/2$; $b = \sqrt{3}/2$):

$$\begin{array}{rlr} A_1: & dn_1 = dy_1 - b\cdot dx_2 - a\cdot dy_2 + b\cdot dx_3 - a\cdot dy_3 & \text{deformation}, \\ A_2: & dn_2 = dx_1 - a\cdot dx_2 + b\cdot dy_2 - a\cdot dx_3 - b\cdot dy_3 & R_z, \\ E: & dn_3 = dx_1 + dx_2 + dx_3 & T_x, \\ & dn_4 = dy_1 + dy_2 + dy_3 & T_y, \\ E: & dn_5 = dx_1 - a\cdot dx_2 - b\cdot dy_2 - a\cdot dx_3 + b\cdot dy_3 & \text{deformation}, \\ & dn_6 = dy_1 + b\cdot dx_2 - a\cdot dy_2 - b\cdot dx_3 - a\cdot dy_3 & \text{deformation} \end{array} \tag{29}$$

(Figures 5b–e). Here, the basis displacements have been chosen as in [3, p. 126] to facilitate the comparison. The normal deformations dn_1 and dn_2 are identical with the ones derived in [3], but for the first E representation, these authors have ($c = 3/2$):

$$\begin{array}{rl} E: & dn'_3 = 2\cdot dy_1 + a\cdot dy_2 + a\cdot dy_3 + b\cdot dx_2 - b\cdot dx_3, \\ & dn'_4 = 0\cdot dy_1 + c\cdot dy_2 + c\cdot dy_3 - b\cdot dx_2 + b\cdot dx_3 \end{array} \tag{30}$$

(deformations for the second E representation are not explicitly stated in [3]). It can easily be seen that these normal coordinates are linear combinations of dn_4 and dn_6 given above. To get a clearer picture of the normal deformations, it is desirable, however, to separate the translation T_y from dn'_3 and dn'_4. Analogously, the derivation of deformation coordinates for the second E representation according to the algorithm described in [3, Chapter 6.5] gives

$$\begin{array}{l} dn'_5 = 2\cdot dx_1 + a\cdot dx_2 + a\cdot dx_3 - b\cdot dy_2 + b\cdot dy_3, \\ dn'_6 = 0\cdot dx_1 + c\cdot dx_2 + c\cdot dx_3 + b\cdot dy_2 - b\cdot dy_3. \end{array} \tag{31}$$

From these deformations, dn_3 and dn_5 can be obtained by separating the translation T_x from the genuine deformation.

The matrices for the joint transformation of the E deformations are:

for $\begin{pmatrix} dn_3 \\ dn_4 \end{pmatrix}$:

$$\begin{array}{lll} [\mathrm{E}] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, & [\mathrm{C}_3] = \begin{pmatrix} -a & b \\ -b & -a \end{pmatrix}, & [\mathrm{C}_3^2] = \begin{pmatrix} -a & -b \\ b & -a \end{pmatrix}, \\ [\sigma'] = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, & [\sigma''] = \begin{pmatrix} a & b \\ b & -a \end{pmatrix}, & [\sigma'''] = \begin{pmatrix} a & -b \\ -b & -a \end{pmatrix}, \end{array} \tag{32a}$$

for $\begin{pmatrix} dn_5 \\ dn_6 \end{pmatrix}$:

$$\begin{array}{lll} [\mathrm{E}] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, & [\mathrm{C}_3] = \begin{pmatrix} -a & -b \\ b & -a \end{pmatrix}, & [\mathrm{C}_3^2] = \begin{pmatrix} -a & b \\ -b & -a \end{pmatrix}, \\ [\sigma'] = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, & [\sigma''] = \begin{pmatrix} a & -b \\ -b & -a \end{pmatrix}, & [\sigma'''] = \begin{pmatrix} a & b \\ b & -a \end{pmatrix}. \end{array} \tag{32b}$$

The translations T_x and T_y are symmetry-preserving, of course, in any arbitrary linear combination. Among the genuine deformations dn_5 and dn_6, only dn_6 preserves a non-trivial symmetry element (*viz.*, σ'), and thus corresponds to a transition to $\mathbb{D}_1^*$. For the sake of symmetry, there must equally well be possibilities to preserve σ'' and σ'''. They can be found by arranging dn_5 and dn_6 in other linear combinations:

$$\begin{array}{l} dn''_5 = -a\cdot dx_1 - b\cdot dy_1 - a\cdot dx_2 + b\cdot dy_2 + dx_3 = -a\cdot dn_5 - b\cdot dn_6, \\ dn''_6 = +b\cdot dx_1 - a\cdot dy_1 - b\cdot dx_2 - a\cdot dy_2 + dy_3 = +b\cdot dn_5 - a\cdot dn_6, \end{array} \tag{33a}$$

or

$$\begin{array}{l} dn'''_5 = -a\cdot dx_1 + b\cdot dy_1 + dx_2 - a\cdot dx_3 - b\cdot dy_3 = -a\cdot dn_5 + b\cdot dn_6, \\ dn'''_6 = -b\cdot dx_1 - a\cdot dy_1 + dy_2 + b\cdot dx_3 - a\cdot dy_3 = -b\cdot dn_5 - a\cdot dn_6. \end{array} \tag{33b}$$

It can easily be checked by looking at the corresponding transformation matrices that, first, dn_6'' preserves σ'' and dn_6''' preserves σ''', and secondly, the linear combinations given above are the only ones which preserve a mirror line.

For a configuration with $\mathbb{D}_1^*$ symmetry (an isosceles triangle), the character set is $\chi(\Gamma) = \{6, 0\}$ which reduces to $\Gamma = 3A_1 + 3A_2$. The normal deformations are then:

$$\begin{array}{lll} A_1: & dn_1 = dx_2 - dx_3 & \text{totally symmetric deformation,} \\ A_1: & dn_2 = dy_1 - dy_2 - dy_3 & \text{totally symmetric deformation,} \\ A_1: & dn_3 = dy_1 + dy_2 + dy_3 & T_y, \\ A_2: & dn_4 = dx_1 + dx_2 + dx_3 & T_x, \\ A_2: & dn_5 = dx_1 + dy_2 - dy_3 & R_z, \\ A_2: & dn_6 = dx_1 & \text{deformation to } \mathbb{C}_1^*. \end{array} \tag{34}$$

These expressions have been calculated by the method of the projection operator. Since the deformations dn_1 to dn_3 belong to A_1, and dn_4 to dn_6 belong to A_2, one can equally well use linear combinations of them. In order to have consistent deformations throughout the form space, the normal deformations for $\mathbb{D}_3^*$ symmetry may be taken over to $\mathbb{D}_1^*$ configurations giving the same numbers of symmetry species A_1 and A_2 as those in equation (34).

The problem of form variation in triangles can also be treated with reduced coordinate sets. One example has been given in Section 2. Another possibility is to fix points P_2 and P_3 and to take the coordinates x_1 and y_1 of point P_1 as coordinate set (Figure 6a). Rotation and translations will be omitted this way. The symmetry diagram for this system is displayed in Figure 6b. Here, the y axis corresponds to $\alpha = \beta$ (angles are located as in Figure 1) in the example of Section 2, the left circle to $\alpha = \gamma$, and the right circle to $\beta = \gamma$. The intersection points of these three curves give $\alpha = \beta = \gamma$ and hence, $\mathbb{D}_3^*$ symmetry. On the other hand, the right intersection point of the left circle with the x axis corresponds to the configuration with $P_1 = P_3$ ($\mathbb{D}_1^*$). Starting from this configuration, two types of deformation retaining the symmetry $\mathbb{D}_1^*$ are possible: a shift of point P_1 either along the x axis or on the arc of the left circle. On the other hand, the left intersection point of the left circle and the x axis gives a line P_1P_3 bisected by P_2 which displays $\mathbb{D}_2^*$ symmetry.

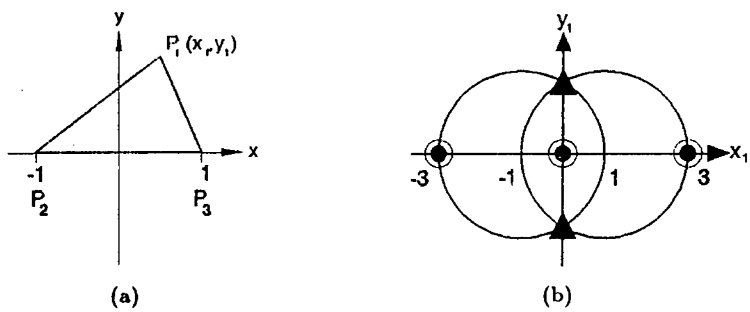

Figure 6. Triangle with reduced degrees of freedom (a): only point $P_1 = (x_1, y_1)$ can be varied. Symmetry diagram (b) with symmetries $\mathbb{D}_3^*$ (▲), $\mathbb{D}_2^*$ (⊙), $\mathbb{D}_1^*$ (circles and axes), and $\mathbb{C}_1^*$ ("background").

5.4. Four Points in a Plane (Arbitrary Quadrilaterals)

The highest possible symmetry in this system (besides $\mathbb{D}_\infty^*$ for an incidence of all vertices) is $\mathbb{D}_4^*$ (a square). The deformations of the square and their analysis have already been presented in Section 3 (Figure 2).

Under $\mathbb{D}_2^*$ symmetry (rectangle or rhombus) and also under $\mathbb{D}_1^*$ (trapezium or unsymmetric rhombus) one gets the same normal deformations, but they belong to different irreducible representations; the correlation is as follows:[11]

[11]For correlation tables, see [3, p. 333 ff]. If in $\mathbb{C}_{nv}$ only one mirror line is preserved, the resulting group is

representation in $\mathbb{D}_4^*$:	A_1	A_2	B_1	B_2	E
representation in $\mathbb{D}_2^*$:	A_1	A_2	A_1	A_2	$B_1 + B_2$
representation in $\mathbb{D}_1^*$:	A_1	A_2	A_1	A_2	$A_1 + A_2$

This means that the representation of the 8 Cartesian displacements reduces under $\mathbb{D}_2^*$ symmetry to $\Gamma = 2A_1 + 2A_2 + 2B_1 + 2B_2$, and under $\mathbb{D}_1^*$ symmetry to $\Gamma = 4A_1 + 4A_2$. Since the normal deformations have the same composition in all symmetry groups, their spatial directions are constant everywhere in the form space.

Analogously to the case of arbitrary triangles (Section 5.3), there is a degeneracy in the normal deformations belonging to the symmetry species E. For these normal deformations, the relevance of linear combinations has therefore to be considered. The translations T_x and T_y, of course, span an isosymmetric plane since arbitrary linear combinations of them are symmetry-preserving. For dn_7 and dn_8 (equation (14)), it follows from the transformation matrices and also from their pictures (Figure 2g) that dn_7 preserves σ_y, and dn_8 preserves σ_x. The only linear combinations of dn_7 and dn_8 which preserve a symmetry line are[12]

$$\begin{aligned} dn'_7 &= dn_7 - dn_8 \quad (\text{preserving } \sigma_q), \\ dn'_8 &= dn_7 + dn_8 \quad (\text{preserving } \sigma_d). \end{aligned} \tag{35}$$

The pictures of these deformations can easily be inferred by vector addition from Figure 2g.

The full network of possible deformations of a square is given in Figure 7.

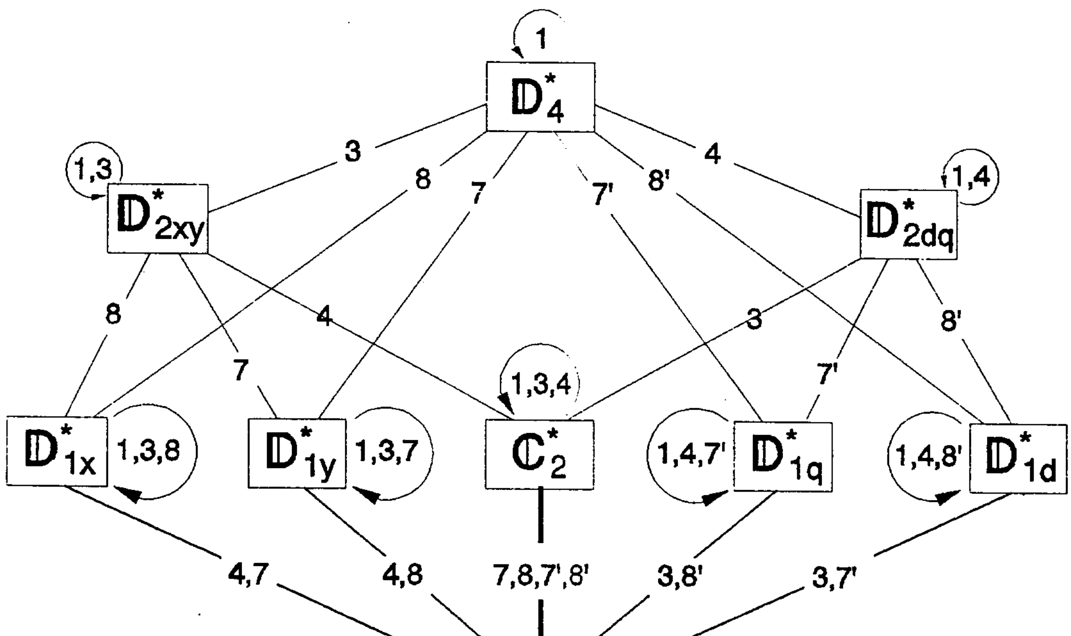

Figure 7. Graph showing the network of normal deformations starting from a square ($\mathbb{D}_4^*$ symmetry) down to an asymmetric ($\mathbb{C}_1^*$) quadrilateral. Symmetry-preserving deformations are shown as loops. Numbers denote the different normal deformations (for the sake of clarity, "dn_1" has been replaced by "1," etc.).

given there as $\mathbb{C}_s$. However—as can be inferred from the Mulliken symbols for $\mathbb{C}_s$ (A', A'')—this group is regarded as being the $\mathbb{C}_{1h}$ group (with a horizontal mirror plane), whereas "genetically" it should be $\mathbb{C}_{1v}$ (with a vertical mirror plane). Since the genetic relationship between the groups is essential for the consideration of form transitions, I denote the resulting group by $\mathbb{C}_{1v}$ (here: $\mathbb{D}_1^*$) and classify its irreducible representations as A_1 and A_2, respectively.

[12]The four mirror lines of the square will be termed here after their locations σ_x, σ_y (along the x and y axes, resp.), σ_d ("diagonal," bisecting the first quadrant), and σ_q (transverse, in German "quer," bisecting the second quadrant). The subgroups of $\mathbb{D}_4^*$ will be termed after the mirror lines they contain as $\mathbb{D}_{1x}^*$, $\mathbb{D}_{1y}^*$, $\mathbb{D}_{1d}^*$, $\mathbb{D}_{1q}^*$, $\mathbb{D}_{2xy}^*$, and $\mathbb{D}_{2dq}^*$.

The relationships for the square itself and the $\mathbb{D}_2^*$ forms derived from it ($\mathbb{D}_{2xy}^*$: a rectangle, and $\mathbb{D}_{2dq}^*$: a rhombus) are illustrated in Figure 8. Normal coordinates have been used here to give a clearer picture of this part of the form space. In the (n_7, n_8) plane, it is obvious (Figure 8a) that the square ($\mathbb{D}_4^*$ symmetry) forms an intersection point of four $\mathbb{D}_1^*$ isosymmetric lines, each preserving one of the four mirror lines of the square. The action of dn'_7 and of dn'_8 (leading to $\mathbb{D}_{1q}^*$ and $\mathbb{D}_{1d}^*$, resp.) is also clearly visible. On the contrary, given a $\mathbb{D}_2^*$ form (Figures 8b–c), the effect of the degenerate E deformations depends on which mirror lines are present in the starting form: in $\mathbb{D}_{2xy}^*$, dn_7 and dn_8 preserve σ_y and σ_x, resp., whereas in $\mathbb{D}_{2dq}^*$, dn'_7 and dn'_8 preserve σ_q and σ_d, resp., in accordance with what has been said above.

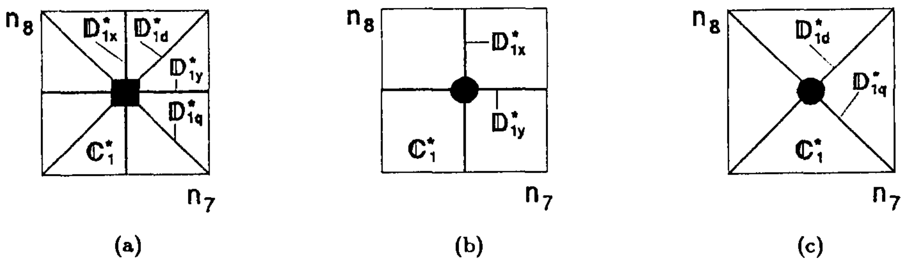

Figure 8. Isosymmetric manifolds for the deformation of a square in the (n_7, n_8) plane near a $\mathbb{D}_4^*$ point ($n_1 \neq 0$, $n_3 = n_4 = 0$) (a), near a $\mathbb{D}_{2xy}^*$ point ($n_1 \neq 0$, $n_3 = 0$, $n_4 \neq 0$) (b), and near a $\mathbb{D}_{2dq}^*$ point ($n_1 \neq 0$, $n_3 \neq 0$, $n_4 = 0$) (c), see text. Symmetries are: $\mathbb{D}_4^*$ (■), $\mathbb{D}_2^*$ (•), $\mathbb{D}_1^*$ (bold lines), and $\mathbb{C}_1^*$ ("background").

5.5. Two Point Pairs on Two Circles (Two Concentric Ellipses)

An interesting case is given by two rotatable ellipses whose fixed centres are at some distance. Reducing the ellipses to point pairs on circles, this gives two distinct circles with one pair of points on each (Figure 9a).

The highest possible symmetry is $\mathbb{D}_2^*$. Under this symmetry, the character set $\chi(\Gamma) = \{2, 0, -2, 0\}$ for the representation reduces to $\Gamma = A_2 + B_2$, and the corresponding normal deformations are:

$$\begin{array}{lll} A_2: & dn_1 = d\alpha_1 - d\alpha_2 & \text{deformation to } \mathbb{C}_2^*, \\ B_2: & dn_2 = d\alpha_1 + d\alpha_2 & \text{deformation to } \mathbb{D}_1^*. \end{array} \tag{36}$$

There exists no symmetry-preserving deformation, but the two deformations lead to the two subgroups of $\mathbb{D}_2^*$, *viz.*, $\mathbb{D}_1^*$ and $\mathbb{C}_2^*$, and give rise to two isosymmetric lines in the symmetry diagram (Figure 9f).

Deformations starting at points on the $\mathbb{D}_1^*$ isosymmetric line (configuration of Figure 9c) belong to symmetry species A_1 or A_2 ($\Gamma = A_1 + A_2$):

$$\begin{array}{lll} A_1: & dn_2 = d\alpha_1 + d\alpha_2 & \text{totally symmetric deformation}, \\ A_2: & dn_1 = d\alpha_1 - d\alpha_2 & \text{deformation to } \mathbb{C}_1^*. \end{array} \tag{37}$$

On the $\mathbb{C}_2^*$ isosymmetric line, we have $\Gamma = A + B$ and

$$\begin{array}{lll} A: & dn_1 = d\alpha_1 - d\alpha_2 & \text{totally symmetric deformation}, \\ B: & dn_2 = d\alpha_1 + d\alpha_2 & \text{deformation to } \mathbb{C}_1^*. \end{array} \tag{38}$$

It is surprising that besides the $\mathbb{D}_1^*$ isosymmetric lines, there exist also isolated $\mathbb{D}_1^*$ points in the form space which correspond to the configuration of Figure 9d. That they *must* be isolated will be clear from the analysis of deformations starting from such a point: the basis deformations give rise to a representation with $\chi(\Gamma) = \{2, -2\}$ which reduces to $\Gamma = 2A_2$: both deformations destroy the $\mathbb{D}_1^*$ symmetry of the form leading to $\mathbb{C}_1^*$. Since there is no symmetry-preserving deformation at all, the $\mathbb{D}_1^*$ point must be an *isolated* point.

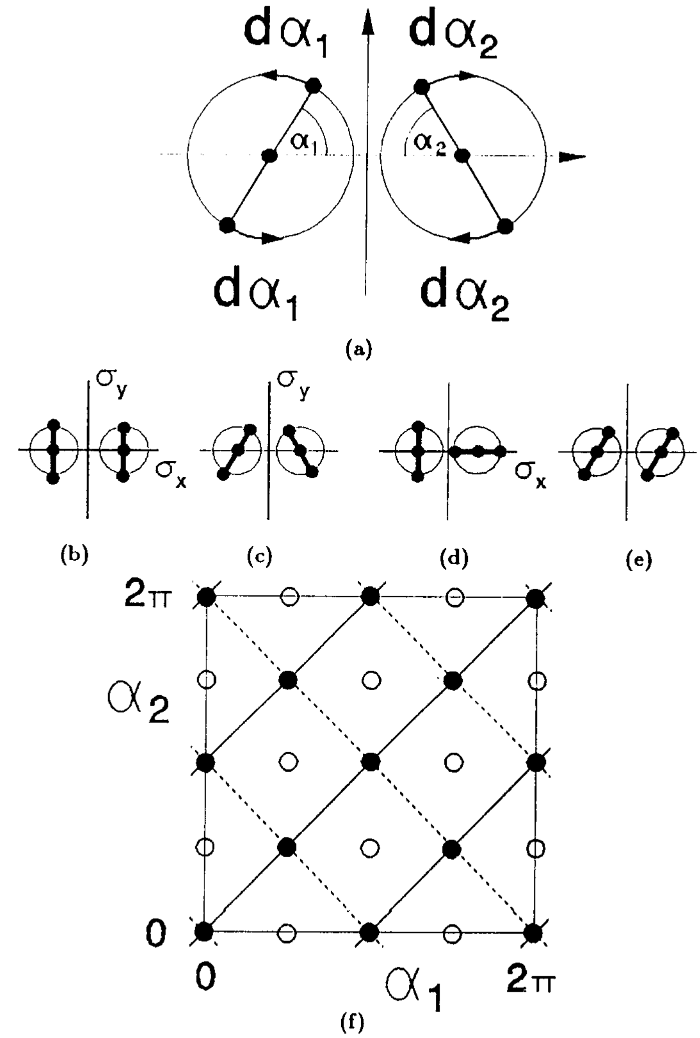

Figure 9. Two point pairs on two circles: coordinates and basis displacements (a), configurations with symmetries $\mathbb{D}_2^*$ (b), $\mathbb{D}_1^*$ (c and d), and $\mathbb{C}_2^*$ (e), and symmetry diagram with symmetries $\mathbb{D}_2^*$ (•), $\mathbb{D}_1^*$ (o and —), $\mathbb{C}_2^*$ (- - -), and $\mathbb{C}_1^*$ ("background").

5.6. Mixing of Three Forms

As has been stated in Section 2, a form variation may also be performed by a mixing of forms by weighted addition of their form functions or their Fourier coefficients [1]. Here, forms will be constructed by mixing pure Fourier coefficients of different symmetries according to

$$R(\varphi) = \beta_1 \cdot \cos k\varphi + \beta_2 \cdot \cos l\varphi + \beta_3 \cdot \cos m\varphi \tag{39}$$

with

$$\beta_1 + \beta_2 + \beta_3 = 1. \tag{40}$$

For the β_m's we take $0 \leq \beta_m \leq 1$, so they are located within the positive orthant $\mathbb{R}^3_+$ of the Euclidean space. Because of the restriction equation (40), the form space $\mathbb{F}$ is reduced to the *simplex* $\mathbb{S}^3$, i.e., the triangle between the points $P_1 = (1,0,0)$, $P_2 = (0,1,0)$, and $P_3 = (0,0,1)$ of $\mathbb{R}^3_+$. Figure 10 shows some examples of such form variations. It is evident that if the symmetry group at the vertex point P_i is $\mathbb{G}(P_i)$, then we must have on the edge E_{ij} connecting the points P_i and P_j

$$\mathbb{G}(E_{ij}) = \mathbb{G}(P_i) \cap \mathbb{G}(P_j), \qquad \text{(see footnote[13])} \tag{41}$$

and in the interior I of the simplex

$$\mathbb{G}(I) = \mathbb{G}(P_1) \cap \mathbb{G}(P_2) \cap \mathbb{G}(P_3) \tag{42}$$

so that the topology of isosymmetric lines is always very simple.

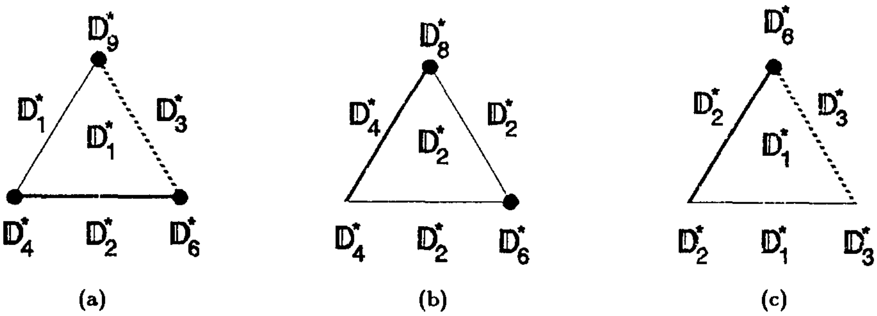

Figure 10. Simplices for the mixing of three Fourier coefficients:

$R(\varphi) = \beta_1 \cdot \cos 4\varphi + \beta_2 \cdot \cos 6\varphi + \beta_3 \cdot \cos 9\varphi,$ (a)

$R(\varphi) = \beta_1 \cdot \cos 4\varphi + \beta_2 \cdot \cos 6\varphi + \beta_3 \cdot \cos 8\varphi,$ (b)

$R(\varphi) = \beta_1 \cdot \cos 2\varphi + \beta_2 \cdot \cos 3\varphi + \beta_3 \cdot \cos 6\varphi,$ (c)

with $\beta_1 + \beta_2 + \beta_3 = 1$.

6. ISOSYMMETRIC MANIFOLDS IN FORM SPACES

6.1. Types of Isosymmetric Manifolds

The symmetry analysis of the form space shows that there are isolated points, lines, surfaces, and also volumes (in summary: *manifolds*) of constant symmetry. They have been termed "isosymmetric manifolds" here. In most cases considered in this paper, these manifolds are straight lines and planes, respectively, but in general, also curved lines and surfaces can be found (cf. the example in Figure 6).

The dimension N of the form space $\mathbb{F}$ is given by the number of coordinates that will be considered. Then there will be N normal deformations dn_i starting from every point P in $\mathbb{F}$. According to the irreducible representation to which a certain dn_i belongs, it leads from the symmetry $\mathbb{G}$ of the starting point to a second symmetry $\mathbb{G}_i$ in the neighbourhood of it. These relationships can be best displayed by a *deformation graph* (Figure 11) showing all N deformations starting from a point of given symmetry and the resulting symmetries,[14] symmetry-preserving deformations being represented by a loop. Since the kind of analysis performed in this paper will primarily predict a *descent* but not an ascent in symmetry, graphs have been directed to subgroups but not to supergroups (see, however, Section 6.2). In turn, every type of deformation graph results in a certain topology of the isosymmetric manifold in the vicinity of the point of the form space which is considered. The most important types for two-dimensional form spaces are shown in Figure 11.

In general, two normal deformations dn' and dn'' applied to a form $\mathfrak{F}$ (corresponding to a point P in the form space) with symmetry $\mathbb{G}$ will result in forms $\mathfrak{F}'$ and $\mathfrak{F}''$ with symmetries $\mathbb{G}'$ and $\mathbb{G}''$. Then, a linear combination

$$dn''' = \beta' dn' + \beta'' dn'' \qquad \text{with } \beta', \beta'' \neq 0 \tag{43}$$

(β', β'': weight factors) will result in a form $\mathfrak{F}'''$ with symmetry $\mathbb{G}'''$ where

$$\mathbb{G}''' = \mathbb{G}' \cap \mathbb{G}''. \tag{44}$$

[13] $\mathbb{G}_1 \cap \mathbb{G}_2$ means the section of the sets of symmetry elements of both groups.

[14] If non-equivalent points with the same symmetry occur in the form space, then there is a separate deformation graph for each point (compare isolated $\mathbb{D}_1^*$ points with points on $\mathbb{D}_1^*$ lines in Section 5.5).

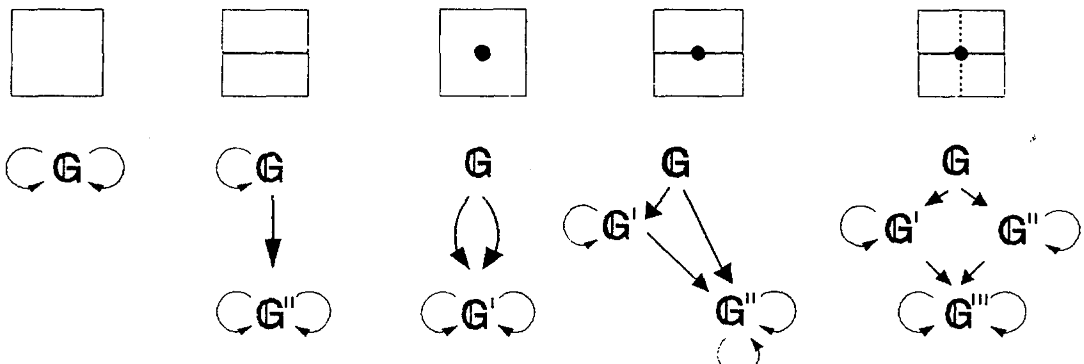

Figure 11. Topologies of isosymmetric manifolds around a reference point and the corresponding deformation graphs for this point taking into account only non-degenerate deformations (a–e). The reference point is always the centre of the square which is presumed to have symmetry $\mathbb{G}$. This point has been made to stand out only if its symmetry differs from that of neighbouring points. The directions of the normal coordinates n' and n'' corresponding to the two deformations dn' and dn'' (see text) are horizontal and vertical, respectively.

For two-dimensional form spaces, there are 5 possibilities displayed in Figure 11: if both normal deformations dn' and dn'' are symmetry-preserving[15] (i.e., $\mathbb{G} = \mathbb{G}' = \mathbb{G}'' = \mathbb{G}'''$), then P is part of an isosymmetric plane of $\mathbb{G}$ (Figure 11a). If dn' is symmetry-preserving and dn'' leads to some subgroup $\mathbb{G}''$ ($\mathbb{G} = \mathbb{G}' \supset \mathbb{G}'' = \mathbb{G}'''$), then we have P as a part of an isosymmetric line of $\mathbb{G}$ embedded in an isosymmetric plane of $\mathbb{G}''$ (Figure 11b). If both deformations lead to the same subgroup $\mathbb{G}'$ ($\mathbb{G} \supset \mathbb{G}' = \mathbb{G}'' = \mathbb{G}'''$), P is embedded in an isosymmetric manifold of $\mathbb{G}'$ (Figure 11c). If dn' and dn'' result in two subgroups $\mathbb{G}'$ and $\mathbb{G}''$ of $\mathbb{G}$ with $\mathbb{G}''$ being in turn a subgroup of $\mathbb{G}'$ ($\mathbb{G} \supset \mathbb{G}' \supset \mathbb{G}'' = \mathbb{G}'''$), then the point P with symmetry $\mathbb{G}$ lies on an isosymmetric line of $\mathbb{G}'$ embedded in a plane of $\mathbb{G}''$ symmetry (Figure 11d). The case of two deformations leading to two different subgroups ($\mathbb{G} \supset \mathbb{G}'$ and $\mathbb{G} \supset \mathbb{G}''$ with $\mathbb{G}''' = \mathbb{G}' \cap \mathbb{G}''$ and $\mathbb{G}' \neq \mathbb{G}'' \neq \mathbb{G}'''$) which corresponds to the example described in Section 5.5 is shown in Figure 11e. Thus, Figure 11 summarises the topologies of isosymmetric manifolds found for two non-degenerate deformations.

In sum:

(i) If there are s symmetry-preserving normal deformations starting in P (with symmetry $\mathbb{G}$), then P is part of an s-dimensional isosymmetric manifold of $\mathbb{G}$ spanned by the directions of the corresponding deformations. If all N deformations lead to the same subgroup $\mathbb{G}'$, then P is an isolated point (0-dimensional isosymmetric manifold) of $\mathbb{G}$ embedded in an N-dimensional isosymmetric manifold of $\mathbb{G}'$.

(ii) If in an N-dimensional form space there are only 2 symmetries $\mathbb{G}$ and $\mathbb{G}'$, s normal deformations starting from P (with symmetry $\mathbb{G}$) being symmetry-preserving, and s' deformations leading to symmetry $\mathbb{G}'$ ($s + s' = N$), then P lies in an s-dimensional isosymmetric manifold of $\mathbb{G}$ which comprises the whole form space if $s = N$, $s' = 0$, otherwise it will divide an N-dimensional isosymmetric manifold of $\mathbb{G}'$. If there are more then two symmetries in the form space, their mutual subgroup-supergroup relationships will determine the topology of the isosymmetric manifolds.

(iii) Intersection manifolds of isosymmetric manifolds are themselves isosymmetric manifolds. For the symmetry $\mathbb{G}(\mathbb{M}_1 \cap \mathbb{M}_2)$ of the intersection manifold of two isosymmetric manifolds $\mathbb{M}_1$ and $\mathbb{M}_2$, we have

$$\mathbb{G}(\mathbb{M}_1 \cap \mathbb{M}_2) = \mathbb{G}(\mathbb{M}_1) \cup \mathbb{G}(\mathbb{M}_2) \tag{45}$$

[15]Note that in the present context these are not only the totally symmetric deformations but also rotation and translations, if they are possible. In the following, $\mathbb{G}$, $\mathbb{G}'$, $\mathbb{G}''$, and $\mathbb{G}'''$ always refer to the symmetries of the reference point and the symmetries induced by dn', dn'', and dn''', respectively. The nomenclature in Figure 11 has been adapted to this convention.

(and analogously for more than two intersecting manifolds). Thus, the intersection manifold corresponds to a *supergroup* of the symmetries of the intersecting manifolds if the groups $\mathbb{G}(\mathbb{M}_i)$ are different as in the case of the $\mathbb{D}_2^*$ intersection point in Section 5.5, or if the intersecting manifolds belong to the same ($\mathbb{D}_n^*$) symmetry, but on the intersection manifolds the mirror lines have different positions (cf. the $\mathbb{D}_3^*$ point in Section 5.2). On the other hand, if the intersecting manifolds have the same ($\mathbb{D}_n^*$) symmetry, and the mirror lines of the intersecting manifolds coincide on the intersection manifold, then the latter has the same symmetry as the $\mathbb{M}_i$'s (cf. the $\mathbb{D}_1^*$ intersection point in Section 5.2).

6.2. Descent and Ascent in Symmetry

The symmetry analysis of deformations gives, in principle, informations about a ***descent in symmetry***: if a genuine deformation dn starting at a point P with symmetry $\mathbb{G}$ does not belong to the totally symmetric representation, then neighbouring points in the direction given by dn will have a certain lower symmetry. But what about an *ascent in symmetry*: how does the system pass to a higher symmetry? By combination of the symmetry analysis and the transformation of form space coordinates, this question can be answered unambigously:

(i) An ascent in symmetry is only possible through a genuine deformation belonging to the totally symmetric representation. This is simply since other deformations invariably *lower* the symmetry.

(ii) An ascent in symmetry is possible only through the one deformation which brings about the corresponding descent in symmetry. This is because the reversibility of deformations. The statements (i) and (ii) are connected as follows: since a normal deformation which induces a symmetry transition $\mathbb{G} \rightarrow \mathbb{G}'$ must preserve the symmetry elements of $\mathbb{G}'$, it will under $\mathbb{G}'$ belong to the totally symmetric representation. These relationships are illustrated in Figure 12 for the case of two point pairs on two circles (cf. Section 5.5). Here, in the subgroups $\mathbb{C}_1^*$, $\mathbb{C}_2^*$, and $\mathbb{D}_2^*$, the totally symmetric deformations lead either to the same group or to the supergroup. If, for instance, the deformation $dn = d\alpha_1 - d\alpha_2$ leads from $\mathbb{D}_2^*$ to $\mathbb{C}_2^*$, then this deformation must under $\mathbb{C}_2^*$ belong to the totally symmetric representation and potentially lead back to $\mathbb{D}_2^*$.

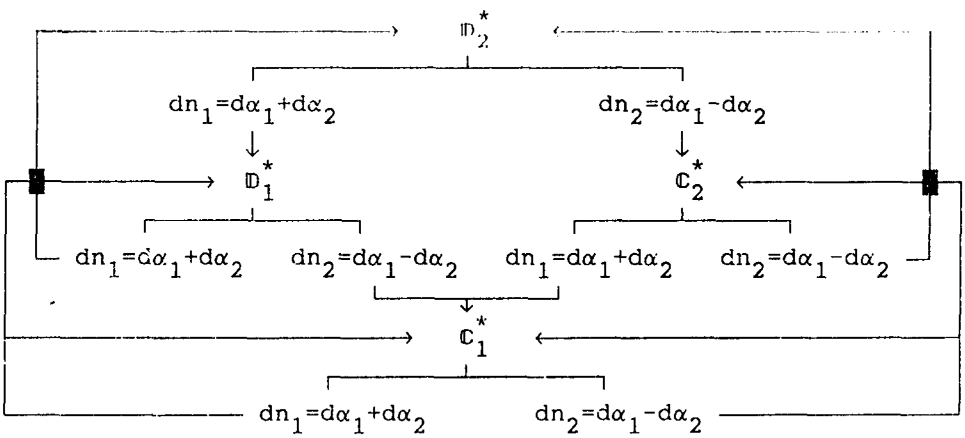

Figure 12. Routes between the different symmetries for two point pairs on two circles in relation to the two possible normal deformations (see text).

(iii) If a certain deformation dn' leads from symmetry $\mathbb{G}$ to its subgroup $\mathbb{G}'$, then it is possible to go back from $\mathbb{G}'$ to $\mathbb{G}$ along the very same deformation coordinate if, by this process, the value of the corresponding normal coordinate n' of the form space is brought to zero. In this way, the symmetry-reducing deformation can be cancelled. If there is more than one path between $\mathbb{G}$ and $\mathbb{G}'$ (cf. Figure 11c), then the normal coordinates corresponding to all of these ways have to be brought to zero. This is since $n' = 0$ means that there is no symmetry-reducing deformation at all in the direction of dn' (see next section). By the way, in Sections 5.3 and 5.4, the totally symmetric deformations should potentially lead to the supergroup of the respective system, *viz.*, $\mathbb{D}_\infty^*$ which will be reached if all points coincide. From the pictures of the totally symmetric deformations of both systems, it can be seen that this is possible. In this case, we find $n_1 = 0$.

6.3. Symmetry Analysis of a Form by Means of Its Normal Coordinates

The symmetry of a form can in an easy way be inferred from the values of its normal coordinates. This will be illustrated here for a square (cf. Sections 3 and 5.4). From the normal deformations of the square (equations (14) and (35)), the following normal coordinates of the form space can be derived by integration (see Section 4):

$$
\begin{aligned}
n_1 &= x_1 + y_1 - x_2 + y_2 - x_3 - y_3 + x_4 - y_4, & \\
n_2 &= x_1 - y_1 + x_2 + y_2 - x_3 + y_3 - x_4 - y_4, & (R_z), \\
n_3 &= x_1 - y_1 - x_2 - y_2 - x_3 + y_3 + x_4 + y_4, & \\
n_4 &= x_1 + y_1 + x_2 - y_2 - x_3 - y_3 - x_4 + y_4, & \\
n_5 &= x_1 + x_2 + x_3 + x_4, & (T_x), \\
n_6 &= y_1 + y_2 + y_3 + y_4, & (T_y), \\
n_7 &= x_1 - x_2 + x_3 - x_4, & \\
n_8 &= y_1 - y_2 + y_3 - y_4, & \\
n'_7 &= x_1 - y_1 - x_2 + y_2 + x_3 - y_3 - x_4 + y_4, & \\
n'_8 &= x_1 + y_1 - x_2 - y_2 + x_3 + y_3 - x_4 - y_4. &
\end{aligned}
\tag{46}
$$

For some simple forms resulting from a square by the different normal deformations (Figure 13), Cartesian and normal coordinates are given in Table 1.

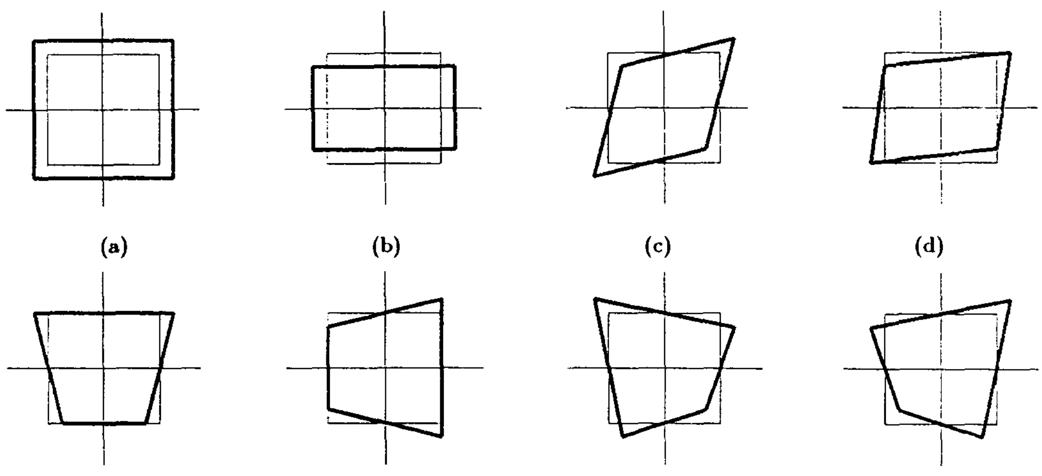

Figure 13. Schematic drawings of the forms resulting from a square (faint lines) by the normal deformations dn_1 (a), dn_3 (b), dn_4 (c), $dn_3 + dn_4$ (d), dn_7 (e), dn_8 (f), dn'_7 (g), and dn'_8 (h); compare with Table 1.

It is obvious that the normal coordinates, corresponding to the normal deformations by which the forms result from a square, have nonzero values; all others (except n_1, corresponding to the totally symmetric deformation, and linear combinations of nonzero coordinates like n'_7 and n'_8) vanish. This way, a simple and efficient symmetry analysis is possible by deducing the symmetry elements of a form as the set of symmetry elements which will be preserved by *all* deformations corresponding to nonzero normal coordinates of the form.

This type of analysis is possible, if the forms to be analysed are aligned with the coordinate system so that the orientation of their mirror lines and the numbering scheme of the vertices match the standard arrangement of Figure 2. It can, however, not necessarily be taken over to general orientations of the forms. Using the expressions for the normal coordinates in equations (46) for forms of arbitrary orientation means that the directions of the deformation vectors will be retained regardless of the orientation of the square. Figure 14 illustrates how the normal deformations change if point P_1 of the square is rotated.

Table 1. Cartesian and normal coordinates for the forms of Figure 13 resulting from a square by normal deformations dn_1 to dn'_8 (see text). Values for n_5 and n_6 (corresponding to the translations T_x and T_y, resp.) have been omitted: they vanish since the reference square is centered at the origin. Below the form names, the deformations by which they result from the square are given.

Form/ Deformation	Fig. 13		x_1 n_1	y_1 n_2	x_2 n_3	y_2 n_4	x_3 n_7	y_3 n_8	x_4 n'_7	y_4 n'_8	Symmetry
Square	a	x_i	1.2	1.2	−1.2	1.2	−1.2	−1.2	1.2	−1.2	$\mathbb{D}_4^*$
dn_1		n_i	9.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
Rectangle	b	x_i	1.2	1.0	−1.2	1.0	−1.2	−1.0	1.2	−1.0	$\mathbb{D}_{2xy}^*$
dn_3		n_i	8.8	0.0	0.8	0.0	0.0	0.0	0.0	0.0	
Rhombus	c	x_i	1.2	1.2	−0.8	0.8	−1.2	−1.2	0.8	−0.8	$\mathbb{D}_{2dq}^*$
dn_4		n_i	8.0	0.0	0.0	1.6	0.0	0.0	0.0	0.0	
Quadrilateral	d	x_i	1.2	1.0	−1.0	0.8	−1.2	−1.0	1.0	−0.8	$\mathbb{C}_2^*$
$dn_3 + dn_4$		n_i	8.0	0.0	0.8	0.8	0.0	0.0	0.0	0.0	
Trapezium	e	x_i	1.2	1.0	−1.2	1.0	−0.8	−1.0	0.8	−1.0	$\mathbb{D}_{1y}^*$
dn_7		n_i	8.0	0.0	0.0	0.0	0.8	0.0	0.8	0.8	
Trapezium	f	x_i	1.0	1.2	−1.0	0.8	−1.0	−0.8	1.0	−1.2	$\mathbb{D}_{1x}^*$
dn_8		n_i	8.0	0.0	0.0	0.0	0.0	0.8	−0.8	0.8	
Rhomboid	g	x_i	1.2	0.8	−1.2	1.2	−0.8	−1.2	0.8	−0.8	$\mathbb{D}_{1q}^*$
dn'_7		n_i	8.0	0.0	0.0	0.0	0.8	−0.8	1.6	0.0	
Rhomboid	h	x_i	1.2	1.2	−1.2	0.8	−0.8	-0.8	0.8	−1.2	$\mathbb{D}_{1d}^*$
dn'_8		n_i	8.0	0.0	0.0	0.0	0.8	0.8	0.0	1.6	

It can be seen that dn_1 (expansion of the square) continuously transforms into dn_2 (rotation), dn_3 transforms into dn_4, and *vice versa*, whereas dn_5, dn_6, dn_7, and dn_8 do not transform into one another. From the pictures it can be seen that in Figure 14a, the $\mathbb{D}_4^*$ symmetry of the square is preserved for all rotation angles (only the area of the square changes). In Figure 14b, the C_2 rotation axis is preserved under all circumstances, whereas the two mirror lines are preserved only in special orientations (first, third, and fourth one). In Figure 14c, for general rotation angles, the symmetry of the form is reduced to $\mathbb{C}_1^*$, and only for special orientations (first, third, and fourth), one mirror line is preserved. From these results, the following can be deduced:

(i) If, for an arbitrary quadrilateral, only n_1 and/or n_2 have nonzero values,[16] then this quadrilateral must be a square.

(ii) If n_3 and/or n_4 have nonzero values, the minimum symmetry of the form is $\mathbb{C}_2^*$, but in special cases it may be $\mathbb{D}_2^*$.

(iii) If n_7 and/or n_8 have nonzero values, then the symmetry of the quadrilateral will be $\mathbb{C}_1^*$, or in special orientations, $\mathbb{D}_1^*$.

Thus, for this special choice of normal coordinates (which can be checked very fast by a computer program), a reduced symmetry analysis of forms is possible. To take full advantage of the possibilities of such an analysis, one has to formulate the expressions for the normal coordinates in a rotation-invariant manner. This can be done by using analogues to the internal coordinates of molecules (radial and angular displacements of the vertices of the form). Then, $n_3 \neq 0$ and $n_4, \ldots, n_8 = 0$ would mean that the form has $\mathbb{D}_{2xy}^*$ symmetry,[17] $n_3 = 0$, $n_4 \neq 0$, and $n_5, \ldots, n_8 = 0$ would denote a $\mathbb{D}_{2dq}^*$ symmetry, whereas n_3, $n_4 \neq 0$, $n_5, \ldots, n_8 = 0$ would characterise a form with $\mathbb{C}_2^*$ symmetry. This way, a precise analysis of the form symmetry could unambiguously determine all symmetries of deformed squares displayed in Figure 7.

The restrictions described above are, of course, not relevant to the normal deformation analysis performed in Sections 3 and 5.1 to 5.6. There, the analysis is made for a precisely defined

[16]The normal coordinates corresponding to translations, i.e., n_5 (T_x) and n_6 (T_y), will not be considered here; they may have arbitrary values.

[17]$\mathbb{D}_{2xy}^*$ symmetry would mean in this enlarged context of rotated forms that the mirror lines bisecting the edges of the form are preserved; in $\mathbb{D}_{2dq}^*$, these would be the mirror lines running through the vertices of the form.

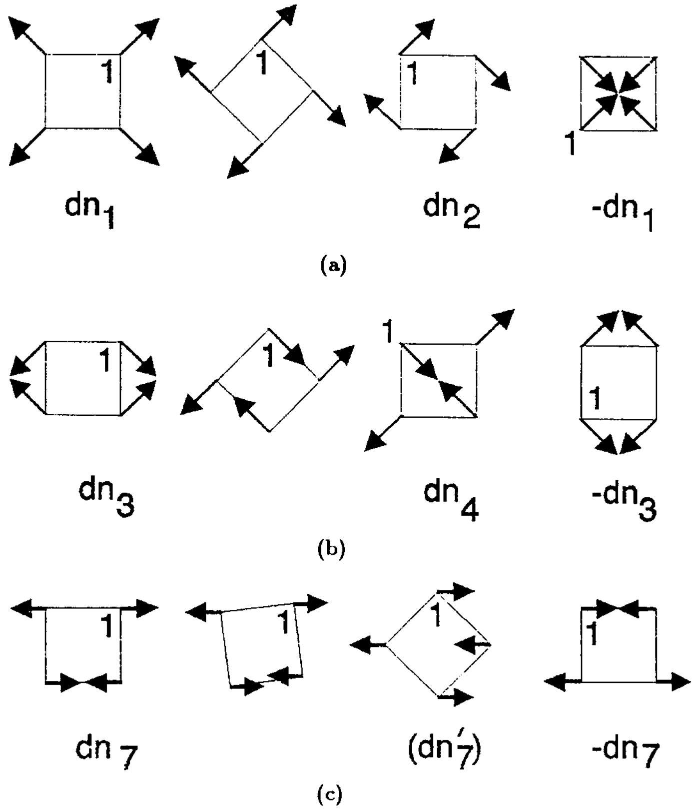

Figure 14. Effect of a rotation of the form on the normal deformations of a square when the respective directions of the displacement vectors are retained during the rotation, shown for dn_1 (a), dn_3 (b), and dn_7 (c); see text. The rotation angle can be inferred from the position of point P_1 which is marked by "1."

arrangement of the form. The conclusions drawn there about matrix representations are valid for arbitrary orientations of the form, in contrast to the mathematical expressions for the normal coordinates which can be taken over to arbitrary orientations only with the information loss detailed here.

7. CONCLUSIONS

The symmetry analysis of deformations presented here is in effect a local one: a certain point within the form space (a form) for which the analysis is to be made, has to be set in advance. Conclusions can then be drawn primarily for certain surroundings of this point. This is analogous to the analysis of vibrating molecules: there the analysis is performed in the vicinity of the equilibrium configuration of the molecule. In the form space, however, such a privileged configuration does not exist so that the restriction to a local analysis would be a drawback.

However, global predictions can be made at least for form spaces spanned by non-angular coordinates if throughout the form space, the same normal deformations are used. As has been shown in Section 5.2, under a subgroup symmetry, the projection operator technique may give a different composition of a normal deformation, but in such cases, the corresponding normal deformation for the supergroup will belong to the same symmetry species (cf. dn_2 and dn_2^* there). Conclusions about an ascent in symmetry and a simple and efficient symmetry analysis of forms based on their normal coordinates are also possible for these form spaces.

For form spaces spanned by angular coordinates, the situation is somewhat more complicated. Here, the isosymmetric manifolds give periodic structures since the angular coordinates are periodic, and singular points with higher symmetry (see Section 5.5) can arise. The locations of such points cannot be predicted in a conclusive manner up to now. It is hoped, however, that the utilisation of the fuzzy symmetry concept [1] can help in the search for points in the form space where such higher symmetries (compared to their surroundings) emerge. This will be the theme of a forthcoming paper.

In sum, the methods presented here are able to facilitate the analysis of isosymmetric manifolds in form spaces, to describe these high-dimensional spaces in an efficient way, to perform a fast and (in case of a rotation-invariant formulation of the normal coordinates) detailed symmetry analysis of forms, and to put the analysis of symmetry consequences of form deformations onto a sound basis.

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