

TOPOLOGICAL CLASSIFICATION OF SYMMETRY DEFECTS AND SOLITONS IN THIN LAYERS OF LIQUID CRYSTALS*

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The topological classification of symmetry defects and solitons in thin, essentially two dimensional, layers is given for some liquid crystals. The method of this classification is based on homotopy groups of a manifold of internal states of a liquid crystal.

1. Introduction

During the last few years there has been many successful attempts to introduce the methods of algebraic topology, such as the homotopy groups [1-3], as working tools into solid state physics. In particular the scheme of classification of defects and solitons¹ in an ordered media was introduced and successfully applied in liquid crystals, normal crystals, magnetic materials and helium 3 and 4 [4-14].

The classification of defects in three dimensional nematics, cholesterics, smectics A and C is in principle already completed [4-8, 12, 14]. However, not much work has been done on other smectics. The same is true for two dimensional problems (i.e., for thin and flat layers of liquid crystals).

Undoubtedly the problem was thought to be simple, especially since the three dimensional case was already solved. There are, however, some subtle aspects to the problem. For example, in three dimensional smectics the topological classification of defects meets one serious obstacle [12]. The possible distortions of the medium in principle cannot include such a class of distortions in which the smectic layers can be considerably bent or in which the thickness of smectic layers can be altered. By attempting to form such distortions we would simply break the layers and the cracks probably would be filled with disordered material (as suggested in slightly different contexts by [9]). The point is that such distortions are topologically possible and "contribute" significantly to the clas-

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¹ By terminology of Finkelstein "kinks" or "homotopons" (see D. Finkelstein, *J. Math. Phys.* 7, 1218 (1966)).

sification of defects. On the other hand, in thin flat layers of liquid crystal the bending of layers and the altering of their thickness are excluded by boundary conditions.

The second reason why the two dimensional problem is interesting follows directly from experiment. At least half of all experiments are being performed on thin layers of liquid crystals (the sample is contained between two glass surfaces — the distance between them is very small). The third reason is valid for one subgroup of smectic liquid crystals, which by de Vries [16, 17] are classified as liquid crystalline fluids². These smectics are of the A, C, B and F types [16]. They show distinct two dimensional, crystal-like, short range order. Each layer can be considered as an independent two dimensional crystal. The correlation between layers is rather weak. Therefore, it would seem that studying defects in short range order structures we can neglect the three dimensional structure of smectic layers and consider them as a stacked pile of independent two dimensional crystals. In the present paper we will study defects (and solitons) for thin essentially two dimensional, layers of nematics and smectics A, C, B and F.

In the second section we will present short range order and long range order symmetries of liquid crystals. We will also introduce the idea of short range order and long range order defects. They will be classified in the third section. The paper closes with very short summary.

2. Symmetry of liquid crystals

The knowledge of symmetry of the medium is crucial for the application of topological methods for the classification of defects. Up till now there was no doubt as to what is the symmetry of nematics, smectics A and C [16–19] (in the terminology of de Vries — smectics A₂ and C₂ [18]).

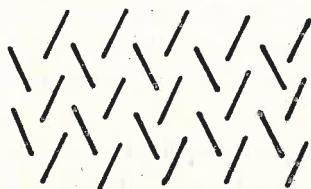


Fig. 1. The herringbone packing of molecules of liquid crystals. The long axes of the molecules are perpendicular to the plane of the drawing. Dashes denote "cross sections" of the molecules. The molecules, even if asymmetric, are represented as symmetric thanks to the two fold rotational disorder around their long axes and thanks to the symmetry up and down (the long axes point as frequently upwards as downwards).

There was, however, much doubt about the structure of other smectics. Now, the situation seems to be clarified [16]. Without going into details, we will give a short summary of the main results of papers [16, 17].

First of all, at any single instant of time, the natural packing of molecules in any liquid crystal is a herringbone packing (see Fig. 1). Such a packing is the true picture even

² In contrast to some smectics which are called liquid crystalline solids, [16, 17] because they show crystal-like three dimensional short range order.

for nematics! There is, of course, much additional molecular disorder, thanks to frequent reorientations around the long axes of the molecules. Therefore, on the average there is no symmetry at all. Sometimes a different situation can occur. A typical "disordered" molecule which, on the average, shows some symmetry, such as for example in smectic B [16], is represented on Fig. 2. The site symmetry at the point *P* in Fig. 2 is now *mmm* (i.e., three



Fig. 2. The disordered molecule for the smectic B

mirror planes perpendicular to one another). It should be stressed that such symmetry is statistical symmetry or mean symmetry. This means that if we could measure all positions and orientations of the molecules in one definite moment of time we would find no symmetry, i.e., complete disorder. In a sense the same situation occurs even in perfect crystals. In the crystal, however, if we average positions of atoms over a short time interval (say 10^{-13} sec) we find perfect order. The similar scale of time for smectics is undoubtedly many orders of magnitude longer (say 10^{-9} – 10^{-5} sec). The numbers given above are based on some typical experimental data which can be found in any handbook on physics, or chemical physics under the heading "relaxation times".

Summing up all what was said above, we see that sometimes in a statistical sense local symmetry can be quite high in liquid crystals. However, the liquid crystals behave much like fluids or, at most, as super soft solids [19, 20]. Therefore, it follows that local crystal-like symmetry (if any) can extend over distances of the order of a few molecular lengths. Such symmetry can be detected by X-ray diffraction [17]. The whole sample of the liquid crystal can be considered as a more or less random collection of minicrystals differently oriented. That is what we mean by the term: short range order symmetry. We can study the defects in a single minicrystal and we call them "short range order defects".

Sometimes, however, such a collection of minicrystals is not distributed completely randomly, and there is some average symmetry which extends over long "macroscopic" distances. We can study this symmetry with the aid of a microscope. Such symmetry can exist even in the absence of local short range order symmetry. The best example is the smectic A_2 . There is no short range order symmetry. However, the smectic as a whole has very high symmetry. Let us consider, for simplicity, a single layer of A_2 . It is invariant under translations on a plane and under rotation about the axis perpendicular to the plane. The molecules look on the average like trees in an infinitely large forest.

That is what we mean by long range order. Similarly we can introduce the definition of "long range order defects".

To finish this short discussion we will present a table where the symmetries for very thin layers of liquid crystals are given.

TABLE I

The symmetry groups for very thin layers of some liquid crystals according to [16]. The symbols which denote the symmetry groups are given both in Schoenflies and in the international notation (when possible). \wedge denotes semi-direct product. R denotes the group of one dimensional translations. I denotes operator of inversion for centrosymmetric molecules. For noncentrosymmetric molecules it denotes inversion multiplied by an operator \mathcal{P} which changes a left molecule into the right one. C_∞ denotes the group of all possible rotations around a fixed axis. D_∞ denotes the group C_∞ plus all possible two fold rotations around axes perpendicular to the axis C_∞ .

Miscibility symbol of liquid crystal	Short range order	Long range order
nematic or cholesteric ^a	—	$R^2 \wedge (D_2 \otimes I)^b$
A ₂	—	$R^2 \wedge (D_\infty \otimes I)$
A ₃	—	$R^2 \wedge (C_2 \otimes I)$
C ₂	—	$R^2 \wedge (C_2 \otimes I)$
B	$D_2^0 \otimes I$ (or $C_{222} \otimes I$)	$R^2 \wedge (D_\infty \otimes I)$
F	$C_2^3 \otimes I$ (or $C_2 \otimes I$)	$R^2 \wedge (C_2 \otimes I)$

^a In very thin layers of cholesteric liquid crystals the samples behave like nematics. There is simply no space for cholesteric pitch to develop.

^b We assume that the molecules of nematic are parallel to the surface of the layer.

3. The topological classification of defects and solitons

The general scheme of topological classification of symmetry defects in an ordered media can be presented in the following way [4–8, 11, 12, 14]:

Consider an infinite ordered media in a perfect state, which is a broken symmetry state. For example, if we have an isotropic molecular liquid invariant under the group G (in this case G is an Euclidean group in three dimensions, i.e., a semi-direct product of rotational group $O(3)$ and the three dimensional translational group R^3 — $G = R^3 \wedge O(3)$) and there is an isotropic to the nematic phase transition, then there appears a spontaneous nematic alignment n which breaks G invariance.

Putting examples aside and saying it directly: the symmetry group is broken from G , the group of physical laws, into H , subgroup of G which is the invariance group of the perfectly ordered state of the medium. In most cases G is simply a symmetry group of the high temperature phase [6].

In the example given above H is the subgroup of operations of $R^3 \wedge O(3)$ which do not change the orientation of the nematic director [20].

The perfect state of our medium is represented by one point of the orbit G/H . When the medium is not in the perfect state i.e., when it is distorted, we may still recognize a local state (represented also by a point of G/H) and this state varies from one point of the medium

to another. This situation can be described with the aid of a function φ which is defined in the space of our medium and valued in the orbit G/H . The points or lines where φ is not defined correspond to point or line defects.

A defect is called topologically stable if it is not possible to continuously extend φ over the defect. The trivial example of φ is $\varphi = \text{const}$. Such a function can always be continuously extended — therefore it cannot define any stable defects. On the other hand if φ is not homotopic to a constant (homotopic loosely speaking means — continuously deformable [1–3]) on an n dimensional sphere S^n surrounding a d' , dimensional defect (where $d' + n - 1 = d$, d is the dimension of the medium [5]) then φ can not be continuously extended inside the sphere and as a consequence the defect is topologically stable.

Generally speaking all possible φ can be divided into homotopy classes; the trivial one, homotopic to a constant, and non trivial ones. The two different φ can be continuously deformed the first into the second one, if and only if, they belong to the same single class.

The homotopy classes of the functions φ from S^n to G/H form a group called the n -th homotopy group or the n -th fundamental group $\Pi_n(G/H)$. Non-trivial elements of Π_n are in a one to one correspondence with types of stable d' dimensional defects. There is one exception for Π_1 . If Π_1 is non-abelian, the correspondence is between the types of the defects and conjugation classes of Π_1 . The simplest proof of the last statement can be found in reference [12].

The meaning of the trivial element of Π_n is that the medium inside S^n is in a perfect state or in a state which can be obtained from the perfect state by continuous deformation of the medium.

Summarizing all what was said above: if we want to have the topological classification of defects, then the knowledge of homotopy groups Π_n is crucial.

In a very similar way we can define topological solitons [10–13] i.e., linear, planar or three dimensional structures usually with a dense core (hence the name “point-like solitons”), for which the function φ is defined everywhere (no defects) but is not homotopic to a constant. However, the knowledge of Π_n is not always sufficient, or, to say it more strictly, appropriate for the classification of solitons [13].

The next remark is about the computation of G/H . The orbit G/H can be identified with the so called manifold of internal states V , which is also a topological space. Intuitively speaking, we can think of V as the manifold of all possible states the order parameter of the medium can take. For example, if $G/H = C_\infty$ i.e., the group of all possible rotations around one fixed axis, then C_∞ can be identified with a one dimensional sphere, $V = S^1$. In the present paper the identification is simple and we do not need any strict mathematical formulation (which can be found, for example, in reference [21]).

Before going to calculations let us make the very last remark about a different approach to defect classification. Such a classification is by the Volterra processes [22, 23]; to each Volterra process correspond one or several well known Burgers paths [6, 22, 23]. This approach was shown to be equivalent to the topological classification in a brilliant paper by Kleman [6].

Now we will proceed to explicit calculations.

3.1. Long range order

3.1.1. Nematics

In the case of a very thin layer of nematic we have

$$G = R^2 \wedge (D_\infty \otimes I), \quad H = R^2 \wedge (D_2 \otimes I), \quad (3.1)$$

where we assume that the z axis is perpendicular to the layer and coincides with the axis C_∞ .

The calculation of the manifold of internal states proceeds as follows:

$$G/H \sim D_\infty/D_2 \sim C_\infty/C_2 \sim P^1 \sim S^1, \quad (3.2)$$

where the axes C_∞ and C_2 are parallel with the axis z and where P^1 denotes the one dimensional projective plane which is topologically equivalent to the circle S^1 .

It is well known that

$$\Pi_0(S^1) = 1, \quad \Pi_1(S^1) = Z, \quad \Pi_2(S^1) = 1, \dots, \quad (3.3)$$

where 1 denotes the trivial one-element group and Z denotes the additive group of integers.

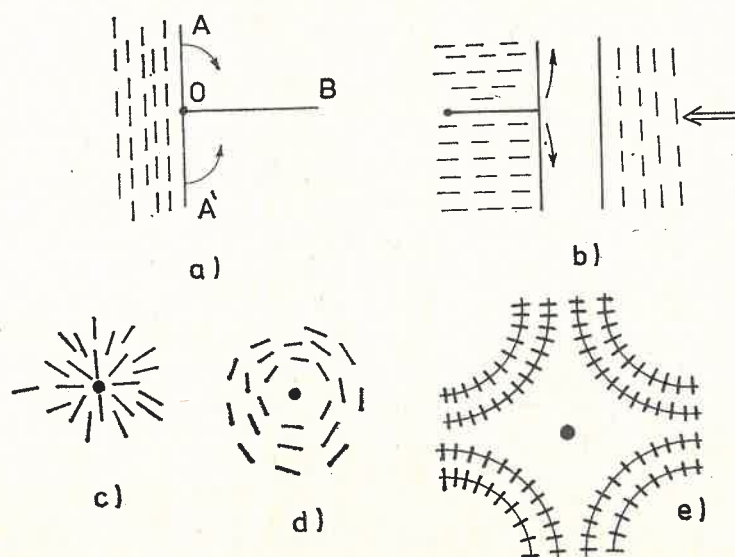


Fig. 3. The graphic representations of long range order point defects in a thin layer of nematic liquid crystal: a. the defect which can be labelled by the element $1/2$ belonging to Z ; the thick line denotes the line of cut and arrows denote the following deformation to the sample after which the lines OA and OA' will coincide with the line OB and the defect will be created; b. the defect $-1/2$; the double arrow denotes the motion of extra material which has to be added to the sample to create the disclination $-1/2$. The meaning of other symbols is the same as in a; c. the defect $+1$ — the so called two dimensional hedgehog; d. the same defect $+1$ — the configuration c can be continuously deformed into the configuration d; e. the defect -1 . The topologically stable defects c-e in the three dimensional case correspond to line defects which are not topologically stable [12]

(in this case the group of integers, and integers plus minus 1/2). The interpretation is as follows [4-6, 10-14]:

$\Pi_0 = 1$ — no line defects,

$\Pi_1 \neq 1$ — there are stable point defects,

$\Pi_2 = 1$ — no point-like solitons.

The graphic representation for the point defects is obvious [20] (see Fig. 3). The last thing to consider is the existence of linear solitons. For simplicity let us demand the following boundary conditions in the xy plane:

$$\lim_{|x| \rightarrow \infty} \mathbf{n}(x, y) = (0, 1). \quad (3.4)$$

The vector \mathbf{n} denotes the local nematic director which on the right and left hand sides of the plane at infinity is supposed to be parallel with the axis y . Such boundary conditions can be easily achieved in an experiment. (Let us note that for the nematic director \mathbf{n} and $-\mathbf{n}$ are equivalent.)

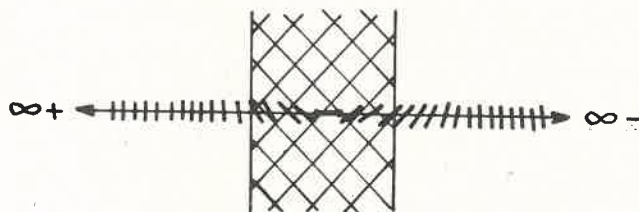


Fig. 4. The linear soliton $+1$ in thin layer of a nematic liquid crystal. The shaded region where the nematic director varies most quickly is called a core of the soliton. The core of the soliton in two dimensions or a core of a wall soliton in three dimensions is nothing else but the so-called "domain walls"

The nontrivial soliton configurations of \mathbf{n} can be distinguished by non trivial mappings of the line, which crosses soliton, into S^1 . This line can be chosen to be the x axis. The classes of topologically non-equivalent mappings:

$$[-\infty, \infty] \rightarrow S^1$$

with

$$\{-\infty\} \text{ and } \{+\infty\} \rightarrow (0, 1) \quad (3.5)$$

can be identified with $\Pi_1(S^1)$.

The graphical representation of linear soliton can be deduced from an example in Fig. 4.

3.1.2. Smectic A_2

This case is the simplest one:

$$G = R^2 \wedge (D_\infty \otimes I), \quad H = G. \quad (3.6)$$

Therefore, V consists of only one point. There are no defects and no solitons because all the groups Π_n are trivial.

3.1.3. Smectic C_2 or smectic A_3

When considering a single layer, C_2 and A_3 are identical. The group H is

$$H = R^2 \wedge (C_2 \otimes I) \quad (3.7)$$

and

$$G/H \sim D_\infty/D_2 \sim C_\infty \sim S^1, \quad (3.8)$$

where in (3.8) the two fold axis C_2 is perpendicular to the C_∞ axis which belongs to D_∞ . Therefore $D_\infty = C_\infty \wedge C_2$ and the quotient corresponds to C_∞ .

The homotopy groups Π_n are identical like that in section 3.1.1 and the classification of defects and solitons is similar to that for nematics. The appearance of defects will however be different, because in smectic C_2 the local order parameter can be represented by an arrow, the tip of which is, for example, the end of a molecule which makes contact with the glass bottom of a sample container.

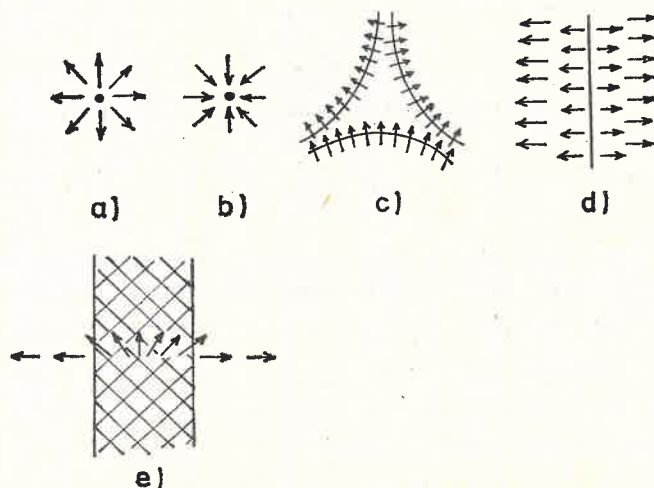


Fig. 5. The picture of long range order point defects in smectics A_3 and C_2 : a. the defect $+1$; b. the defect -1 ; c. a defect analogous to the defect $-1/2$ from Fig. 4 is not possible. It would result in at least one line in the medium where the order parameter looks like it does in Fig. 5d. Such configurations, as from Fig. 5d, at a closer look may either turn out to be solitons with very dense cores (see Fig. 5e) or are topologically unstable [12]

The group $\Pi_1 = Z$ in this case consists only of integers. For the rest see Fig. 5. The linear solitons in smectic C_2 look very similar to those for nematics. There is, however, a different kind of solitons which corresponds to different boundary conditions:

$$\lim_{x \rightarrow -\infty} n(x, y) = (0, 1), \quad \lim_{x \rightarrow \infty} n(x, y) = (0, -1), \quad (3.9)$$

where n denotes the local order parameter in C_2 (the same notation as for nematics).

Such solitons cannot be assigned to elements of any homotopy group [13]. As the boundary conditions (3.9) look quite natural the existence of such solitons, unfortunately, cannot be ignored.

Finally let us notice that long range order defects in smectics B are the same as in smectics A_2 (that is there are none) and the same in smectics F as in smectics C_2 .

3.2. Short range order

For nematics, and smectics A_2 , C_2 , A_3 there is simply no short range order symmetry. Therefore, we will consider only smectics B and F because only these are non-trivial.

3.2.1. Smectics B

The group H in two dimensions is

$$H = C222 \otimes I. \quad (3.10)$$

The body centred elementary cell is represented in Fig. 6. The quotient G/H can be expressed as (see Appendix A):

$$G/H \sim (R/Z)^2 \wedge (C_\infty/C_2). \quad (3.11)$$

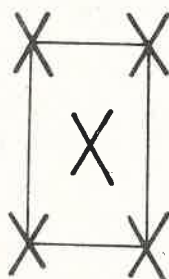


Fig. 6. The elementary cell for smectic B. The cell dimensions are a and b respectively

Owing to the fact that the semi-direct product is also the topological product [14] we obtain

$$\Pi_n((R/Z)^2 \wedge (C_\infty/C_2)) = \Pi_n(R/Z)^2 \wedge \Pi_n(C_\infty/C_2).$$

The groups $\Pi_n(C_\infty/C_2)$ are as we remember trivial with the exception that $\Pi_1(C_\infty/C_2) = Z$.

To calculate $\Pi_1(R/Z)$ we can use the theorem about the sequence of exact homomorphism [3, 12, 14]:

$$\dots \Pi_2(R) \rightarrow \Pi_1(R/Z) \rightarrow \Pi_0(Z) = Z$$

and the result is that $\Pi_1(R/Z) = Z$. The other $\Pi_n(R/Z)$ are trivial.

The final result is

$$\Pi_0 = \Pi_2 = 1, \quad \Pi_1 = (Z^{\text{tr}})^2 \wedge Z^{\text{rot}}, \quad (3.13)$$

where subscripts tr, rot (translational, rotational) were added simply for convenience.

Only short range order *point* defects can exist. These defects can combine translational dislocations (Z^{tr}) and disclinations (Z^{rot}) [22, 23]. As Π_1 is certainly non-abelian whole classes of conjugate elements of Π_1 (whole classes of Burgers circuits) will correspond to one type of defect (to one definite Volterra process). In reality disclinations (non-trivial elements of Z^{rot}) require much energy and are associated with very large strains [23]. In

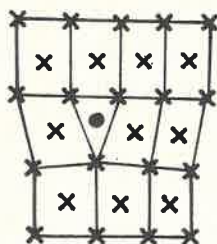


Fig. 7. A simple edge dislocation in smectic B

small short range structures which behave as super soft crystals they are not likely to occur. We are left in this case only with translational dislocations (edge dislocations) which require much less energy (see Fig. 7).

As for solitons, we will not look for them. The scale of length is too small.

3.2.2. Smectics F

The smectic F is simply a tilted smectic B. The symmetry group is $C2 \otimes I$. The elementary cell is represented in Fig. 8. The quotient G/H is equal to

$$G/H = (R/Z)^2 \wedge C_\infty.$$

The topological space is hence identical to the space for smectic B and $\Pi_1 = (Z^{tr})^2 \wedge Z^{rot}$. This case is formally the same as for smectic B. The difference would appear for disclina-

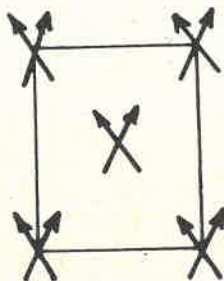


Fig. 8. The elementary cell for smectic F. The thick arrow shows the direction of the two fold axis

tions. We can remember that a similar situation occurred for long range order disclinations in nematics and smectics C_2 which also had the same group Z .

However, as disclinations in smectics B and F are not likely to occur, all this discussion is not necessary. To support this statement once more let us recall that the strain increases

linearly with the distance from the centre of disclination [22, 23]. Therefore, in each new "belt" of elementary cells surrounding the disclination there must appear many cracks or edge dislocations (if the period of translation is to remain at least approximately constant). Indeed, much more probable would be a transition of such a "would be disclination" to a completely disordered state [9].

4. Short summary

To sum up all the results of section 3 we collect them into Table II. Linear solitons in thin flat layers of liquid crystals (long range order) do exist for nematics and smectics A_3 and C_2 . For suitable boundary conditions at infinity, they can be classified by first homotopy group which in all cases is isomorphic with Z .

I would like to thank Dr K. Sokalski who aroused my interest in the present problems. Thanks are also due for his valuable comments.

TABLE II

Point defects in thin layers of liquid crystals. The topological classification by the first homotopy group

Liquid crystal	Long range order	Short range order
nematic	Z	1
A_2	1	1
C_2	Z	1
A_3	Z	1
B	1	$Z^2 \wedge Z$
F	Z	$Z^2 \wedge Z$

APPENDIX A

Let us calculate the quotient G/H for

$$G = R^2 \wedge (D_\infty \otimes I), \quad H = Z^2 \wedge (D_2 \otimes I).$$

The international symbol for $Z^2 \wedge D_2$ is $C222$. Z^2 denotes the group of two dimensional discrete translations.

1. First of all we will consider a simpler problem the solution of which will be useful for further considerations:

$$D_\infty = C_\infty^z \wedge C_2^x \quad \text{and} \quad D_2 = C_2^z \wedge C_2^x,$$

where the upper indices z, x show that the appropriate symmetry axis coincides with the z or with x axis respectively. Then

$$D_\infty/D_2 \sim C_\infty^z/C_2^z \sim P^1 \sim S^1$$

2. Now the group of matrices isomorphic with G and H are respectively:

$$\text{for } G: \begin{bmatrix} 1 & 0 & 0 & x \\ 0 & 1 & 0 & y \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c & s & 0 & 0 \\ -s & c & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & \text{sgn}_1 & & \\ & & \text{sgn}_1 & \\ & & & 1 \end{bmatrix},$$

where $c = \cos \psi$, $s = \sin \psi$, ψ is an angle and where $\text{sgn}_1 = \pm 1$;

$$\text{for } H: \begin{bmatrix} 1 & 0 & 0 & n \frac{a+b}{2} \\ 0 & 1 & 0 & m \frac{a-b}{2} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \text{sgn}_2 & & & \\ & \text{sgn}_2 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & \text{sgn}_3 & & \\ & & \text{sgn}_3 & \\ & & & 1 \end{bmatrix},$$

where n, m are integers and $\text{sgn}_2, \text{sgn}_3$ are ± 1 . The letters a, b denote the dimensions of the elementary cell.

3. The set of cosets G/H can be given by the generating elements $\{\alpha_1, \dots, \alpha_k\}$

$$G = \alpha_1 H + \alpha_2 H + \dots + \alpha_k H;$$

α_1 is the trivial element of G . It is easy to check that the general form of α is

$$\alpha = \begin{bmatrix} \tilde{c} & \tilde{s} & 0 & \tilde{x} \\ -\tilde{s} & \tilde{c} & 0 & \tilde{y} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

where

$$\tilde{c} \text{sgn}_2 = c, \quad \tilde{s} \text{sgn}_2 = s,$$

$$x = \tilde{x} + \tilde{c} \frac{n}{2} (a+b) + \tilde{s} \frac{m}{2} (a-b),$$

$$y = \tilde{y} - \tilde{s} \frac{n}{2} (a+b) + \tilde{c} \frac{m}{2} (a-b).$$

From this we see that one coset is obtained from the elements of G by choosing a given

angle ψ and x, y such that

$$x = \tilde{c}\varrho \frac{a+b}{2} + \tilde{s}\xi \frac{a-b}{2},$$

$$y = -\tilde{s}\varrho \frac{a+b}{2} + \tilde{c}\xi \frac{a-b}{2},$$

$$0 \leq \varrho < 1, \quad 0 \leq \xi < 1.$$

After this we take with this element all the other ones with the same ψ (or with $\psi' = \psi + \pi$) and with x, y such that ϱ, ξ can be increased by any integer. All the just mentioned elements together are the single element of the orbit G/H . This means that:

$$G/H \sim (R^2/Z^2) \wedge (C_\infty/C_2).$$

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