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DISTORTIONS WITH DOUBLE TOPOLOGICAL CHARACTER : THE CASE OF CHOLESTERICS

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Résumé. — La classification topologique des distorsions dans les milieux ordonnés conduit naturellement à une distinction entre distorsions singulières (défauts) et distorsions non singulières. Cependant, dans les cristaux liquides cholestériques, où le paramètre d'ordre contient des composantes de rigidités différentes, les distorsions optiquement observées présentent à la fois des aspects singuliers et non singuliers : elles ont un double caractère topologique. Ce phénomène, que l'on prédit exister aussi dans d'autres systèmes ordonnés, est analysé ici en termes de l'indice de Hopf pour un champ de directeurs.

Abstract. — The topological classification of distortions in ordered media leads naturally to a distinction between singular distortions (defects) and non singular distortions. However, in cholesteric liquid crystals, where the order parameter contains components with different rigidities, the optically observed distortions present both singular and non singular aspects : they have a double topological character. This phenomenon, which is predicted to exist also in other ordered systems, is analysed here in terms of the Hopf index for a director field.

In a 1974 paper [1], which is the basic reference for the present paper, one of us (Y. Bouligand) has presented various optical observations in cholesteric liquid crystals, together with a review of preceding work and theoretical interpretations.

Since then, a general topological classification of distortions in ordered media, based on homotopy theory (homotopy groups), has been developed. Obviously, it was interesting to examine what progress in understanding this topological theory could bring to the observations in cholesterics, which are among the most convenient materials for the experimental study of defects, due to the applicability of direct optical techniques. However, from the theoretical point of view, the order which exists in cholesterics is rather complex, with several subtleties ; as shown below, these subtleties have required refinements of the theoretical analysis, which promise to be of general interest.

1. **Brief history of theoretical interpretations.** — In 1969, before the developments of the topological analysis, Kléman and Friedel [2] introduced a classification of defects in cholesterics : they defined three types of disclination lines (called χ, λ, τ), each type with an index (+ or −).

In 1976, when the topological analysis was systematically applied to distortions in ordered media [3],

it was soon realized that, for some materials, the first homotopy group of the manifold of internal states, which describes linear defects in three-dimensional media, could be non commutative, with remarkable consequences [4, 6]. The best example, from a theoretical point of view, was found to be in biaxial nematic liquid crystals, which unfortunately have not yet been discovered nor synthesized.

In the meantime, Volovik and Mineev [7] were the first to apply the topological analysis to cholesterics and they showed that, in this case also, the first homotopy group was non commutative; in fact, $\pi_1 = Q$, the discrete quaternion group with eight elements, i.e. the same group that is predicted for biaxial nematics. In the light of the analysis of Volovik and Mineev, the early Kléman-Friedel classification reveals some insufficiencies, which is not surprising because they could hardly be guessed without the homotopic tools.

Another step had to be made before the theory could be usefully applied to the observations, such as those referred to earlier [1]. This was the full recognition, presented here, of the following fact : the order parameter, in cholesterics, is a frame of three orthogonal directions, but, among those, one is the direction of the elongated constituent molecules and, for energetic reasons, it, more than the other directions, *dislikes* any singularity. Therefore, the commonly observed distortions in cholesterics tend to be singular for the full order parameter and non singular for one part of the order parameter, the direction of the molecules. This double topological character can be seen as a complication, or, more accurately, as an enrichment compared to the standard situation, with simpler order parameters.

2. **General topological analysis and specificities of the cholesterics.** — The symmetry group of a medium with cholesteric order contains mixed translation and rotation elements. The cholesteric manifold of internal states, which is the quotient space of the disordered phase symmetry group by the ordered phase symmetry group [6, 7], is homeomorphic to $SO(3)/D_2$, as shown by Volovik and Mineev [7].

In the case of biaxial nematics [4], only rotation symmetry elements are actually relevant, and this leads to a complete picture in terms of a local order parameter, which is an orthogonal frame of three directions. The biaxial nematic manifold of internal states is $SO(3)/D_2$ and therefore the classification of distortions, by homotopy groups, is the same for biaxial nematics as for cholesterics.

The term *distortion* is used here as a general name to include singular distortions (defects), as classified [3], in dimension three, by the three first homotopy groups (π_0, π_1, π_2), and non singular distortions, as classified by the third homotopy group (π_3).

For $V = SO(3)/D_2$, one has

$$\pi_0(V) = 0\,, \qquad \pi_2(V) = 0\,, \qquad \pi_1(V) = Q\,,$$

where Q is the discrete quaternion group with eight elements. Using the notations of reference [4], rather than those of reference [7], these elements will be denoted

$$I, J, e_1, (-e_1), e_2, (-e_2), e_3, (-e_3)$$

with the combination rules

$$e_1 e_2 = -e_2 e_1 = e_3$$
$$e_1^2 = e_2^2 = e_3^2 = e_1 e_2 e_3 = J$$
$$J^2 = I\,.$$

So this group describes linear disclination defects in cholesterics or biaxial nematics. Because this is a non commutative group, it is not possible in general to attribute to a concrete disclination line an absolute name, and this leads to important physical consequences, as has been described [5]. A concrete disclination line can be named as belonging to a conjugacy class (for instance $\pm e_1$), and if the conjugacy class consists of only one element commuting with all the others, i.e. belonging to the centre of the group (for instance J), then the naming takes place as usual with commutative groups.

In biaxial nematics, where the local order parameter is a frame of three directions (called 1, 2, 3), on a loop surrounding an $\pm e_1$ line, the order parameter undergoes a rotation of angle π around the e_1 direction and similarly, respectively, for e_2 and e_3. On a loop surrounding a J line, the order parameter undergoes a rotation of angle 2π (no direction needs to be specified).

In cholesterics, one may introduce also a local frame of three directions (with, conventionally, direction 1 for the molecular director, direction 3 for the cholesteric direction, and direction 2 for the bi-normal) but some caution has to be exercised. Thus, in an undistorted configuration, this local frame is not homogeneous in space since the direction of molecules rotates. Therefore, in cholesterics a distortion cannot be simply regarded as a non homogeneity in space of this local frame, whereas it could be so defined in biaxial nematics. This difference is easily traced back to the presence or absence of translation elements in the ordered phase symmetry group. Although non mysterious in origin, this fact leads to some practical difficulties, in particular in the analysis of non singular configurations. We show below how this difficulty can be overcome.

Among the three directions of the cholesteric local frame, one direction does not *like* to have singularities : this is the direction of the molecules or molecular director. This can be taken as an experimental fact, but it is intuitively reasonable in terms of energy costs [1]. Thus the commonly observed defects are $\pm e_1$ or, most commonly, J disclination lines. Isolated J linear defects are observed forming rings (see for instance Fig. 5*a*, *b*, *o*, *p*, *q*, *r* in Ref. [1]) with

either two apparent cusps (*fuseau*) or one apparent cusp (*larme*), or in the form of two linked rings (*double anneau*). We are going to interpret and discuss these observed forms, with due account of the continuity of the molecular director. To do this, we need some results on the non singular configurations of three-dimensional vectors or directors.

3. **Hopf mappings for three-dimensional vectors or directors.** — The manifold of internal states for an order parameter which is a three-dimensional vector (resp. director) is the two-dimensional sphere (resp. projective plane)

$$V = S^2 \qquad (\text{resp. } P^2) .$$

In three-dimensional space, the non singular configurations of a vector (resp. director) field with homogeneous boundary conditions at infinity are mappings $S^3 \to V$ and they are classified by $\pi_3(V)$, where $V = S^2$ (resp. P^2).

In 1931, H. Hopf [8] was able to prove that

$$\pi_3(S^2) = \mathbb{Z} .$$

His proof is an historic achievement in algebraic topology, making manifest the difference between homology and homotopy groups. These Hopf mappings for a three-dimensional vector field were introduced in physics by D. Finkelstein [9], and they have recently attracted much attention in various domains [7, 10].

To each homotopy class of these mappings $S^3 \to S^2$ is attached an integer number, called the Hopf index. Before giving the rules for computing the Hopf index of a given configuration, we present a standard construction for mappings representative of the various classes. In this construction a continuous map $S^3 \to S^2$ will be described in terms of a vector field $\mathbf{V}(x, y, z)$ in R_3, such that for $x^2 + y^2 + z^2 \to \infty$ the limit of $\mathbf{V}(x, y, z)$ is well-defined and is independent of direction.

At the origin, is placed a vector which is arbitrarily chosen as vertical. At a point M(**r**), the orientation of the vector is obtained, from the orientation of the vector at the origin, through a rotation around **r** with an angle which is a monotonous function $f(r)$ of $r = |\mathbf{r}|$, with $f(0) = 0$. If $f(r \to \infty) = 2\pi$, one gets a configuration with a Hopf index equal to one. Generally, if $f(r \to \infty) = 2\pi h$, h integer, one gets a configuration with a Hopf index equal to h. (This construction can be generalized to change the Hopf index in an already distorted configuration.)

For a given configuration, which may be highly non symmetrical, the Hopf index can be computed as follows.

Consider the inverse image of one point in $V = S^2$, which is in general position. This inverse image in the three-dimensional base space will consist of a number of closed loops (this is easily seen on the standard mappings given above). Now, if one contracts smoothly this locus of the inverse image into one point, the image in $V = S^2$ of the contracting locus is going to sweep over S^2 a number of times, since it is, initially and finally, just one point. The algebraic number of times S^2 is swept during this process is a topological invariant (independent of the initial point chosen in S^2, if in general position, and independent of the contraction path), and this number is the Hopf index [11].

Another computation, first given by Hopf himself, expresses the index as the linking number of the inverse images of two points in general position in $V = S^2$. Consider two such points $x, y \in S^2$; their inverse images in real space are curves called, respectively, C_x and C_y. The sphere S^2 is orientable; let us choose one orientation. Let us choose also one orientation for the three-dimensional base space; then, from these two orientations, C_x and C_y become oriented curves. The linking number of these two oriented curves is an integer, denoted $lk(C_x, C_y)$, which is a topological invariant, equal to the Hopf index h

$$h = lk(C_x, C_y) .$$

It is easily shown that $lk(C_x, C_y) = lk(C_y, C_x)$; the linking number is independent of the orientation chosen in S^2; it changes sign when the orientation of the three-dimensional base space is reversed. Therefore, the sign of the Hopf index for one configuration is arbitrary but the relative sign of two distant configurations is well-defined. Again this computation is best visualized by considering the standard configurations presented above.

We examine now the same problem for a director field instead of a vector field. Because S^2 is a covering space for P^2, it follows that $\pi_i(S^2) = \pi_i(P^2)$ for $i \geqslant 2$; in particular one also has :

$$\pi_3(P^2) = \mathbb{Z} .$$

The standard construction given above for a vector field applies also for a director field. One might think for a moment that new configurations exist for a director field, corresponding for instance to $f(r \to \infty) = \pi$, but it is soon realized that such a choice does not provide homogeneous boundary values. In fact, the following theorem can be proved : any non singular configuration for a director field, on a simply connected manifold, gives a non singular configuration for a vector field, obtained by putting arrows on the directors. It is always possible to put arrows, whenever the director field is non singular, and one does not meet any contradiction in doing so. One can prove this by the following list of remarks : *a*) if one orients a director field at some point p, this induces, automatically, a well-defined orientation of the director field in some neighbourhood of p; *b*) if q is some other (let us say distant) point, and C is a path joining p to q one can propagate the orientation from p to q continuously, along the path; *c*) this could, of course, lead to problems since in general

different paths could lead to different results at q, but not so in the simply connected case.

The computation of the Hopf index, from a linking number, as given above for a vector field, would need adjustments to be extended to a director field since P^2 is a non orientable manifold. However, with the preceding theorem, there is an easy way out of this difficulty, which consists in putting arrows first on the directors, and this brings one back to the vector case. Since two diametrically opposite points on S^2 are just one point on P^2, one sees that it is actually possible to determine the Hopf index for a director field from the inverse image of only one point of P^2.

4. **Interpretation of the optical observations in cholesterics.** — When examined in suitably polarized light [1], a distorted cholesteric sample exhibits black lines which give the locus of points where the molecular director is vertical, that is precisely the inverse image of one point of P^2. This experimental feature allows therefore an easy determination to be made for the Hopf index of the director field as a linking number (which justifies the considerations presented in the previous section).

Let us examine successively the ring structures depicted on figure 5 of reference [1] : *anneaux en fuseau, anneaux en forme de larme, double anneau.* In all these cases, as explained in the drawings of figure 6 and figure 10 of reference [1], along the rings there are lines of singularity, of type *J*, for the full cholesteric order parameter. Because the element *J* of $\pi_1 = Q$ commutes with all elements of the group Q, there is no topological obstruction, at this level, for the crossing of two lines [5].

Then, when it is realized that these ring structures are also non singular configurations for the molecular director field (which is only one part of the full cholesteric order parameter), several questions may be raised : What are the Hopf indices associated with these various structures ? That is, can they be created or transformed into one another continuously, i.e. without ever creating a singularity in the molecular director field ? Can the linked rings of figure 5*r* be unliked continuously ?

a) *Anneau en fuseau* (Fig. 5*a* [1]). — Its Hopf index is $h = 0$. This can be determined in various ways. The most direct way consists in recognizing that the black line is the inverse image of one point of P^2 ; to have a non trivial configuration of the molecular director field, this inverse image would have to be self-linked, which is not the case.

Therefore, an *anneau en fuseau* can be created from a non distorted configuration, without ever making a singularity in the molecular director field. There is no topological barrier for creation, at this level.

b) *Anneau en forme de larme* (Fig. 5*b* [1]). — Its Hopf index is again $h = 0$. The preceding argument applies here also, and also the preceding conclusion. Moreover, an *anneau en fuseau* may be transformed into an *anneau en forme de larme*, without any break of continuity in the molecular director field. This is not so obvious when looking at the drawings of figure 6 [1].

c) *Double anneau* (Fig. 5*o, p, q, r* [1]). — Its Hopf index is $h = -1$. This is best seen by putting arrows on the molecular directors in the drawings of figure 10*f* [1]. Then one black line is recognized as the locus of up vectors and the other black line as the locus of down vectors. These inverse images of two points in S^2 have a linking number equal to (-1). The arbitrariness in sign, due to the arbitrariness in the orientation of space, is removed if one chooses the orientation of space according to the natural orientation provided by the cholesteric order.

As a consequence, there is a topological obstruction to the unlinking of such double rings, which comes not from the singular nature of the distortion but from its non singular nature. Thus, these double rings may be termed topological atoms.

It is worth pondering on the fact that the simplest non trivial Hopf configuration for a director field, as seen in polarized light optical techniques, appears as a linked double ring. This double ring is a beautifully direct manifestation of the double connectedness of projective space. This fact is of importance for all liquid crystals, nematics, smectics, ... and not only for cholesterics.

In appendix I, it is shown how detailed predictions can be made for more complicated distortions, with double topological character, in cholesterics. In appendix II, a formula for linking numbers, which is useful to compute higher Hopf indices, is presented.

5. **Conclusion.** — In conclusion, some remarks may be useful to unveil the generality of the phenomenon studied in this paper.

Consider a material which can exist in three phases (named P_1, P_2, P_3) whose symmetry groups are $G_1 \supset G_2 \supset G_3$. For instance, one may have a cholesteric phase (P_3), a nematic phase (P_2), an isotropic phase (P_1).

The general topological classification of defects leads naturally to a classification of the defects of phase P_3 which have a P_1 core. However, it may be of interest, for energetic reasons, to consider the restricted class of defects of phase P_3 which have a P_2 core. In our example, this meant considering defects in a cholesteric phase which have a nematic core (no singularity in the molecular director). In this way, energetic considerations can be progressively introduced into the topological analysis.

If, by varying some external parameters (temperature, pressure, ...) one is able to drive the material successively from phase P_1 to phase P_2, and then to phase P_3, some new questions appear. In phase P_2, various topologically stable distortions (singular and non singular) may exist. What will happen after the transition from phase P_2 to phase P_3 takes place ? For instance, does a non singular configuration (with a

given Hopf index) in a nematic phase imply the apparition of cholesteric defects, after a (gedanken) transition from a nematic phase into a cholesteric phase ?

This sort of problems appears, more generally, whenever several types of order coexist in the same material. The distortions associated with one type of order may act as obligatory sources of distortions of another type of order. This problem meets and enlarges the idea of frustration, which was introduced to describe the coupling between a matter field and a gauge field [12].

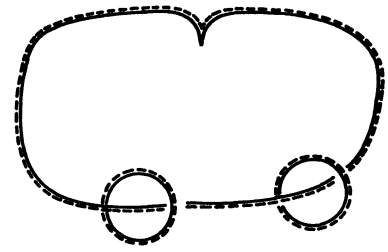

FIG. 1. — This triple ring structure, with Hopf index $h = -2$, is predicted to be observable in a right-handed cholesteric. The dotted line represents the optically observed whitish line, discussed in appendix I.

Appendix I. — Experimental determination of the orientation of a defect line of type J (Bouligand convention) and conservation laws for one ring.

In reference [1], it was shown that a defect line of type J (*fil épais*) its seen in suitably polarized light as a black line, locus of vertical directors, with a whitish line on one side, the side with one extra cholesteric pitch. The presence of the whitish line allows one to give an orientation to the black line and the following convention was adopted : looking in the positive direction, the whitish line is on the right side, for a right handed cholesteric, and on the left side, for a left handed cholesteric.

Once the inverse image of the vertical direction has received an orientation, according to the preceding recipe, the determination of the Hopf index of a give distortion readily follows.

Actually, there are stronger conservation laws, one for each closed ring, due to the discrete nature of the cholesteric translation periodicity. When circumnavigating along a closed ring, one must come back to the same height on the cholesteric axis. This rule can be expressed as

$$N_q + N_t + N_c = 0 ,$$

where N_q is the change of height due to rotation of the J line in space (a 2π rotation in the positive sense, according the cholesteric orientation, gives a lift of + 1, in cholesteric pitch units) ; N_t is the change of height due to traversals of another J type ring (its value is − 1 per traversal) ; N_c is the change of height due to cuspoidal points (its value can be either 0 or + 1, per cuspoidal point). For illustrative drawings, see reference [1].

With these rules, one can make detailed predictions for the observable distortions. For instance, the triple ring structure, depicted in figure 1, with Hopf index $h = -2$, should be observable.

Appendix II. — A formula for linking numbers.

We give below a certain formula for computing linking numbers of composite curves, which is both useful for our purposes and physically suggestive.

Let us start by considering a simple closed (oriented) curve $C_1 \subset S^3$. It can be shown that C_1 is always the boundary of some orientable (in general non simply connected) surface $\Sigma \subset S^3$, called a *Seifert surface* for C_1. If K is some other curve, disjoint from C_1, then lk (C_1, K) is simply the number of points in $\Sigma \cap K$, correctly counted (which means each intersection point being given the appropriate sign).

In particular, if one pushes C_1 slightly into Σ, one gets a curve C_1', which follows closely C_1, without *spiraling around* C_1, and $lk(C_1, C_1') = 0$. In general, if some curve C_1' follows closely C_1, there will be a certain amount of spiraling and this is measured exactly by $lk(C_1, C_1')$.

Consider now two disjoint curves C_1, C_2 and two other curves C_1', C_2', following them closely (with a certain amount of spiraling around). Using the Seifert surfaces, it can be easily shown that the linking number for the composite curves $C = C_1 + C_2$, $C' = C_1' + C_2'$ is :

$$lk(C, C') = lk(C_1, C_1') + lk(C_2, C_2') + 2\, lk(C_1, C_2) .$$

So there are three terms : the first two coming from the spiraling of C_1' (respectively C_2') around C_1 (respectively C_2) and a third *interaction* or *orbital term* reflecting the way C_1 and C_2 are linked together.

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