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ON THE CLASSIFICATION OF DEFECTS IN THE SMECTIC PHASES Sm A AND Sm C

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Résumé. — On calcule les groupes d'homotopie qui donnent la classification topologique des défauts des phases smectiques A et C. On obtient d'abord ces résultats par un usage direct des méthodes classiques de la topologie algébrique, avant de les discuter par une méthode plus intuitive et plus géométrique, qui repose sur le fait qu'une ligne de disinclinaison particulière doit disparaître dans la transition physique d'une phase C à une phase A.

Abstract. — We calculate the homotopy groups which yield the topological classification of defects for the smectic A and C phases. After having shown how a direct use of classical methods in algebraic topology lead to the required results, a more intuitive and geometrical discussion of the results is given, which relies on the fact that a specific disclination line should disappear in a physical transition from the Sm C to the Sm A phases.

It has been shown in [1] that, given an ordered medium, the homotopy groups of the manifold of its internal states V permit a classification of the topologically stable defects in this medium. The manifold V is a representation of the topological properties (dimensionality, connectivity) of the *order parameter* and it has been demonstrated in [2] that V is an orbit G/H of the thermodynamic group G (generally the Euclidean group E') with respect to the subgroup H, the symmetry group of the ordered medium.

In this note we give the homotopy groups which yield the topological classification of defects in the smectic A and C phases. We think it useful to explain to physicists how one can compute such groups, using the powerful methods of algebraic topology (first paragraph); but in the following paragraphs a more intuitive and geometrical discussion will also be given which uses the fact that the symmetry group of the Sm C phase is a subgroup of the Sm A phase symmetry group.

These symmetry groups are respectively [3, 4] ([1])

$$H'_C = (Z \times R^2) \square C_{2h} \quad H'_A = (Z \times R^2) \square D_{\infty h} . \tag{1}$$

([1]) We use the following notations for groups : Z, R additive group of integer, real numbers ; Z_n ,cyclic group of n elements ; $\times$ direct product, $\square$ semi-direct product of groups ; $SU(2)$ is the group of 2×2 unitary matrices with determinant 1. We follow Landau and Lifschitz [14] notations for the point groups C_{2h}, $D_{\infty h}$, C_i, D_i etc... and we refer to them for their definition.

1. — We shall call E the connected subgroup of E' (i.e. without reflections) and $H_A = E \cap H'_A$, $H_C = E \cap H'_C$. We denote by $\overline{E}$ the universal covering of E and by θ the surjective homomorphism $\overline{E} \xrightarrow{\theta} E$; its kernel, the center of $\overline{E}$ is the two-element group generated by the rotation through 2π. Equivalent definition of the orbits V_A and V_C are :

$$E'/H'_x = E/H_x = \overline{E}/\overline{H}_x = V_x$$

where

$$x = \text{A or C} \tag{2}$$

and where $\overline{H}_x = \theta^{-1}(H_x)$, the inverse image of H_x by θ.

Note that V_A and V_C are both connected since they are bases of connected fiber bundles E or $\overline{E}$, with fibers H_x or $\overline{H}_x$; hence

$$\pi_0(V_A) = 1 = \pi_0(V_C) . \tag{3}$$

In order to compute the homotopy groups π_i, $i = 1, 2, 3$, of V_A and V_C we use the long homotopy exact sequence for a principal fiber bundle [6, para. 17.11] ([2]) which is here applied to the total space $\overline{E}$ with base V_x and fiber $\overline{H}_x$; this is the best of

([2]) These physicists who find this group theory heavy going can skip this paragraph and go to para. 2. But they can get knowledge of the necessary concepts in ref. [5] and [6]. However, it remains that a few concepts, and in particular that of exact homotopy sequence, are essential throughout this paper.

the possible choices in eq. (2), because $\pi_1(\overline{E}) = 1$, so that the long homotopy sequence *breaks more*.

$$\begin{aligned}\to \pi_3(\overline{H}_x) \to \pi_3(\overline{E}) \to \pi_3(V_x) \to \pi_2(\overline{H}_x) \to \\ \to \pi_2(\overline{E}) \to \pi_2(V_x) \to \pi_1(\overline{H}_x) \to \pi_1(\overline{E}) \to \\ \to \pi_1(V_x) \to \pi_0(\overline{H}_x) \to 1 .\end{aligned} \quad (4)$$

This sequence ends with 1 because $\overline{E}$ is connected [7]. Moreover $\overline{E}$ has the homotopy of its maximal compact subgroup $SU(2)$ ([3]).

$$\pi_n(\overline{E}) = \pi_n(SU(2)) \quad (5)$$

hence

$$\pi_1(\overline{E}) = 1 = \pi_2(\overline{E}) \quad \text{(see ref. [8])} \quad (6)$$

$$\pi_3(\overline{E}) = Z \quad \text{(see ref. [9])} \quad (7)$$

which yields

$$\pi_2(V_x) = \pi_1(\overline{H}_x) ; \quad \pi_1(V_x) = \pi_0(\overline{H}_x) . \quad (8)$$

Sm C. We have to compute $\overline{H}_C$. We remark that a rotation of π is of order 2 in E (i.e. its square is 1) and of order 4 in $\overline{E}$ (its square, i.e. the rotation of 2π, is indeed the non-trivial element of the center of $\overline{E}$), so $\overline{H}_C = (Z \times R^2) \square Z_4$, and from the remark in foot-note ([3]) $\pi_n(\overline{H}_C) = \pi_n(\overline{K}_C)$ where $\overline{K}_C = Z \square Z_4$. Since $\overline{K}_C$ is a discrete group, $\pi_0(\overline{H}_C) = \overline{K}_C$ and, for $n > 1$, $\pi_n(\overline{H}_C) = 1_C$. So the long exact sequence splits for each n, and for $n > 1$ it yields the isomorphisms $\pi_n(\overline{E}) = \pi_n(V_C)$.

To summarize :

$$\begin{aligned}\pi_3(V_C) = Z ; \quad \pi_2(V_C) = 1 ; \\ \pi_1(V_C) = Z \square Z_4 ; \quad \pi_0(V_C) = 1\end{aligned} \quad (9)$$

Sm A. We have first to compute $\overline{D}_\infty = \theta^{-1}(D_\infty)$. The abstract groups D_∞ and $\overline{D}_\infty$ are both extensions of Z_2 by C_∞ with the same action (α, the non-trivial element of Z_2, changes $r \in C_\infty$ into r^{-1}), but while D_∞ is the semi-direct product, $\overline{D}_\infty$ is a non-trivial extension ; the square of each element of the connected component $\neq C_\infty$ is now the non-trivial square root of 1 in $\overline{C}_\infty$; in geometrical terms, in D_∞ the elements $\notin C_\infty$ are rotations of π with square 1 in E and, when pulled-back in $\overline{E}$ by θ^{-1}, their square is the rotation of 2π. So, although $K_A = \pi_0(H_A) = K_C$, we have

$$\pi_0(\overline{H}_A) = K_A = Z \square Z_2 . \quad (10)$$

The higher homotopy depends only on the connected component : containing the unit element of $\overline{H}_A$, it is $\overline{C}_\infty$, the double covering of C_∞ but isomorphic to it, hence, for $n > 0$, $\pi_n(\overline{H}_A) = \pi_n(S^1)$, i.e.

$$\pi_1(\overline{H}_A) = Z ; \quad \pi_n(\overline{H}_A) = 1 \quad \text{for} \quad n > 1 . \quad (11)$$

Again, the long exact sequence splits at $\pi_n(\overline{H}_A)$ for each $n > 2$, i.e., for $n > 2$

$$\pi_n(V_A) = \pi_n(\overline{E}) = \pi_n(SU(2)) = \pi_n(V_C) . \quad (12)$$

For $n \leqslant 2$, the splitting is obtained by

$$\pi_2(\overline{E}) = 1 = \pi_1(\overline{E}) ,$$

so that we have

$$\pi_2(V_A) = \pi_1(\overline{H}_A) . \quad (13)$$

Finally, collecting our results obtained on the homotopy sequence of $\overline{H}_A$, $\overline{E}$, V_A :

$$\begin{aligned}\pi_3(V_A) = Z ; \quad \pi_2(V_A) = Z ; \\ \pi_1(V_A) = Z \square Z_2 ; \quad \pi_0(V_A) = 1 .\end{aligned} \quad (14)$$

2. — Now, let us be more intuitive and physical. According to [2] we have, for Sm C, the following results :

a) There are no topologically stable walls in the Sm C phase, since $\pi_0(E'/H'_C) = 1$: both E' and H'_C contain a symmetry by reflection, and we have $E'/H'_C = E/H_C$.

b) The homotopy groups $\pi_i(V_C)$ for $i \geqslant 2$ are all equal to $\pi_i(E)$ (ex. : $\pi_2(E) = 1$: there are no stable singular points ; $\pi_3(E) = Z$: there are topological solitons.)

c) $\pi_1(V_C)$ is isomorphic to the lifting of H_C in the covering group of E, ($\overline{E} = SU(2) \square R^3$), and one gets $\pi_1(V_C) = Z \square Z_4$ (see eq. (9)), where Z corresponds to the dislocations of translation, and Z_4 to the disclinations. This group is non-abelian. Write an element of $\pi_1(V_C)$ as (p, α) where p is an integer and α one of the elements of $Z_4 = (I, a, a^2, a^3)$. One has the following composition law

$$(p, \alpha)(q, \beta) = (p + \alpha(q), \alpha\beta) \quad (15)$$

where

$$\alpha(q) = q \quad \text{if} \quad \alpha = I, a^2$$

$$\alpha(q) = -q \quad \text{if} \quad \alpha = a, a^3 .$$

The change of sign indicates that the rotations of angle $\pm\pi$ (the elements a and a^3) reverse the translations. The only dyad axis in the Sm C phase is perpendicular to the plane of symmetry and the dislocations (p, a) and (p, a^3) are obtained by applying a Volterra process about that axis [10]. The element $(0, a^2)$ corresponds to the fabrication of a disclination by a 2π rotation Volterra process about any axis, but it is enough to consider for the sake of clarity those defects built about the normal to

([3]) A semi-direct product of groups is a topological product considered as a topological space. The homotopy groups of a topological product are direct products of the homotopy groups of the factors. In such a topological product we can omit the contractible factor such as R^3 since its homotopy is trivial.

the layers. The element $(0, a^4)$ corresponds to a 4π rotation and is also the unit element of $\pi_1(V_C)$ $(a^4 = I)$: the 4π disclinations are not topologically stable. The Volterra process applied successively to the normal to the layer (2π rotation) and to any axis (4π rotation) brings a $(0, a^2)$ disclination (formerly built along the normal to the layers), along the direction of the 4π object. A detailed description of all the defects of the Sm C phase is to be found in [10]. We refer to ref. [2] for the coalescence of line defects according to homotopy classes and to ref. [15] for their possibility of crossing.

3. — The physical process of continuous phase change between the Sm C and the Sm A phases consists in tilting the optical axis towards the normal to the layers. This geometrical description can be expressed as follows : let us assume that we know the manifold of the internal states $V_A = V(\text{Sm A})$. To each point in V_A we put in correspondence a one-parameter family of orientations of the Sm C phase, by keeping the orientation of layers constant but moving the optical axis on a cone about the normal to the layer ; all these positions define a circle S^1 ; in mathematical terms S^1 is the fiber of the fiber bundle with base V_A, and bundle V_C [6] : all the orientations of the Sm C phase are indeed reached once and only once when one performs the former geometrical operation at all points of V_A.

Reciprocally, let us consider, the set of all loops on V_C whose homotopy class is $(0, a^2)$; we know from § 2 that they correspond to 2π disclination lines about the normal to the layers (Fig. 1). These loops clearly deal with the geometrical operation just considered, and the fibers S^1 are in the same homotopy class. The 2π disclination lines disappear when the Sm C phase is transformed to the Sm A phase. Therefore, V_A is obtained from V_C by identifying on V_C all the points of each loop of a family of $(0, a^2)$ loops fibering V_C. In the same way, all the elements in $\pi_1(V_C)$ which are in the conjugacy class (4)

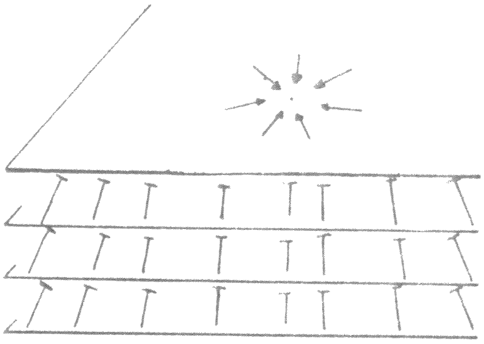

FIG. 1. — Typical $(0, a^2)$ disclination line in a Sm C phase. The vectors represent the projection of the optical axis on the layer. We have used the symbolism of the *nails* for the molecules in the vertical plane afore the singularity. It is assumed in this drawing that the line is transverse to the layers, but this is not essential.

(4) It happens that $(0, a^2)$ is the only element of its conjugacy class.

of $(0, a^2)$, or which pertain to the smallest subgroup containing this conjugacy class, disappear when $V_C \to V_A$. This subgroup consists of the elements $(0, 1)$ and $(0, a^2)$. It is isomorphic to Z_2 and is the kernel of the mapping $\pi_1(V_C) \to \pi_1(V_A)$. Hence

$$\pi_1(V_A) \simeq \frac{\pi_1(V_C)}{Z_2} = Z \,\square\, Z_2 . \tag{16}$$

Let us notice furthermore that $(0, a^2)$ is equal to its own inverse. Geometrically, this means that an oriented loop of this class can change orientation after each of its point has performed a closed path on V_C. This indicates clearly that V_C cannot be obtained as a direct product of V_A by S^1 : rather it is a situation analogous to that one in which one obtains a Moebius ribbon by fibering a circle (the base) by a line segment (the fiber), letting this line segment suffer a π rotation along the basis.

4. — The other homotopy groups in Sm A follow by using a classical property relating the homotopy groups of the fiber, the bundle, and the base, stating that the following semi-infinite sequence :

$$\cdots \to \pi_2(S^1) \to \pi_2(V_C) \to \pi_2(V_A) \to \pi_1(S^1) \to \to \pi_1(V_C) \to \pi_1(V_A) \tag{17}$$

terminating with $\pi_1(V_A)$ is a sequence of group homomorphisms and is exact [6].

The groups $\pi_n(V_A)$ are easily calculated for $n \geqslant 3$. We get indeed, using the fact that $\pi_n(S^1) = 1$ for $n \geqslant 2$, the results of eq. (13), i.e. $\pi_n(V_C) \simeq \pi_n(V_A)$ $n \geqslant 3$.

The calculation of $\pi_2(V_A)$ is less trivial but can be done the same way, using the fact demonstrated in § 3 that the kernel of the mapping $\pi_1(V_C) \to \pi_1(V_A)$ is Z_2. By going up the homotopy sequence, one obtains :

$$\pi_2(V_A) = Z \tag{18}$$

i.e. singular topologically stable points are allowed in Sm A, in contrast with Sm C.

Note that the Z_2 factor of $\pi_1(V_A)$ acts on $\pi_2(V_A)$ by changing the sign of the elements so this sign is not defined for isolated point defects. For a pair of point defects the relative sign can be observed when they combine (e.g. they can annihilate if they have some strength and opposite sign) but this relative sign will change if a disclination line is moved between them.

5. — The existence of point defects in Sm A is related to the geometrical property of the fiber bundle (V_C, V_A, S^1) that this bundle has no cross-section, i.e. that it is not possible to construct a mapping of the base V_A into the bundle V_C which is everywhere continuous. In physical terms, this means that, it one starts from a Sm A phase which is *sufficiently* full of defects, the transformation to the Sm C phase is attended by the appearance of $(0, a^2)$ disclination

lines. For example, start from a droplet in which the Sm A layers are piled in concentric spheres; this droplet contains a singular point (eq. (18)); cool it to the Sm C phase : assume that the layers keep the same orientation through the transition; at least two $(0, a^2)$ lines must appear, which will begin on the singular point. This is reminiscent of the transformation of a t'Hooft-Polyakov monopole [11, 12] into a Dirac monopole [13] with a singular string by a singular gauge transformation. Notice that we have specifically assumed that the layers keep a constant orientation during the phase transformation. If it is not the case, there is no obstruction to a transition towards a line $(0, 1) = (0, a^2)^2$ with a non-singular core; however, inspection of corresponding configurations (see [10]) indicates that this requires a complete destruction of the topology of the sphere.

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