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CLASSIFICATION OF TOPOLOGICALLY STABLE DEFECTS IN ORDERED MEDIA

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Résumé. — Les défauts de symétrie d'un milieu ordonné qui sont topologiquement stables, sont classés par des groupes d'homotopie. A titre d'exemple, nous établissons une classification complète de ces défauts de symétrie cristalline.

Abstract. — Topologically stable symmetry defects in ordered media can be classified by some homotopy groups. As an example we establish a complete classification of such defects for crystals.

Two of us, G. T. and M. K., have proposed [1] a classification of elementary stable defects by the homotopy groups of the manifold of states. In this letter we will give a more systematic approach and present some applications of this classification, particularly for crystals.

1. — Let G be the symmetry group of the physical laws governing a thermodynamical system M. Among the statistical equilibrium states of M, there generally exist not only a phase with symmetry G, but also other phases with less symmetry : in a *perfect state* (i.e., without defects, and idealized as an infinite system) such a phase is invariant under a subgroup H of G ; the action of G on this state yields an orbit G/H of states with identical physical properties ; this orbit is the manifold of states of ref. [1]. If there are defects, H invariance is only local : different domains of M correspond to different points of the orbit G/H (i.e., these different local states are transformed into each other by G). Ideally, this situation defines a function φ, taking its values in G/H, at each point of the continuous medium outside the defects. (These considerations also apply to any model of statistical mechanics in a space of dimension d.) The restriction of the function φ to an r-dimensional sphere S_r defines a homotopy class $\alpha_r \in \pi_r(G/H)$. If $\alpha_r = 0$, $\in \pi_r$, the function φ can be extended to an $(r + 1)$-dimensional disc bounded by S_r and, on this (contractible) disc, this extended function is homotopic to a constant, i.e., to the function of the *perfect state*. When $\alpha_r \neq 0$, S_r encloses a topologically stable defect of dimension $d' = d - 1 - r$. If $\alpha_r = 0$ for all r such that

$$0 \leqslant r \leqslant d - 1 ,$$

then by continuous deformation the state of the system can be made perfect in the interior of the sphere S_{d-1} ($d = 3$ in our space). When some α_r are nontrivial, there is a topologically stable defect (= t.s. defect in this letter).

We are naturally led to a classification of t.s. defects ; of course such a classification cannot depend on the base point chosen for computing the homotopy classes. In all applications G will be a Lie group (which might be of dimension zero, i.e., discrete) ; when G and H are connected, G/H is n-simple for

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every n (see ref. [2], theorem 16.11): then the t.s. defects of dimension d' can be classified by the elements of $\pi_r(G/H)$ with $r = d - 1 - d'$. When H is not connected, $\pi_1(G/H)$ may act nontrivially on $\pi_n(G/H)$ and the t.s. defects will be classified by the orbits of π_1 in π_n; for instance if π_1 is not abelian, the line defects (when $d = 3$) will be classified by the conjugation classes of π_1.

In ref. [1], these ideas have been applied to several systems, e.g., superfluid ^{4}He and ^{3}He. For all applications here, $G = E(3)$ the Euclidean group in 3-dimensions. It is the semi-direct product $R^3_\square O(3)$ of the translation group R^3 by O(3). We denote by E_0 its connected component and by $\overline{E}_0$ the universal covering of E_0 ($\overline{E}_0$ = semi-direct product $R^3_\square SU(2)$ of R^3 by SU(2)); finally we denote by θ the surjective group homomorphism :

$$\overline{E}_0 \xrightarrow{\theta} E_0 . \qquad (1)$$

2. **Nematics.** — As a first illustration, we consider a case already dealt with in ref. [1] in order to show that we do reach the same conclusions. Nematic phases are invariant by translations but not by rotations because the non-spherical molecules of these liquids are oriented (at least partially) so the thermodynamic properties of the nematic phase are described by a quadrupole (symmetric tensor with null trace of O(3)). There are two types of orbits :

$$E(3)/(R^3_\square(D_{\infty h})) \sim O(3)/D_{\infty h} \sim SO(3)/D_\infty \sim P(2, R)$$

(the projective real plane) and

$$E(3)/(R^3_\square D_{2h}) \sim O(3)/D_{2h} \sim SO(3)/D_2 .$$

The first kind of orbit corresponds to uniaxial nematics with the homotopy $\pi_0 = 0$, $\pi_1 = Z_2$, $\pi_2 = Z$ as found in ref. [1]. The second kind of orbits would correspond to biaxial nematics (the quadrupole has three unequal axes) and by a computation similar to that in 3 below one finds $\pi_0 = 0$, $\pi_2 = 0$ (no t.s. point defects in that case !) and $\pi_1 = Q$ the quaternion group (i.e., the group generated by the $i\sigma_k$ where σ_k are the Pauli matrices); π_1 is not abelian and has five conjugation classes : 1 (the perfect state), -1, $\pm i\sigma_1$, $\pm i\sigma_2$, $\pm i\sigma_3$.

3. **Crystal.** — We can now sketch the classification of the t.s. defects in a crystal. Let H be the crystallographic group of the crystal under consideration (it belongs to one of the 230 crystallographic classes) : H is a discrete subgroup of E(3) such that the orbit E(3)/H is compact. Since E(3) is a covering space of the orbit :

$$r > 1 , \qquad \pi_r(E(3)/H) = \pi_r\, E(3) \qquad (2)$$

(see e.g., ref. [2]), so for any crystal

$$\pi_2 = 0 , \qquad \pi_3 = Z \qquad (2')$$

(see refs. [3] and [4] respectively).

Let $H_0 = H \cap E_0$. If $H = H_0$, the point group H/Z^3 does not contain reflections, so the orbit E(3)/H has two connected components i.e., $\pi_0 = Z_2$; the only other case is when H_0 is a subgroup of index two of H: then the orbit is connected and $\pi_0 = 0$. To summarize

$$\pi_0 = Z_2 \quad \text{if} \quad H \subset E_0 , \qquad \pi_0 = 0 \text{ otherwise} . \qquad (3)$$

When $\pi_0 = z_2$, there can be wall defects; they are a special type of twin boundary, the twin by reticular merihedry in the terminology of G. Friedel [5]. If $\pi_0 = Z_2$, the two connected components of the orbit are homeomorphic so, in all cases, to compute $\pi_1(E/H)$ we need only to consider E_0/H_0 which is homeomorphic to the orbit $\overline{E}_0/\theta^{-1}(H_0)$; since $\overline{E}_0$ is simply connected

$$\pi_1 = \theta^{-1}(H_0) \quad \text{where} \quad H_0 = H \cap E_0 . \qquad (4)$$

In general this group is not abelian, so *isolated* line singularities in a crystal can be classified by the conjugation classes of $\theta^{-1}(H_0)$, the covering in $\overline{E}_0$ of the crystallographic group without reflections.

4. What happens when two t.s. defects of the same dimension coalesce ? If each one is described by an element of an abelian group, they combine according to the (abelian) group law. For instance any two wall singularities in a crystal (twin boundaries) annihilate, as do two t.s. line defects in uniaxial nematics and as two vortices in phase A of ^{3}He should do, as was predicted in ref. [1]. If two isolated line defects are described by conjugation classes of π_1, the composition law of these conjugation classes is that of an abelian algebra (which is the centre of the group algebra). However the function φ, defined in 1 above, yields more information : indeed the π_1 orbit (by π_1 inner automorphisms) of the product $\alpha\beta$ of a pair of elements of π_1 lies in a *unique* conjugation class, which is independent of the order since $\alpha\beta$ and $\beta\alpha$ are conjugated : $\alpha\beta = \alpha(\beta\alpha)\,\alpha^{-1}$.

5. The two following remarks will help the interpretation of paragraph 1.

a) The local states of non-perfect media are not simply obtained from each other by Euclidean displacements, but more generally by linear or even by differentiable transformations. In the case of crystals, consider for instance the figures of ref. [6] Ch. 3. So the function φ defined in 1 above takes its values in (Diff R^d)/H where Diff R^d is the group of diffeomorphisms of the d-dimensional Euclidean space. This does not change our conclusions : indeed, using the work of Stewart [7], we obtain

$$\pi_r(\text{Diff } R^n/H) = \pi_r(E(n)/H) .$$

(It is for pedagogical reasons that we first introduced the Euclidean group.)

b) One can also consider instead of G/H a family of orbits (G/H) (η) corresponding to the different values of the Landau [7] (scalar) order parameter η. This positive parameter decreases as a function of T and reaches zero at the temperature T_c of the phase transition to the symmetrical phase. For $\eta > 0$ all orbits are homeomorphic and the family

$$\{ (G/H)(\eta), \quad 0 < \eta_1 \leqslant \eta \leqslant \eta_2 \}$$

is the topological product of G/H and a line segment, so it has the homotopy of G/H. However, when the fluctuations of η to the value $\eta = 0$ can no longer be neglected (when T goes nearer to T_c i.e. usually when T increases) the manifold of states to be considered is the union $\{ (G/H)(\eta), 0 \leqslant \eta \leqslant \eta_2 \}$. It is contractible into the point $\eta = 0$, so its homotopy is trivial i.e., the defects become unstable (e.g. annealing process).

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After this work was finished, our attention was called to the paper of D. Rogula in *Trends in applications of pure Mathematics to Mechanics*, p. 311-331, edited by G. Fichera, Pitman Publ. London 1976. This paper proposes homotopy for classification of defects and gives some applications to Bravais lattices.

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