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Spontaneous Breaking of Euclidean Invariance and Classification of Topologically Stable Defects and Configurations of Crystals and Liquid Crystals

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We show how many mesomorphic states illustrate the following general scheme: The symmetry group of an equilibrium state of Euclidean-invariant quantum statistical mechanics is a subgroup H of the Euclidean group E such that the orbit E/H is compact. Moreover, the homotopy groups of E/H yield a classification of the topologically stable defects and configurations of these ordered media. This suggests a predictive value of this scheme for yet unobserved media and for defects.

Homotopy theory has already been used explicitly by physicists for the study of topological stability of kinks,[1] t' Hooft–Polyakov monopoles,[2,3] and instantons[4]; it also appears that topological notions are used for the study of defects in ordered media, e.g., Burgers circuit and Volterra process, which can be related in some way to homotopy.[5] Toulouse and Kleman have proposed a topological classification of defects by the homotopy groups of the "manifold of internal states" and, as an application, have predicted that vortex lines in superfluid He^3-A should annihilate by pairs.[6,7] Michel has shown[8] how this classification can be related to the spontaneous symmetry breaking of the invariance group G of physical laws (e.g., gauge group, Euclidean group, etc.) into a subgroup H, the symmetry group of the perfect media (i.e., without deformations): The manifold of internal states of Ref. 6 is the orbit G/H. Several applications[9-13] and extensions[14,15] of these ideas have been published recently.

Here we present a synthetic classification of the possible symmetries of media with long-range order, their defects, and their configurations[16] with the hope that such classification has some predictive value. The complete list of the possible global-symmetry groups H of equilibrium states with spontaneously broken Euclidean symmetry has been given by Kastler *et al.*[17]: In quantum statistical mechanics if an invariant state is a mixture, it can be decomposed, in the transitive case, into an integral over an orbit G/H of pure states and this orbit has to carry a finite G-invariant measure. When G is the Euclidean group E, this means that the orbit E/H is compact. We first recall the classification of these subgroups H, up to conjugation in the affine group: For instance, for H discrete, one obtains all the 230 crystallographic classes predicted last century. Consider the Euclidean group E given as the semidirect product $T\square O(3)$ and let $T_H = T \cap H$ be the intersection of H with the group T of translations. T_H is an invariant subgroup of H; so H is a subgroup of $N(T_H)$ the normalizer of T_H in E [i.e., $N(T_H)$ is the largest subgroup of E which has T_H as an invariant group]. $N(T_H)$ may be written as the semidirect product $T\square Q_H$. There are then five cases to study[18]:

Case	T_H	Q_H
I	R^3	O(3)
II	$R^2 \times Z$	$D_{\infty h}$
III	$R \times Z^2$	Discrete
IV	Z^3	Discrete
V	R^2	$D_{\infty h}$

In each case, the possible H are all closed subgroups of E such that

$$T \cap H \equiv T_H \subset H \subset T \square Q_H . \tag{1}$$

Below we give some known examples corresponding to each case.

Case IV.—This case corresponds to crystals.

Case I.—In this case, the largest possible proper subgroup of E is $T\square D_{\infty h}$. This is the symmetry group of the *nematics*: They are constituted of aspherical, randomly distributed, but aligned, molecules; their refraction index and electric or magnetic susceptibilities are axially symmetric quadrupoles.

Cases II and V.—Here $N(T_H) = T\square D_{\infty h}$; its identity component can be written as $R^2 \square [R \times SO(2)]$,

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where $R \times SO(2)$ is the group generated by the translations along an axis and the rotations about it. Figure 1 represents several possible subgroups, with either $H \cap R = Z$ (case II) or $H \cap R = \varnothing$ (case V). Known classes of liquid crystals corresponding to these cases are given as follows:

Subcase IIa, cholesterics.—Here $H = R^2 \square (R_h \square D^2)$, where R_h denotes an helicoidal group [see Fig. 1(a)]. The molecules are algned in the planes orthogonal to the cholesteric axis but the azimuth of this alignment is a linear function of the axis coordinate.

Subcase IIb, smectic-A.—Here $H = (R^2 \times Z) \square L_{\infty h}$; the molecules are in parallel layers and are oriented perpendicularly to them [see Fig. 1(b)].

Subcase IIc, smectic-C.—Here $H = (R^2 \times Z) C_{2h}$; the molecules are all aligned, but obilquely so, relative to the layers.

Subcases IId and V, chiral smectic-C.—The oblique orientation of the molecules makes a constant angle with the axis orthogonal to the layers, but it turns from layer to layer by an angle θ about this axis; the two subcases correspond, respectively, to θ/π rational or irrational [the latter subcase is given in Fig. 1(c)].

Case III.—This case is illustrated by a lattice of vortex lines in a type-II superconductor in the intermediary state[19] or by the hexagonal rod lattice of lyotropic crystals[20]; then $H = (Z^2 \times R) \square D_{6h}$.

One expects that other examples of mesomorphic states, corresponding to other possible subgroups H, will be discovered (see, for example, Ref. 11). The states which are not covered by this classification are those which do not have a global-symmetry group, *either* because E has only an ergodic action (ergodic states of Ref. 17) —e.g., in case of helimagnetic crystals or modulated crystals when the ratio of the two superposed periods is irrational—*or* by lack of long-range order correlations in some directions in the last case the local order cannot be preserved macroscopically, e.g., in the smectic-B or -E which has a hexagonal or tetragonal structure in the layers; so they are very crystal-like locally, but the order correlation disappears along the direction orthogonal to the layers).

Consider again the media with global-symmetry groups (transitive states of Ref. 17). Acting on them by the Euclidean group, one obtains the whole orbit E/H of its positions. The state of a perfect medium is characterized by its position beside temperature, pressure, etc. In an imperfect medium the position varies locally; this variation defines a function φ valued in E/H and whose domain is the volume V occupied by the medium excepting the defects. If φ can be extended continuously over a defect, this defect is not topologically stable. If φ cannot be extended continuously over a defect Δ, around this defect it must belong to a nontrivial homotopy class of E/H. This yields the topological classification of defects: Elements of $\pi_n(E/H)$, $n = 0, 1, 2$ classify wall, line, and point defects, respectively. It may also happen that φ may be made constant over a whole sphere S^2 and defined everywhere inside without being homotopic to a constant: This defines a topologically stable configuration,[16] classified by the elements of $\pi_3(E/H)$.

To compute the homotopy groups $\pi_n(E/H)$, for $n > 0$, first note that they are also those of $E_0/H' = \overline{E}_0/\overline{H}'$, where E_0 is the connected subgroup of E (no reflections) and $\overline{E}_0$ is the (double) universal covering of E_0: The kernel of the homomorphism $\theta: \overline{E}_0 \to E_0$ is the center of $\overline{E}_0$ (it is generated by the rotation of 2π); finally $H' = H \cap E_0$ and $\overline{H}' = \theta^{-1}(H')$. Then one can use the long exact homotopy sequence for principal fiber bundles[21] and other basic facts of homotopy.[22] Since $\pi_0(\overline{E}_0) = 1$, $\pi_1(\overline{E}_0) = 1$, and $\pi_2(\overline{E}_0) = 1$,[23] we deduce

$$\pi_1(E/H) = \pi_0(\overline{H}'), \quad \pi_2(E/H) = \pi_1(\overline{H}'). \tag{2}$$

Let H_0' be the connected subgroup of H'. We have to distinguish two cases:

In case (i), $H \supset SO(2)$. Then $\pi_1(\overline{H}') = \pi_1[SO(2)] = Z = \pi_2(E/H)$: There are *point* defects—this is the

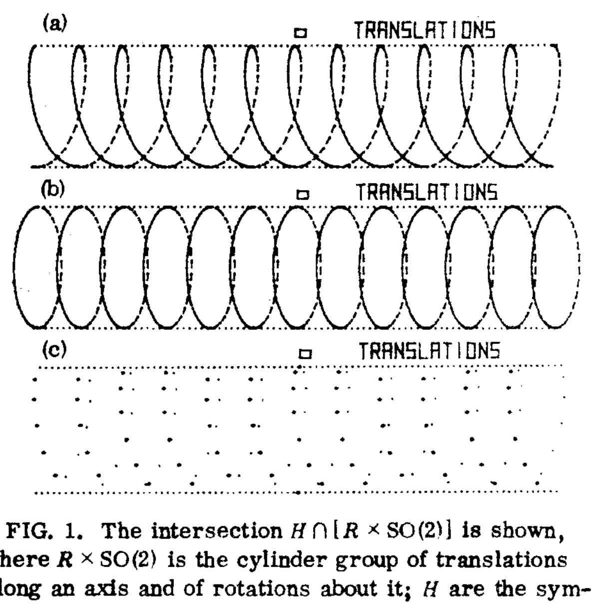

FIG. 1. The intersection $H \cap [R \times SO(2)]$ is shown, where $R \times SO(2)$ is the cylinder group of translations along an axis and of rotations about it; H are the symmetry groups of (a) cholesterics, (b) smectic-A, and (c) chiral smectic-C with θ/π irrational.

case of nematics and smectic-A. The *line* defects are classified by

$$\pi_0(\overline{H}') = H'/H_0' = \pi_1(E/H). \tag{3}$$

In case (ii), $H \not\supset \mathrm{SO}(2)$. Then $\pi_1(\overline{H}') = 1 = \pi_2(E/H)$: There are no stable point defects and

$$\pi_0(\overline{H}') = \overline{H}'/\overline{H}_0' = \pi_1(E/H).$$

In all cases $\pi_n(\overline{H}') = \pi_n(H) = 1$ when $n > 1$ so that, for $n > 2$, E/H and E_0 have the same homotopy—that of SU(2); and from Bott,[24] $\pi_3(E/H) = Z$, which classifies the *configurations* of all media. We recall in Table I the explicit homotopy groups of all previously listed mesomorphic states. Of course, defects are studied and should be studied from the point of view of energy stability. However, this simple topological classification is already interesting and has some predictive power.

We remark that, except for the nematics, all $\pi_1(E/H)$ are non-Abelian; so isolated line defects are characterized only[9,10] by conjugation classes of π_1. However, pairs of line defects correspond to conjugated pairs of π_1 elements: These line defects can coalesce[9] but, as shown by Poenaru and Toulouse,[14] they cannot cross each other when they correspond to noncommuting elements of $\pi_1(E/H)$. Note also that $\pi_1(E/H)$ acts nontrivially on $\pi_2(E/H)$ when the latter is Z. Hence for smectic-A we have the same situation as that described by Volovik and Mineev[10] for nematics: The sign of isolated point defects is undefined; the relative sign of a pair of point defects may change when a line defect is moved between them. In all cases π_1 acts trivially on the configuration group $\pi_3(E/H) = Z$.

As shown in Ref. 9, $\pi_0(E/H)$ is nontrivial for crystals when $H = H'$; then $\pi_0(E/H) = Z_2$ classifies *wall* defects annihilating by pairs (the twins by reticular merihedries[25]). The relation $H = H'$ is also true for cholesterics and chiral smectic-C but these phases seem to exist only for optically active molecules (the existence of twin defects would exist if one could observe the same phases made with racemics).

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Note added.—Since this paper has been written, new examples of thermotropic mesomorphic phases of disklike molecules have been discovered.[26,27]

The topological classification of defects and configurations based on homotopy as presented here and in the quoted references is too coarse for three reasons:

(i) If the domain $\Omega = (V -$ the defects) is not contractible, there might be other topological obstructions to extending the function φ when it is homotopically trivial; they are characterized by the cohomology of Ω valued in the π's of E/H.

(ii) The continuous deformations of φ necessary to show the homotopic equivalence of two defects or configurations may require deformations of the medium beyond the elastic limit and are therefor unphysical. The medium generally deals with this difficulty by creating new defects to which the homotopy classification applies.

(iii) A medium can eventually be submitted to the "conditions of integrability" (e.g., $\hat{n} \cdot \nabla \times \hat{n} = 0$ for smectics or the well-known compatibility conditions of dislocation theory). This additional constraint has to be taken into account. Thom has

TABLE I. List of some predicted subgroups H of the Euclidean group E which are symmetry groups of phases already observed in nature.

Case	H	Name	π_3	π_2	π_1	π_0	Ref.
I	$R^3 \square D_{\infty h}$	Nematics	Z	Z	Z_2	1	6, 9, 10
IIa	$R^2 \square (R_h \square D_2)$	Cholesterics	Z	1	$Q = \overline{D}_2$	$\cdots$[a]	10, 13
IIb	$(R^2 \times Z) \square D_{\infty h}$	Smectic-A	Z	Z	$Z \square Z_2$	1	12
IIc	$(R^2 \times Z) \square C_{2h}$	Smectic-C	Z	1	$Z \square Z_4$	1	12
IId or V	$(R^2 \times Z) \square C_2$	Chiral smectic-C	Z	1	$Z \square Z_4$	$\cdots$[a]	
III	$(R \times Z^2) \square D_{6h}$	Rod lattices	Z	1	$Z^2 \square \overline{D}_6$	$\cdots$	
IV	(Z^3, P)[a]	Crystals	Z	1	$\overline{H}_0 = (Z^3, \overline{P}_0)$[a]	Z_2 if $P = P_0$; 1 otherwise	9

[a]These chiral phases are made only from chiral molecules, and so we should consider only E_0 invariance. The group $\overline{D}_n = \theta^{-1}(D_n)$ has $4n$ elements; it is defined by the generators r, s and relations $r^{2n} = s^4 = 1$, $rsr = s$; for $n = 2$, it is the quaternion group $1, -1, \pm i\tau_k$, where τ_k are the Pauli matrices. The symbol (Z^3, P) means that $H/Z^3 = P$, where P is the point group of the crystal, for which P_0 is its subgroup without reflections and $\overline{P}_0 = \theta^{-1}(P_0)$.

recently made some suggestions in that direction.[28]

This synthesis suggests new types of problems (for instance, at phase transitions).

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