SPONTANEOUS BREAKING OF EUCLIDEAN INVARIANCE AND CLASSIFICATION OF TOPOLOGICALLY STABLE DEFECTS AND CONFIGURATIONS OF CRYSTALS AND CRYSTALS AND LIQUID CRYSTALS

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Abstract. 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.

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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]. G. Toulouse and one of us (M. K.) 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^3A should annihilate by pairs[6,7]. The other author (L.M.) 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 reference 6 is the orbit G/H. Several applications [9,10,11,12,13] 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, 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 was given by one of us (L.M.) with D. Kastler et al.[17] :
In statistical quantum 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 a conjugation in the affine group : for instance, for H discrete, one obtains the 230 crystallographic classes predicted last century. E is the semi-direct product $T \square O(3)$;

let $T_H = T \cap H$ 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 invariant subgroup. $N(T_H)$ is the semi-direct product $T \,\square\, Q_H$. There are 5 cases to study [18] .

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

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

$$T_H \subset H \subset T \,\square\, Q_H \ , \ H \cap T = T_H \tag{1}$$

Here are known examples corresponding to each case :

Case IV corresponds to crystals.

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

Cases II and V. Then $N(T_H) = T \,\square\, D_{\infty h}$; its identity component can be written $R^2 \,\square\, Cyl$ where $Cyl = R \times SO(2)$ is the group generated by the translations along an axis and the rotations about it. Fig.1 represents several possible subgroups, $H \cap R$ = either Z (case II) or empty (case V). Known liquid crystals corresponding to these cases are :

IIa : cholesterics. $H = R^2 \,\square\, (R_h \times D_2)$ where R_h denotes an helicoïdal group (see Fig.1a). The molecules are aligned in the planes orthogonal to the cholesteric axis but the azimuth of this alignment is a linear function of the axis coordinate.

IIb. Smectics A. $H = R^2_{\square}(Z \times D_{\infty h})$; the molecules are in parallel layers and are oriented perpendicularly to them. (See Fig.1b).

IIc. Smectics C. $H = R^2_{\square}(Z \times C_{2h})$; the molecules are all aligned but obliquely to the layers.

IId and V. Chiral smectics 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 to θ/π respectively rational or irrational (The latter case is figure 1c).

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, e.g.[11]. The states which are not covered by this classification are those which have not a global symmetry group, either because E has only an ergodic action (ergodic states of ref.17), e.g. 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. the smectics B or E which have 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).

Let us 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 ... 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 non trivial homotopy class of E/H . This yields the topological classification of defects : elements of $\pi_n(E/H)$, n = 0,1,2 respectively classify wall, line, point defects. 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 t.s. (topologically stable) configuration[16] , classified by the elements of $\pi_3(E/H)$.

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

$$\pi_1(E/H) = \pi_o(\bar{H}') \quad , \quad \pi_2(E/H) = \pi_1(\bar{H}') \tag{2}$$

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

i) $H \supset SO(2)$, then $\pi_1(\bar{H}') = \pi_1(SO(2)) = Z = \pi_2(E/H)$: there are <u>point</u> defects; this is the case of nematics and smectics A . The <u>line defects</u> are classified by

$$\pi_o(\bar{H}') = H'/H'_o = \pi_1(E/H) \tag{3}$$

ii) $H \not\supset SO(2)$, then $\pi_1(\bar{H}') = 1 = \pi_2(E/H)$: no stable point defects and

$$\pi_o(\bar{H}') = \bar{H}'/\bar{H}'_o = \pi_1(E/H) \ .$$

In all cases $\pi_n(\overline{H}') = \pi_n(H) = 1$ when $n > 1$ so for $n > 2$, E/H and E_o have the same homotopy : that of SU(2) and from ref 24 , $\pi_3(E/H) = Z$ which classifies the <u>configurations</u> of all media. We recall in table 1 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 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 non commuting elements of $\pi_1(E/H)$. Note also that $\pi_1(E/H)$ acts non trivially on $\pi_2(E/H)$ when the latter is Z . Hence for smectics 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 [9] , $\pi_o(E/H)$ is non trivial for crystals when $H = H'$: then $\pi_o(E/H) = Z_2$ classifies <u>wall</u> defects annihilating by pairs (the twins by reticular merihedries[25]). The relation $H = H'$ is also true for cholesterics and chiral smectics 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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Table 1.

Case	H	Name	π_3	π_2	π_1	π_o	Ref.
I	$R^3 \square D_{\infty h}$	Nematics	Z	Z	Z_2	1	6,9,10
IIa	$R^2 \square (R \square D_2)$	Cholesterics	Z	1	$Q = \overline{D}_2$	a)	10,13
IIb	$(R^2 \times Z) \square D_{\infty h}$	Smectics A	Z	Z	$Z \square Z_2$	1	12
IIc	$(R^2 \times Z) \square C_2$	Smectics C	Z	1	$Z \square Z_4$	1	12
IId or V	$(R^2 \times Z) \square C_2$	Chiral smectics C	Z	1	$Z \square Z_4$	a)	
III	$(R \times Z^2) \square D_{6h}$	Rod lattices	Z	1	$Z^2 \square \overline{D}_6$	$\left\{ Z_2 \right.$ if $P=P_o$	
IV	(Z^3,P)	Crystals	Z	1	$\overline{H}_o=(Z^3,\overline{P}_o)$	1 otherwise	9

a) These chiral phases are made only from chiral molecules, so we should consider only E_o invariance. The group $\overline{D}_n = \theta^{-1}(D_n)$ has 4 elements; it is defined by the generators r,s and relation $r^{2n} = s^4 = 1$, rsr = S ; for n = 2 , it is the quaternionic 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, P_o is its subgroup without reflections and $\overline{P}_o = \theta^{-1}(P_o)$.

Figure Caption

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

References or Footnotes

1 FINKELSTEIN D., Kinks, J. Math. Phys. 7, 1218 (1966), FINKELSTEIN D. and RUBINSTEIN J., ibid 9, 1762 (1968).

2 TYUPKIN Yu.S., FATEEV V.A. and SHVARTS A.S., JETP Lett. (Translations) 21, 42 (1975).

3 MONASTYRSKII M.I. and PERELOMOV A.M., JETP Lett. (Translations) 21, 43 (1975).

4 BELIAVIN A.A., POLYAKOV A.M., SCHWARTZ A.S., TYUPKIN Yu.S., Phys. Lett. 59b, 85 (1975).

5 KLEMAN M., Relationship between Burger's circuit, Volterra process and homotopy groups, J. Phys. Lett. 38L, 199 (1977).

6 TOULOUSE G., KLEMAN M., Principles of a classification of Defects in ordered media, J. Phys. Lett. 37 L, 149 (1976).

7 We disagree with D. ROGULA,"Large deformations of Crystals, Homotopy and Defects"in "Trends in application of pure mathematics to mechanics", G. Fichera editor, Pitman Publishing Co. 1976, concerning his point of view for the homotopic classification of crystal defects.

8 MICHEL L., 6th Int. Colloq. Group Theoretical Methods in Physics, Tübingen 1977, to appear in Springer Lecture Notes in Physics.

9 KLEMAN M., MICHEL L., TOULOUSE G., Classification of topologically stable defects in ordered media, J. Phys. Lett. 38 L, 195 (1977).

10 VOLOVIK G.E., MINEEV V.P., Study of singularities in ordered systems by homotopic topology methods, Preprint Landau Institute Moscow.

11 TOULOUSE G., Pour les nématiques biaxes, J. Phys. Lett. 38 L, 67 (1977).

12 KLEMAN M. and MICHEL L., in J. Phys. Lett. January 78.

13 KUKULA J., Senior Thesis, Princeton University, unpublished.

14 POENARU V., TOULOUSE G., J. Phys. 38, 887 (1977).

15 GAREL A.T., Boundary conditions for textures and defects, Preprint Lab. Phys. Solides, Orsay.

16 D. FINKELSTEIN has coined the name of kinks for non-singular topologically stable configurations.The term of "texture" has been introduced by P.W. Anderson and G. Toulouse, Phys. Rev. Letters 38 (1977), 508, to connote non-singular non topologically stable configurations (e.g. S = 1 lines in nematics, 4π rotation lines in superfluid He^3- A phase). There is at present time some laxism in terminology, physicists having the trend to call textures what Finkelstein called kinks. We propose to use "configuration", because the words kinks and textures are both used extensively since a long time with a very precise meaning in the physics of dislocations, a kink being a special type of accident on a line of dislocation and a texture being an extensive word to connote an assembly of defects, e.g. J. Friedel, Dislocations, Pergamon Press, Oxford (1964).

17 D. KASTLER, G. LOUPIAS, M. MEBKHOUT, L. MICHEL, Comm. Math. Phys.27(1972)195.

18 R and Z are respectively the additive group of real and integer numbers. For the other groups we use the rotation of L.D. Landau and E.M. Lifschitz, Quantum Mechanics, Chapt. 12.

19 H. TRÄUBLE and U. ESSMANN, Phys. Lett. 24A (1964)256. This pattern was predicted by A.A. ABRIKOSOV, J. Exp. Th. Phys. 5 (1957) 1174, but with a square lattice while the observed hexagonal one was proposed by W.M. KLEINER, L.M. ROTH, S.H. AUTLER , Phys. Rev. 133A (1964) 1226.

20 V. LUZZATI and A. TARDIEU, Ann. Rev. Phys. Chem. 25 (1974)79.

21 STEENROD N. , The topology of fiber bundles, Princeton University Press (1957).

22 The topological space of a semi-direct product of groups is a topological product of the group spaces. In such a product we can omit contractible factors R^k since their homotopy is trivial and the homotopy groups of a topological product are direct products of the homotopy group of the factors.

23 CARTAN E. , La topologie des espaces représentatifs des groupes de Lie, Act. Sci. Ind. 358, Hermann Paris 1936.

24 BOTT R., Proc. Nat. Acad. Sci. U.S. 40, 586 (1954).

25 FRIEDEL G., Leçons de cristallographie, Berger-Levrault, Paris (1929).

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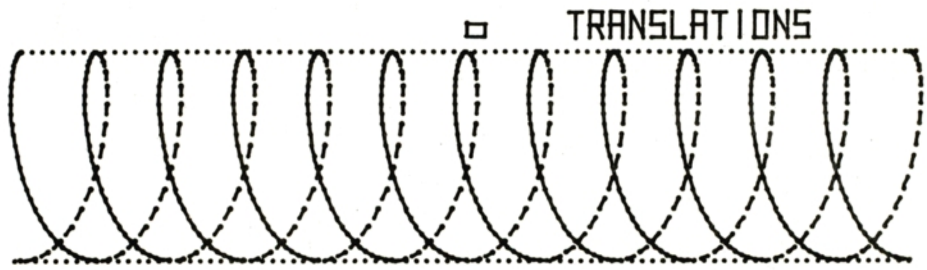

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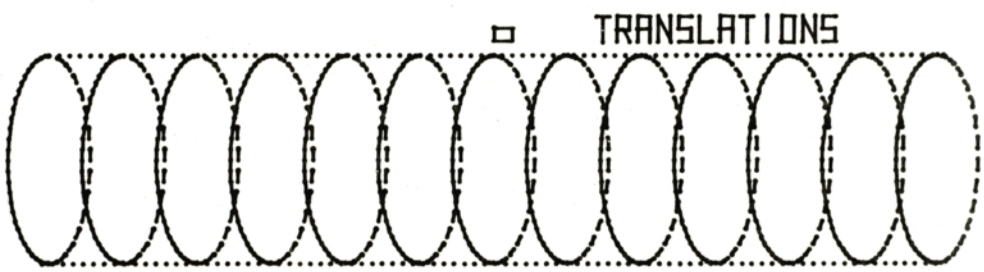

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