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PRINCIPLES OF A CLASSIFICATION OF DEFECTS IN ORDERED MEDIA

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Résumé. — Une classification des défauts dans les milieux ordonnés est présentée. Fondée sur des concepts purement topologiques, elle fournit une distinction entre défauts élémentaires (topologiquement stables) et défauts composés. Cette classification systématique contient des résultats dérivés antérieurement de manière empirique et permet de nouvelles prédictions. Elle révèle une liaison entre la nature des défauts dans une phase ordonnée et les phénomènes critiques à la transition de phase.

Abstract. — A classification of defects in ordered media is presented. Based on purely topological concepts, it provides a distinction between elementary (topologically stable) and compound defects. This systematic classification recovers some previous empirically derived results and allows new predictions. It exhibits a striking connection between the nature of defects in an ordered phase and the critical phenomena at the phase transition.

1. Introduction. — An important part of condensed matter and phase transitions physics is involved with the study of the defects which occur in the ordered phases and give rise to the variety of observed textures. It is a natural inclination of the physicist to try to find elementary objects, which can serve as building blocks to construct the others. What is needed, in other terms, is a classification of elementary defects and the set of rules governing their aggregation. In other words, one wants to apply to the defects in a given ordered medium the program which has been achieved for chemical objects, with a hierarchy of levels : atoms, molecules, condensed states.

Most of the past and considerable effort in the theory of defects has been concerned with energy calculations, although it has been recognized by many that topological concepts are important. It is shown here that it is possible to go far indeed with considerations based merely on continuity properties, that is with topology. For a given ordered medium of arbitrary space dimensionality, it is possible to give a systematic classification of the elementary defects of various dimensionalities (points, lines, walls, ...) and to attribute to them characteristic numbers, which govern the rules for their associations.

2. The space of internal states. — The nature of the ordering in an ordered medium can be characterized by an order parameter. Some examples may help to fix ideas ; for an ordered alloy, the order parameter is a real scalar ; for a superfluid, it is a complex scalar ;

for an isotropic ferromagnet, it is a vector ; many more examples could be given. This order parameter is defined at each point of the ordered medium, and, by definition, it characterizes the internal state of the medium at that point. If there were no distortions, the internal state would be the same in each point of the sample. The presence of defects is accompanied by a variation of the internal state from point to point in the medium.

Now each internal state can be represented by a point in an abstract space, the space of internal states. We shall be interested in the subspace formed by all possible values of equal amplitude of the order parameter, and we shall call this subspace the manifold of internal states (we use the term manifold, instead of space, in order to avoid confusion with the real space in which the medium lies, and also, because it is a topological concept, to stress the topological properties).

Let us take again some examples ; for a real scalar order parameter, the manifold of internal states is two points (± 1) ; for a complex scalar, it is a circle ; for a vector, it is a sphere ; etc... This manifold of internal states has important topological properties. First, its dimensionality. Second, its connectivity properties.

In the theory of critical phenomena, that occur near a phase transition point, much emphasis has been put on the effect of the dimensionality. In this theory of defects, the emphasis will be put on the connectivity properties. Actually, the two topics are closely related.

3. The surrounding of defects. Let us begin with a known simple example, which will be generalized afterwards. Consider a line defect (vortex line) in a three dimensional sample of superfluid. To characterize this line defect, one surrounds it by a closed loop. The phase change $\Delta\varphi/2\pi$ of the complex order parameter as one completes a turn along the loop is a topological invariant : to one turn in real space, around the vortex line, is associated a certain closed path in the manifold of internal states. This closed path (more precisely, the class of equivalent paths into which this path can be continuously deformed within the manifold of internal states) then characterizes topologically our line defect. If the closed path can be continuously deformed into one point in the manifold, then the line defect is not topologically stable (it can be continuously reduced to no defect at all); if the closed path cannot be continuously deformed into one point in the manifold, then the line defect is topologically stable.

Let us generalize this construction to arbitrary space dimensionalities of the medium (d) and of the defect (d'). We wish to *surround* the defect by a subspace of dimensionality r such that :

$$d' + 1 + r = d.$$

The term 1 in the left hand side comes from the distance between the line defect and the subspace which surrounds it. In the preceding example, $d = 3$, $d' = 1$, and the surrounding subspace has dimensionality $r = 1$. Now it is seen that, in three-dimensional space, wall defects will be surrounded by two points (this is the 0-dimensional sphere S_0), line defects by a closed loop (this is the 1-dimensional sphere S_1), point defects by a sphere (this is the 2-dimensional sphere S_2).

In each point of the surrounding subspace S_r exists some internal state which is represented by a point in the manifold of internal states V . This defines a map of S_r into V . The possible maps of S_r into V can be classified into classes of equivalent maps (which can be continuously deformed into one another within V). The ensemble of these classes is called the r th homotopy group of V and is denoted $\pi_r(V)$.

Much is known in mathematics concerning the homotopy groups of many manifolds. In some cases, one simply recovers empirically known facts. For instance, in the preceding example of the three-dimensional superfluid, knowing that the manifold of internal states is $V = S_1$ and that

$$\pi_0(S_1) = 0, \quad \pi_1(S_1) = Z, \quad \pi_2(S_1) = 0,$$

where 0 denotes the trivial group with only one element and Z the additive group of integers, one concludes that there are no stable walls, no stable points, but that there are stable vortex lines which can be characterized by an integer (positive or negative), the strength of the vortex. In three-dimensional

isotropic ferromagnets, for which $V = S_2$, one finds stable points but no stable lines (this corresponds to the empirical phenomenon of *escape in third dimension*).

4. Application to systems where the order parameter is an n -component vector (n -vector model). — This includes a large category of systems which contains the examples previously given (real scalar order parameter : $n = 1$; complex scalar : $n = 2$; ordinary vector : $n = d$) and has been much studied in the context of critical phenomena.

For an n -vector order parameter, the manifold of internal states is $V = S_{n-1}$, since the amplitude is taken constant. Now it is known [1] that

$$\pi_r(S_m) = 0 \quad \text{for } r < m,$$

$$\pi_m(S_m) = Z.$$

Topologically stable defects have therefore the dimensionality

$$d' = d - n,$$

which means that for $n > d$, there are no topologically stable defects, for $0 < n < d$ (this is the *triangle of defects* in the n, d plane) there is one kind of defect (points for $n = d$, lines for $n = d - 1$, walls for $n = d - 2, \dots$; other defects may occur for $d > 4$, see note [1]), and finally for $n < 0$, there is again no topologically stable defect.

Note that the boundaries of the *triangle of defects* in the n, d plane are the diagonal $n = d$, which plays an important role in critical phenomena, and the line $n = 0$, which is known to describe disordered systems; it is interesting to notice that, as far as defects are concerned, the case $n = 0$ corresponds to stable defects having the dimensionality of real space, the whole system being in some sense the core of a defect, with no recognizable ordered domains.

5. Application to some other systems. — Let us consider uniaxial nematic liquid crystals, where the order parameter is a line element, that is a vector with no arrow. For an arbitrary number n of components of the order parameter, the manifold of internal states is $V = P_{n-1}$, which means real projective space of $(n - 1)$ dimensions. For usual nematics in three dimensional space, $V = P_2$, the projective plane; for two-dimensional nematics, $V = P_1 = S_1$.

It is then known that

$$\pi_1(P_m) = Z_2,$$

$$\pi_r(P_m) = \pi_r(S_m) \quad \text{for } r > 1,$$

where Z_2 is the two-element group of the integers modulo 2.

As a consequence, for instance, the usual three-dimensional nematics will have, besides the point defects they share with the corresponding vector

systems, topologically stable line defects which have the property of being their own antiparticle : two nematic line defects can disintegrate into points.

As a last example, let us consider the superfluid A phase of He_3 where the orbital order parameter is now estimated to be a frame of three orthogonal vectors (we neglect here the nuclear spin degrees of freedom, which amounts to considering only defects which do not break the dipolar energy). Then, the manifold of internal states V is $V = \text{SO}(3) = \text{P}_3$, so that the A phase appears as a kind of higher-dimensional nematic. One then predicts for a three-dimensional He_3 sample, no walls, no points and lines which are their own antiparticles (these lines can have a mixed vortex-disgyration [2] character). It is amusing to notice that if one tries to construct a point defect for one of the three orthogonal vectors, there is necessarily a *string* of singularities of the other two vectors, attached to the point; this situation is obviously reminiscent of the Dirac monopoles [3].

At this stage, it may be noticed that, through such a classification, the mere observation of the defects in a given phase may give a clue on the nature of the ordering; this poses a rather interesting inverse problem.

Obviously, this short exposition calls for development of both abstract and concrete aspects of the classification scheme; this will be presented in a more detailed publication [4].

6. Conclusion. — During the course of our study, we have discovered that topological concepts have been previously used in field theory by quite a few people, the emphasis being mainly on point singularities [5] or on global configurations of the whole space [6]. Actually, this similarity of concepts in the study of elementary particles and of defects in ordered media appears as a very promising feature. First, it brings some unity in physics. Second, it will probably lead to cross-fertilization. The field theorists (and the mathematicians) have an experience with rather complicated manifolds, the condensed matter physicists can exhibit many systems, with a lot of experimental control on them.

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