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INVESTIGATION OF DEFECTS IN ORDERED MEDIA BY METHODS OF ALGEBRAIC TOPOLOGY

H.-R. Trebin

Physics Department
City College of CUNY, New York 10031

and

Institut für Theoretische Physik, Universität Regensburg
D-8400 Regensburg, West Germany

The recently introduced scheme to classify defects by their topological stability is reviewed. Applications to the transformation of defects in a phase transition are discussed.

1. Introduction

Ordered media form a large class of condensed matter systems, appearing in either a uniform or a nonuniform state. The uniform state is characterized by the fact that it possesses a definite symmetry group H. H is a subgroup of G, the symmetry group of the physical laws. This higher symmetry group G, from which the symmetry of the uniform medium is broken, can be a geometric group or a gauge group. Examples for ordered media are solid crystals and liquid crystals, where G is the full Euclidean group $E = T(3) \wedge O(3)$ or its proper part $E^0 = T(3) \wedge SO(3)$; and the superfluids and superconductors, where G is the gauge group U(1) or a more complicated gauge group. Uniform ordered media, being systems of broken symmetry, are degenerate with respect to one or more parameters ξ: there exist nonequivalent equilibrium states for which ξ differs but whose thermodynamic potential is the same for prescribed homogeneous external conditions. One of the simplest of such systems (and hence a standard example) is a nematic liquid crystal. The nematics are anisotropic fluids, composed of rod-like molecules whose long axes are preferentially aligned parallel to a unit vector $\hat{n}$. They have translational continuous symmetry and orientational axial symmetry $D_{\infty h}$. The director $\hat{n}$ serves as degeneracy parameter. All nematics of the same chemical composition, temperature and pressure but differing director are degenerate. The range of values of the degeneracy parameter is the "manifold of internal states" V. For nematics V is the projective plane P_2, i.e. the set of points of the surface of a unit sphere, where opposite points are identified, since $\hat{n}$ and $-\hat{n}$ are equivalent.

In nonuniform ordered media the order parameter is a local quantity: these media are described by a continuous mapping

$$\begin{aligned} \phi:\ R^3 - \Delta &\rightarrow V \\ \underline{x} &\mapsto \xi = \phi(\underline{x}), \end{aligned}$$

where to each point $\underline{x}$ a degeneracy parameter $\xi = \phi(\underline{x})$ is assigned. There may be points, lines or walls Λ where ϕ is singular. These constitute the possible defects of the medium. Defects are most striking in liquid crystals: they can easily be detected by use of the polarizing microscope. Efforts to classify defects have been made for almost a century. Recently, a classification scheme has been proposed by Toulouse, Kléman, Michel, Rogula[1] Volovik and Mineev[2] that applies methods of algebraic topology. It is interesting to note that liquid crystals, which have been investigated by physicists as well as chemists and biologists, belong now to the most important systems of condensed matter, to which topological methods are applied, and also attract the curiosity of mathematicians.

2. The topological classification of defects

The idea behind the new classification scheme is roughly the following: let Δ be either a single point, infinite line or wall. Two "defects" $\phi, \phi': R^3 - \Delta \rightarrow V$ are equivalent if in all space R^3, apart from Δ, the fields ϕ, ϕ' can be deformed continuously into each other without creation of new singularities. By "continuously deformable" or, equivalently, "homotopic" is meant that there is a continuous family of fields $\{\phi_t: R^3-\Delta \rightarrow V \mid 0 \leq t \leq 1\}$ such that $\phi_0 = \phi$ and $\phi_1 = \phi'$. Δ, the "core" of the defect, is in physical reality a three-dimensional object, necessarily of a different phase, and a region surrounded by high strain energies. Creation of new defects costs energy. Hence, if topological considerations demand that two fields ϕ, ϕ' are inequivalent in the above sense, they represent metastable equilibrium states separated by a high energy barrier. In particular, a defect is unstable, if ϕ is homotopic to the uniform phase. In systems of gauge symmetry, the defect cores are zeroes of complex wavefunctions whose energy density is lowest at nonzero values.

If Δ is a single point or a single (infinite) line, then the space $R^3-\Delta$ is contractible to a twodimensional sphere S^2 or a circle S^1, respectively. Generally, for defects of dimension d' in a space of dimension d, the set $R^d-\Delta$ is contractible to an r-dimensional sphere S^r, where $d'=d-r-1$; for a topological defect classification it suffices to survey the field ϕ on a sphere S^r surrounding the defect core. Hence, line defects in three dimensions are encircled by a closed loop Γ. Mapping the points of this loop into the manifold of internal states by ϕ results in a closed loop $\phi(\Gamma)$ in V. The above definition of equivalence can be reduced to the following statement: two line defects are considered identical if the mappings into V of the loops surrounding them are homotopic. Thus each type of line defect corresponds to a class of homotopic loops in V. Generally, defects of dimension d' in d-dimensional space are in one-to-one correspondence with the classes of homotopic mappings of r-dimensional spheres into V, $d'=d-r-1$. In a two-dimensional amorphous ferromagnet (or the XY-model of a spin system in continuum approximation), for example, at fixed temperature the length of the magnetization vector is constant, and V is a circle. In going around a point defect on a closed loop, the degeneracy parameter runs an integer number of times n about this circle. This number labels the homotopy class. To change this "winding" number, on each loop at least one point must be made singular. Therefore on an entire ray extending from the point to infinity the magnetic phase must become paramagnetic in an intermediate state. By investigating a defect locally through a loop or a sphere (rather than studying the entire field ϕ) it is now possible to classify parts of a defect network, single defects of many defect systems, or the combination of defects. Thereby it is of importance that the set of homotopic loops in the manifold of internal states possesses an algebraic structure. The sets of homotopic loops in V which start and end at a fixed (base) point ξ_0 form the fundamental group $\pi_1(V,\xi_0)$ of V at ξ_0. Freely homotopic loops, and hence the classes of defects of dimension $d'=d-2$, are in bijective correspondence with the conjugacy classes of $\pi_1(V,\xi_0)$. The homotopy classes of based continuous mappings of two-dimensional spheres S^2 into V form the second homotopy group $\pi_2(V,\xi_0)$. Defects of dimension $d'=d-3$ are labeled by the orbits of $\pi_2(V,\xi_0)$ under a group action of $\pi_1(V,\xi_0)$. These results of homotopy theory, which are standard for mathematicians, have been discussed in a series of introductory review articles.[3]

There is a close relation between the manifold of internal states V and the symmetry group H of the uniform system. The group $G \supset H$ acts transitively on the parameter ξ, i.e., if ξ_0 is an (arbitrary, but fixed) base point in V, then V is the orbit of ξ_0 under the action of G: $V=G\xi_0$. H is the little group of ξ_0: $H\xi_0=\xi_0$. Then, if an element $g\in G$ transforms ξ_0 into $\xi\in V$, all elements of the coset gH produce the same transformation: $\xi=g\xi_0=(gH)\xi_0$, and ξ can be identified with gH. The orbit $V=G\xi_0$ is isomorphic to the coset space of the little group H of ξ_0 (the symmetry group of the uniform medium) in G: $V=G/H = \{gH|g\in G\}$. To obtain the following theorems for the computation of homotopy groups, G must be chosen arcwise and simply connected. For mesomorphous media this can be achieved by using instead of SO(3) the special unitary group SU(2), and instead of SO(2) the group T(1)=R, and lifting the proper part of the isotropy groups into these covering groups. For such a choice of G and H the long exact sequence of homotopy groups[3] provides the following isomorphisms:

$$\pi_1(G/H) = H/H^0 , \tag{1}$$

$$\pi_2(G/H) = \pi_1(H^0) . \tag{2}$$

H^0 is the component of H which is arcwise connected to the unit element and as such is an invariant subgroup of H. The cosets in the factor group H/H^0 are the different connected parts of H. For media of discrete isotropy groups $H^0 = 0$. This is the case for crystals. According to isomorphism (2) crystals have no stable point defects. The fundamental group is the double group of the proper part of the space group. The translational part of this group is just the Bravais lattice of the space group; consequently dislocations are classified by Burgers vectors.

3. Transformation of defects in phase transitions

The behaviour of defects in phase transitions is still far from explained quantitatively. The homotopic classification scheme can provide qualitative answers in the form of selection rules. Given a phase 2 of symmetry group H_2, and a phase 1 of symmetry group H_1, and the labeling scheme of the defect classes, into what defect of phase 1 does a certain defect of phase 2 transform in the phase transition $2 \to 1$? If $H_2 \subset H_1$, then the uniform medium 2, described by the constant field $\phi_2(\underline{r}) \equiv gH_2$, $g \in G$, becomes the uniform medium 1 of field $\phi_1(\underline{r}) \equiv gH_1$, according to the projective mapping

$$\begin{aligned} p: \quad G/H_2 &\to G/H_1 \,, \\ gH_2 &\mapsto gH_1 \,. \end{aligned} \tag{3}$$

p maps each coset of G/H_2 into that of G/H_1 which includes it. The most straightforward model for the phase transition of a nonuniform medium is to assume that at each point (in the volume as well as at boundaries) the symmetry is broken and the degeneracy parameter transforms as in the uniform medium. Thus at a point $\underline{r}$, $\phi_2(\underline{r})$ turns into $\phi_1(\underline{r}) = (p \circ \phi_2)(\underline{r})$, and, consequently, the loop $\phi_2(\Gamma)$ in G/H_2 turns into the loop $(p \circ \phi_2)(\Gamma)$ in G/H_1. p relates loops (and closed surfaces) in both degeneracy spaces and leads to a homomorphism

$$p_*^{(r)} \; : \quad \pi_r(G/H_2) \to \pi_r(G/H_1) \,, \tag{4}$$

between homotopy groups of arbitrary degree $r > 0$. Simultaneously $p_*^{(r)}$ induces a mapping between the orbits of $\pi_r(G/H_j)$ under the group action of $\pi_1(G/H_j)$, $j=1,2$, respectively. This mapping is the selection rule for the phase transition of defects of dimension $d' = d-r-1$ in d-dimensional space.

As a simple example we consider the transition biaxial nematic $\to$ uniaxial nematic. The biaxial nematics are liquid crystals to which much attention has been paid by theorists, but which unfortunately have not yet been found in nature. They are fluids, i.e., systems of continuous translational symmetry, but of discrete rotational symmetry. The simplest biaxial nematics have symmetry D_{2h} and can be imagined as fluids composed of oriented boxlike molecules. The fundamental group of this system is $\bar{D}_2$ (the bar denoting a double group), isomorphic to the quaternion group Q. Since Q is nonabelian, there are topological obstructions for the crossing of line defects, which may have interesting physical consequences.[4] The relevant groups for both phases are:

$$H_2 = T(3) \wedge \bar{D}_2 \quad , \qquad H_1 = T(3) \wedge \bar{D}_\infty \quad ,$$

$$H_2^0 = T(3) \quad , \qquad H_1^0 = T(3) \wedge \bar{C}_\infty \quad ,$$

$$H_2/H_2^0 = \bar{D}_2 = Q \quad , \qquad H_1/H_1^0 = Z_2 \quad ,$$

$$\pi_1(H_2^0) = 0 \quad , \qquad \pi_1(H_1^0) = Z \quad .$$

Z_2 is the two-element group. The homomorphism $p_*^{(1)}$ relates the following elements:

$$\pm 1, \pm i\sigma_z \mapsto 0 \; ,$$

$$\pm i\sigma_x, \pm i\sigma_y \mapsto 1 \; . \tag{5}$$

The 360°-disclination (-1) and 180°-disclination about the z-axis ($\pm i\sigma_z$) become unstable (0), the 180° -disclinations about the x- and y-axes ($\pm i\sigma_x$, $\pm i\sigma_y$) turn into the stable 180°-disclination (1) of the uniaxial nematic. The cholesteric liquid crystals also have the quaternion group as fundamental group. The degeneracy parameter of the cholesterics is a director and a pitch-axis orthogonal to it, along which the director rotates continuously. The cholesteric liquid crystals can therefore be viewed as twisted nematics, and homomorphism (5) establishes a correspondence between the defect structure of both points of view. From homomorphism (4) it follows that in the reverse transition $1 \to 2$ a defect labeled by an element $\chi \in \pi_r(G/H\ )$ can turn into any defect of phase 2 labeled by an element of the inverse image $p_*^{(r)-1}(\chi)$, provided this image is not empty.

If, however, the inverse image is empty, the defects of phase 1 break into defects of higher dimension in phase 2. This fact has been proved by Mermin, Volovik and Mineyev[2,5] for point and line defects in superfluid ^{3}He-A, where a subset relation $V_2 \subset V_1$ exists between the degeneracy parameter spaces of the dipole locked and the dipole free phase. Also Kléman and Michel have presented an example for the phase transition smectic A $\to$ smectic C . Given the mapping ϕ_1: $R^d - \Delta \to G/H_1$ which describes the higher symmetry phase, we have to search for a mapping ϕ_2 and a set $\Delta_2 \supseteq \Delta_1$ for the lower symmetry phase such that the diagram

$$\begin{array}{ccc} R^d-\Delta_1 & \xrightarrow{\phi_1} & G/H_1 \\ q \uparrow & & \uparrow p \\ R^d-\Delta_2 & \xrightarrow{\phi_2} & G/H_2 \end{array}$$

commutes up to continuous deformation. Here $q(\underline{x})=\underline{x}$ for $\underline{x} \in R^d-\Delta_2$. In the following a general method to construct the resulting defect pattern Δ_2 is illustrated by the example of a "hedgehog" point singularity (director parallel to $\hat{r}$) in the transition uniaxial $\to$ biaxial nematic.

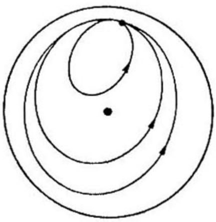

Fig.1a. Resolution of the sphere around a point defect into Burgers circuits.

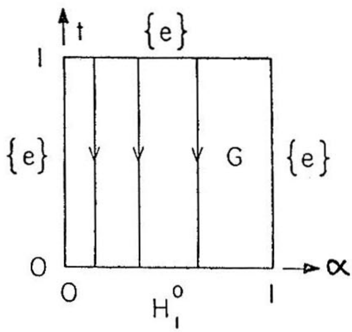

Fig.1b. Domain and range of the "Burgers paths" $\{g(t_1,t_2) \in G | 0 \le t_1, t_2 \le 1\}$ that correspond to the Burgers circuits of Fig.1a.

As in Fig.1, the sphere around the point defect is resolved into loops ("Burgers circuits"), parametrized by $(\alpha,t)\in[0,1]\times[0,1]$, where α labels the loops, t its points. The values of the degeneracy parameter along these loops are described by elements of G acting on the initial point ξ_0: $\xi(\alpha,t)=g(\alpha,t)\xi_0$. Thus a continuous family of "Burgers paths" is obtained in G. When operating in G rather than in G/H, a cut must be made on the sphere (in this case consisting of a single point), and the endpoints of the paths, $\{g(\alpha,t=0)\}$ must form a closed loop in H_1^0. As is known from the isomorphism between absolute and relative homotopy groups[3] for the case of the hedgehog point defect, this loop runs once around $\bar{C}_\infty$. In the phase transition H_1^0 is reduced to the set of discrete points $H_1^0\cap H_2=\{\pm 1,\pm i\sigma_z\}$ (Fig.2).

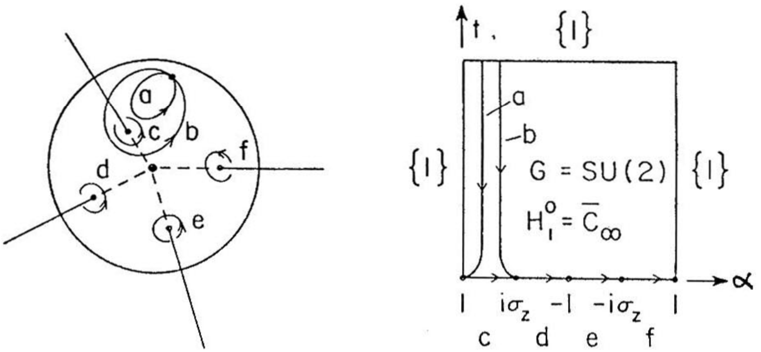

Fig.2a. Line defects arising from a point defect in the transition 1→2 and the circuits to analyse them.

Fig.2b. Domain and range of the corresponding paths in G.

The least molecular rearrangement to meet this situation is required if the image of each vertical line (α=const, t) is bent into the nearest point of $H_1^0\cap H_2$. A path $g(\alpha=\text{const}, t)$ in G, terminating in a component of H_2 different from H_2^0 corresponds to a nontrivial loop $g(\alpha=\text{const}, t)H_2$ in G/H_2. Hence in real space, loop *b* of Fig.2 does enclose a stable line defect, loop *a* does not. Loop *c* is homotopic to $a^{-1}b$ and encircles a 180°-disclination ($i\sigma_z$) in the right sense, with respect to the ray emanating from the point defect , as do loops *d*, *e* and *f*. The homotopy classes labeling these line defects must lie in the kernel of homomorphism $p_*^{(1)}$. One might investigate the transformation of the hedgehog point defect by the long exact homotopy sequence [7]

$$\rightarrow \pi_2(G/H_2) \xrightarrow{p_*^{(2)}} \pi_2(G/H_1) \xrightarrow{\Delta} \pi_1(H_1/H_2) \xrightarrow{i_*^{(1)}} \pi_1(G/H_2).$$

The point defects under consideration are not in the kernel of Δ, but in the kernel of $i_*^{(1)} \cdot \Delta$ which is the entire group $\pi_2(G/H_1)$. The analysis of Δ indicates a situation where the four line defects collapse to a single ray which can escape to infinity. Mathematically, Δ_2 being a single ray is the simplest response of the defect structure to the phase transition, since $R^3 - \Delta_2$ is then contractible not permitting any stable defects. The distortion of the four line defects of Fig.2 to a single ray, however, seems to require too much energy to be realized in nature.

For $r = 3$ homomorphism (4) represents the selection rule for phase transitions of configurations in three-dimensional space. Configurations are nonsingular mappings

$$\phi : R^d \longrightarrow V$$

with the boundary condition $\phi(\underline{r}) \rightarrow \xi_0$ for $|\underline{r}| \rightarrow \infty$. For all mesomorphous phases $\pi_3(V) = Z$ (= set of integers), [8] and relation (4) is an isomorphism. No stable defects can arise in a phase transition between configurations. For the phase transition uniaxial $\rightarrow$ biaxial nematic a construction similar to that of Fig.2 but in one dimension higher, demonstrates, that line defects can appear forming closed loops. There exists an experiment confirming this statement: in cholesteric liquid crystals Bouligand et al.[9] have observed rings of 360°-disclinations in the cholesteric pitch. They assign to them a "double" topological character, locally as line defects corresponding to an element of the fundamental group for cholesterics; globally as a nonsingular configuration of a (twisted) nematic.

4. Conclusion

The geometrical model of a phase transition and the conclusions drawn by topological considerations are qualitative and require a verification by investigation of thermodynamic potentials and strain energies. But even quantitative theories of defect phase transitions must take into account the topological classification in the form of boundary conditions. Our model should be valid in the far field of the defect, where ϕ is nearly uniform and the strain is small. The nature of a defect, however, is also resembled in its far field. If defect transformations break the selection rules provided by homomorphism (4), the far field must be completely rearranged which seems very unfavorable energetically.

It has been suggested that for media of discrete translational symmetry some intermediate states in the continuous deformation of field ϕ into ϕ' might not be physically realizable. Hence there would be a difference between "mathematical" and "physical" homotopy, caused by certain compatibility conditions. These conditions, not yet successfully incorporated in the classification scheme, will lead to a subclassification and refine the selection rules but not break them.

The theory presented above has a number of additional applications. Defects of phase 2 with a nonsingular core of phase 1, for instance, must correspond to homotopy classes in the kernel of homomorphism (4). Sometimes defects in only that part of the degeneracy parameter are considered which can easily be influenced by the form of the vessel. In superfluid ^{3}He-A, for example, the degeneracy parameter is a tripod of which one leg, the angular momentum vector of a Cooper pair, is perpendicular to outer surfaces. In a conjectured phase transition, where phase 1 is governed by the incomplete, phase 2 by the complete order parameter, these defects can be related to the singularities of the actual manifold of internal states.

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