SYMMETRY AND IMPERFECTIONS

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ABSTRACT

This paper gives an introductory survey of the connection between the symmetry of a physical system and the defects that can occur in it. The topological classification of defects is described and illustrated with a simple example. Other possible applications of homotopy theory are then mentioned. Finally a brief outlook for the future is presented.

INTRODUCTION

Solid state physicists traditionally idealize a solid as an infinite, perfect crystal. Though not in conformity with reality, such an assumption provides a convenient and good enough stepping stone to the description of many of the observed properties like thermal, electronic and optical. Indeed, this fiction of perfect order is carried to such an extent that in many well-known books[1,2] on solid state physics, defects receive mention only towards the end (seldom reached by most readers!). There is unquestionable merit in the above simplification but it does ignore an important fact of life namely, real crystalline solids always have defects.

The existence of defects in crystals has been reasoned out on various grounds—thermodynamic (vacancies), flow properties (dislocations) etc. There is, of course, also experimental evidence for their existence. And while, as noted above, some physicists have tended to underplay defects, others, particularly those close to technology (be it semiconductor devices or metallurgical), have always been quite conscious of them and the important influence they (*i.e.* defects) have on certain properties, especially mechanical.

Defects are not a peculiarity of the crystalline state of matter. It is now known that they occur in other ordered systems as well—liquid crystals, superconductors and even superfluid helium (both ^4He and ^3He), to name a few. With due apologies to the poet, it almost seems like: If there is order, can defects be far behind!

In this article, I wish to summarize (in a somewhat descriptive manner), recent developments concerning the connections between symmetry and imperfections[3-8] which enables us to have a unified picture of defects, their classification, their stability and the rules for their aggregation in various types of ordered condensed matter. Much of this unification is through a skilful exploitation of the results of algebraic topology[9]. Lest there should be some skepticism as to whether such high-powered machinery is actually required, I wish to point out that without resorting to it, one could not really come to grip with defects in superfluid ^3He[5]. In a similar fashion, considerable progress has been made in the case of liquid crystals also[10,11]. It further seems as if topological concepts are unavoidable if one has to really understand the structure of glass[12-20]. In a sense therefore, this article could well be titled: Defects and Topology.

SYMMETRY AND ORDERING

Before discussing the connection between symmetry and defects, it is useful to recall some pertinent facts concerning symmetry and order. For purposes of illustration, we shall consider the planar magnet shown schematically in figure 1. We have here a set of spins aranged in a lattice, each spin $S(i)$ having rotational freedom in the plane. At high temperatures the spins at different sites will be oriented at random characteristic of spin disorder (see figure 1a), but at low temperatures the spins will be aligned as in figure 1b. (Strictly speaking this is not true; see, for exam-

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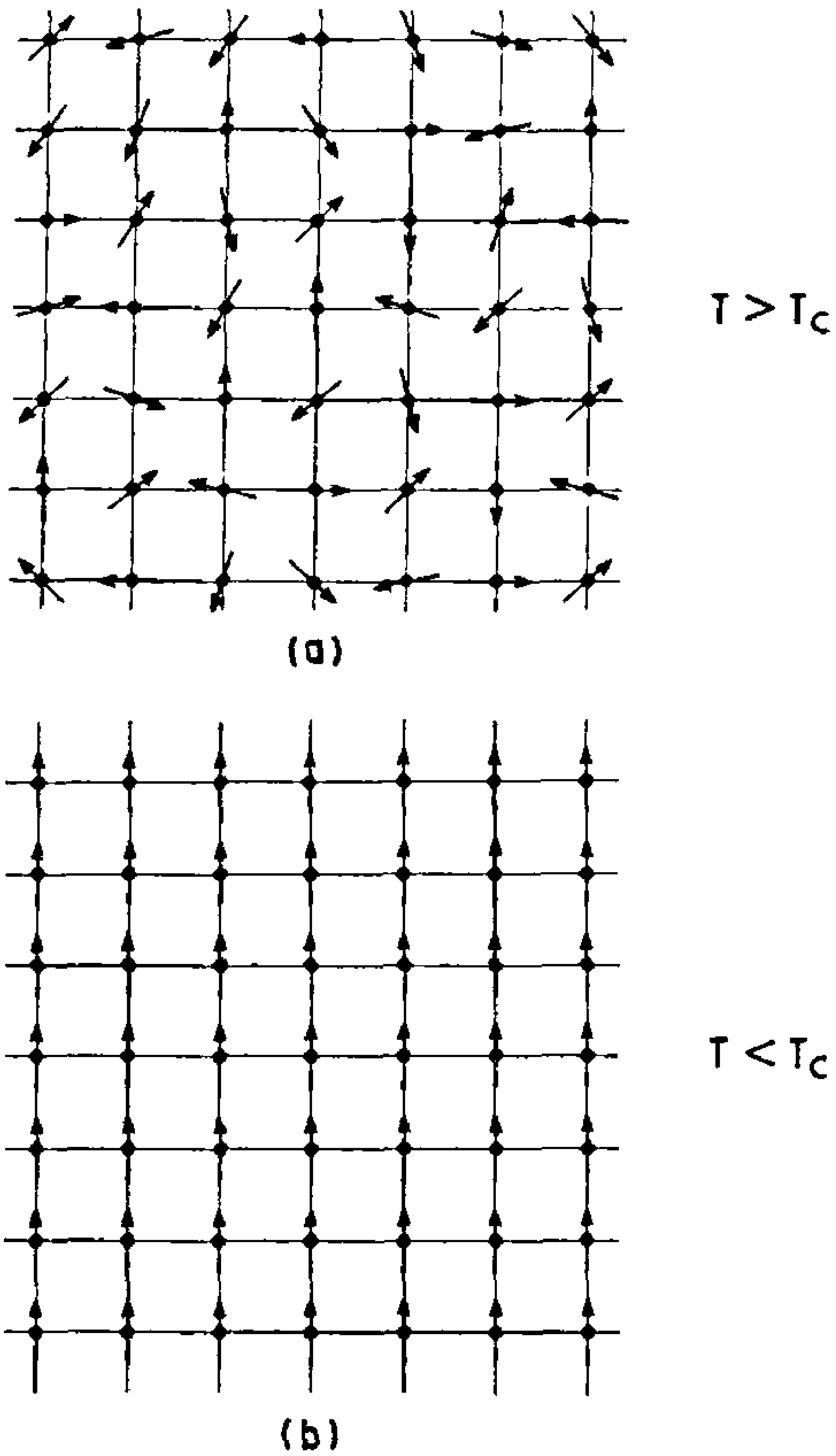

Figure 1. Schematic drawing showing disorder and order in a planar spin assembly.

ple, reference 21. We shall, however, gloss over this technicality!).

It is convenient to introduce the complex order parameter ψ defined by

$$\psi \equiv S_x - iS_y = \psi_0 \exp i\theta \qquad (1)$$

to discuss the transition between the disordered and the ordered states in figure 1. Following Landau, one could write the free energy of the system in terms of ψ as

$$F(\psi) = F_0 + a|\psi|^2 + b|\psi|^4 \quad b > 0 \qquad (2)$$

where $a = \alpha(T - T_c)$ $(\alpha > 0)$, and T_c is the transition temperature. At any given temperature, the system seeks a configuration corresponding to the minimum of the free energy. From figure 2 we see that for $T > T_c$, the configuration chosen has $\psi = 0$, *i.e.* it lacks order (as illustrated in figure 1a). Below T_c, $F(\psi)$ has a shape resembling the bottom of a wine bottle. There is no unique minimum, every point in the bottom edge (shown with a thick line) qualifying equally. Thus, when the system orders, it can choose any of the possibilities in figure 3a. Which one is actually realized during a particular cool down from above T_c to below T_c, is a matter of chance.

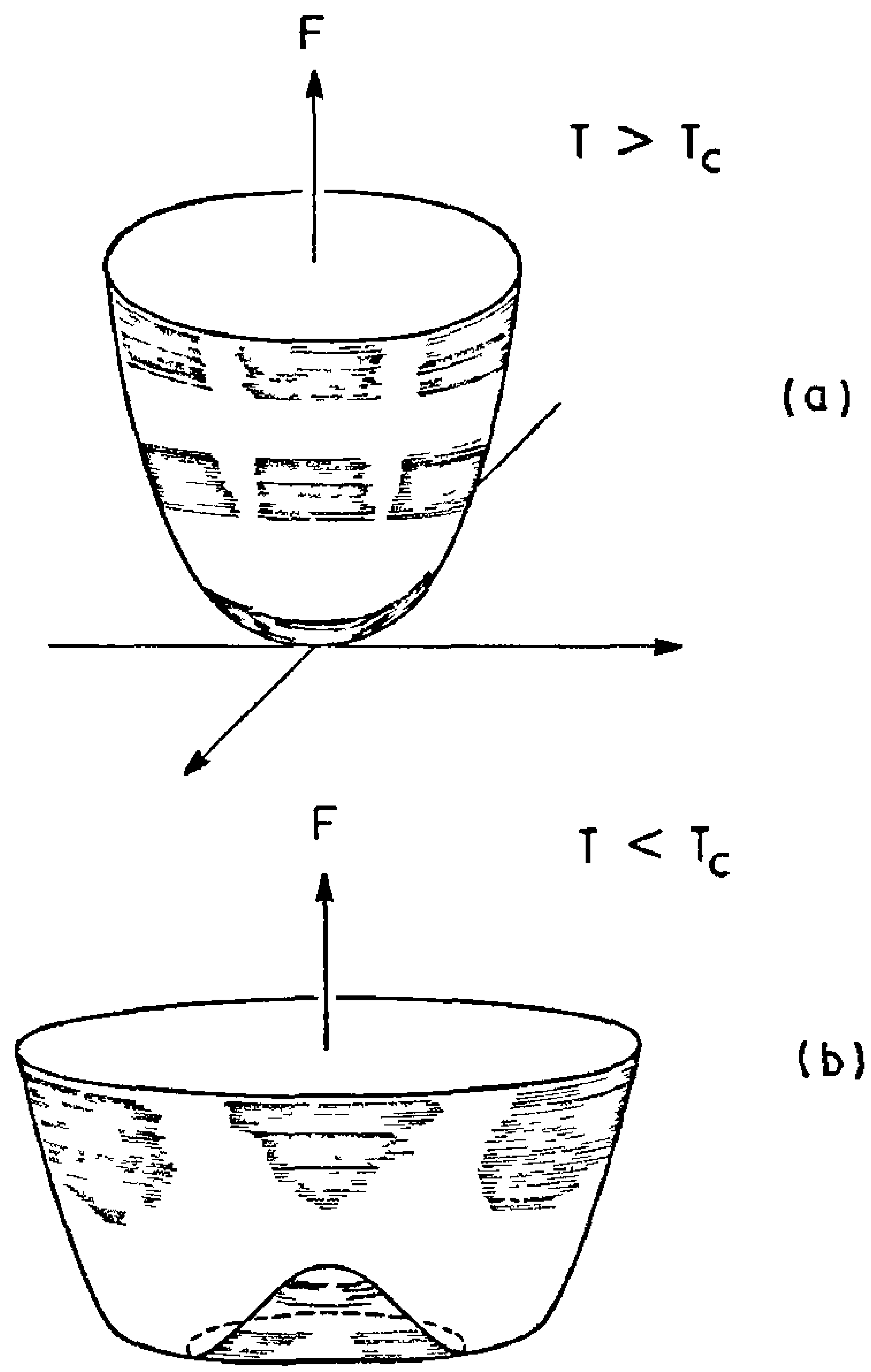

Figure 2. Free energy surfaces for the planar magnet system for $T > T_c$ and $T < T_c$. In equilibrium, the system will be at the free energy minimum. For $T < T_c$, this implies that the system can be anywhere along the rim at the bottom of the "wine bottle" shown in (b).

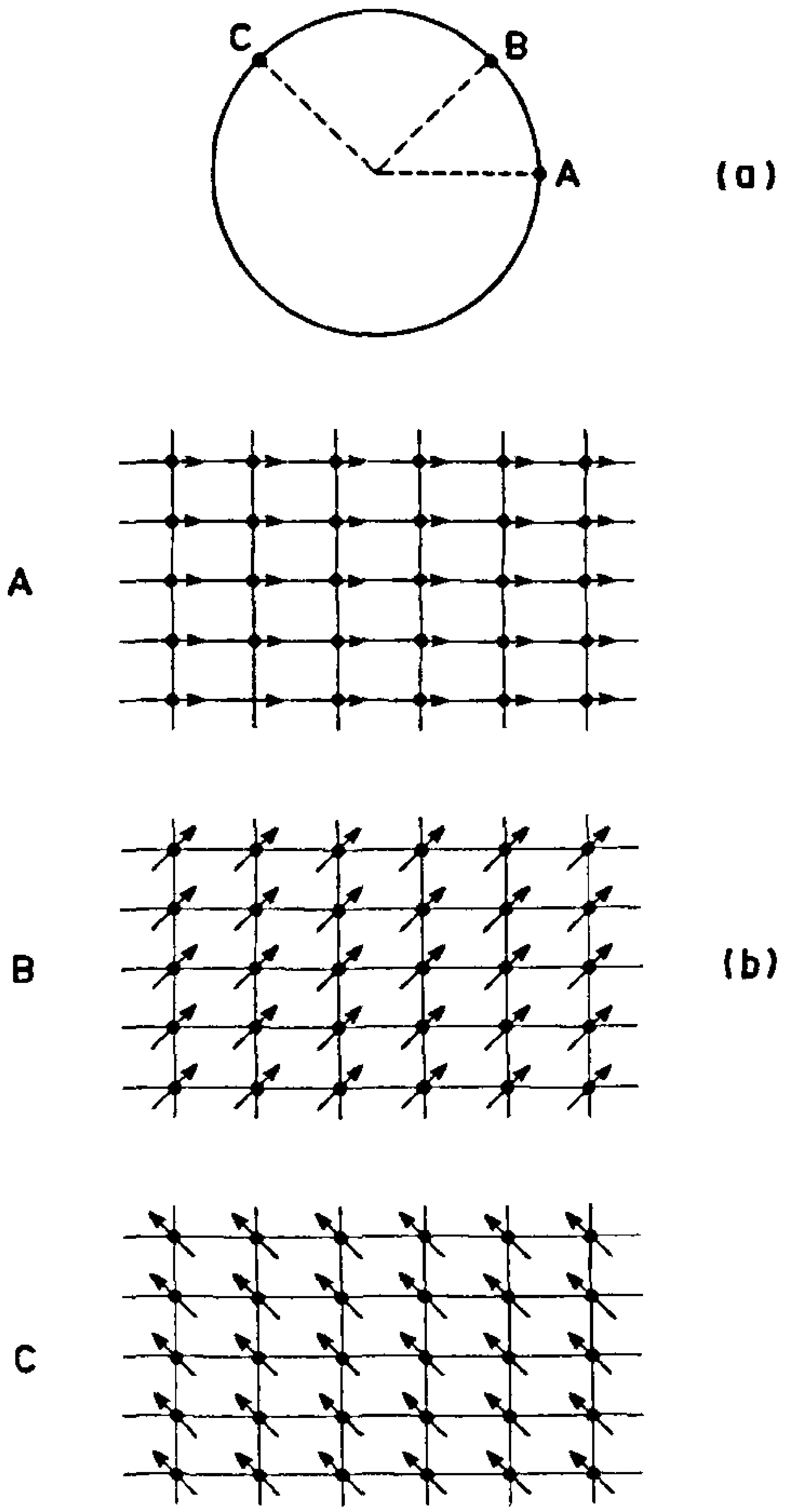

Figure 3. (a) shows the order parameter space for the planar magnet. This is the bottom of the "wine bottle" of the previous figure. In (b) are illustrated various possible ordered states that can arise when the system is cooled to below T_c. The corresponding configurations in the order parameter space are shown in (a).

Several points are worth underscoring at this stage. Firstly, the disordered system has in fact a higher symmetry than the ordered system. Puzzling though this might sound, this is easy to understand when we note that the spins in the disordered systems, *i.e.* the pattern of figure 1a may be rotated in any way we like without our being able to detect the difference. On the other hand, we are definitely able to say that the different patterns in figure 3b, (all of which represent ordered states), are rotated with respect to each other. One formalizes this observation with the statement that whereas the disordered state is invariant under the group G of planar (spin) rotations, the ordered state is not. It is as if the system sheds some symmetry while becoming ordered, a phenomenon technically referred to as symmetry breaking. In the present example, continuous rotational symmetry is the one that is broken.

ORDER PARAMETER SPACE

We next turn to the ordered states illustrated in figure 3b, where also there are a few points to be noted. Firstly, the ordered state too has a symmetry group of H of its own which leaves that particular state invariant. This group H is naturally a subgroup of G and is referred to as the isotropy subgroup. In figure 3a, each ordered state has its own isotropy subgroup but, as is to be expected, all the different isotropy subgroups H_A, H_B, H_C etc are equivalent in a group-theoretial sense. It should also be clear from figure 3 that it is possible to go from any ordered state ψ_A to any other state ψ_B, ψ_C etc by acting on ψ_A with an appropriate element of G (obviously not contained in H_A). In this way, one can build up the entire circle shown in figure 3a. The manifold so built up is variously referred to as the order-parameter space (OPMS) or as the manifold of internal states.

Going back to figure 2, we note that the OPMS is a surface of minimum energy. In general, this surface has a dimensionality $(n-1)$, where n is the dimensionality of the order parameter. Technically, the OPMS $R = (G/H)$, the space of cosets of G with respect to H[6].

ORDER PARAMETER AND IMPERFECTIONS

The space R plays a key role in the topological classification of defects. It is important to appreciate that R is manifold in an abstract space.

The significance of this statement will (hopefully!) become clear shortly.

It might have been noticed that the order parameter in Landau's theory does not involve the spatial coordinate. When a system orders, it has the same value for the order parameter *at all points in space*; in other words, the ordering is perfect. Viewed in this light, an imperfection is a state where the order parameter is a function $\psi(r)$ of r. Such imperfections can either be singular or non-singular[22], and if, of the latter type, are often referred to as textures. Figure 4 shows two examples of singular defects in a planar magnet.

How does one recognize a defect, and how does one classify them? It is in answering these questions in a generalized way that topological concepts enter into the picture. Consider a singular defect. This is one where the order parameter field (like $\psi(r)$ of the planar magnet) becomes singular at some point r. Since matter is actually discrete rather than continuous (being made up of atoms), $\psi(r)$ in real life escapes a singular fate. We shall however sidestep these subtleties by agreeing not to look closely inside a small region called the core which surrounds the defect. Outside the core, the order parameter does not vary so strongly (as it does while approaching the singularity), and it is by scanning these slow variations that we must recognize the defect. The actual identification is effected by a technique familiar in characterizing dislocations in crystal *i.e.* by traversing a closed contour C surrounding the suspected defect, and measuring $\psi(r)$ everywhere along this circuit. Clearly $\psi(r)$ must come back to its initial value when we return to the starting point. However, this does not imply that the phase angle θ in (1) must also come back to its initial value. It could in fact assume the values $(\theta + 2\pi n)$ where n is an integer. If $n = 0$, then there is no defect in the encircled region but if $n \neq 0$ there is a defect, the value of n characterizing the defect (see figure 4).

DEFECT CLASSIFICATION: AN EXAMPLE

Let us now consider the round trip in real space along C *vis-a-vis* R which, remember, is an abstract space[4]. This is illustrated in figure 5. We observe that as C is traversed, *local* regions appear as if perfectly ordered, with the *local* value of ψ corresponding to some point or other of the OPMS R. In other words, as the closed contour C is traversed in real space, a corresponding loop is mapped in the abstract space R.

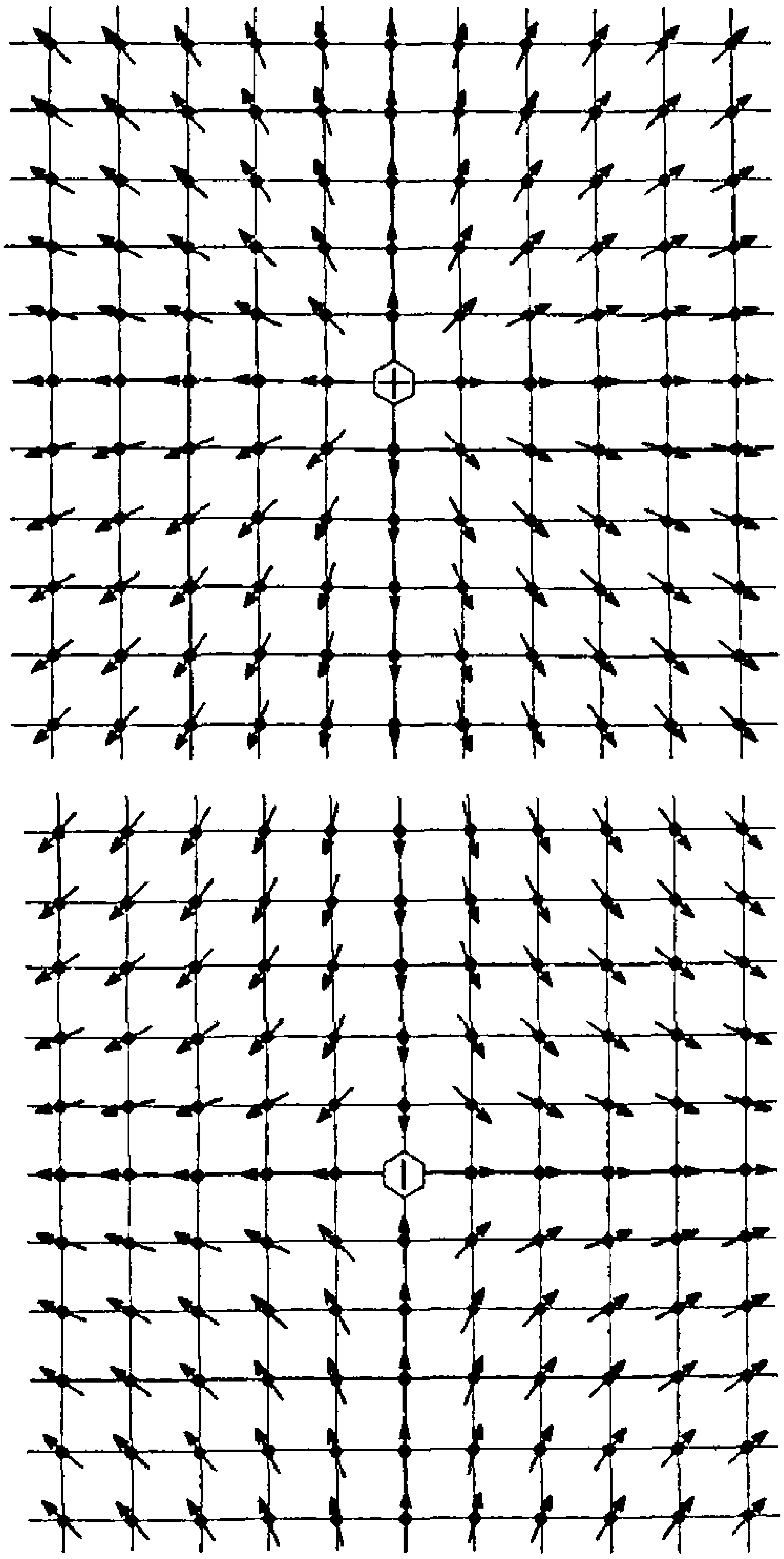

Figure 4. Two of the simplest defects of the planar magnet system.

Figure 6 shows some typical defects of the

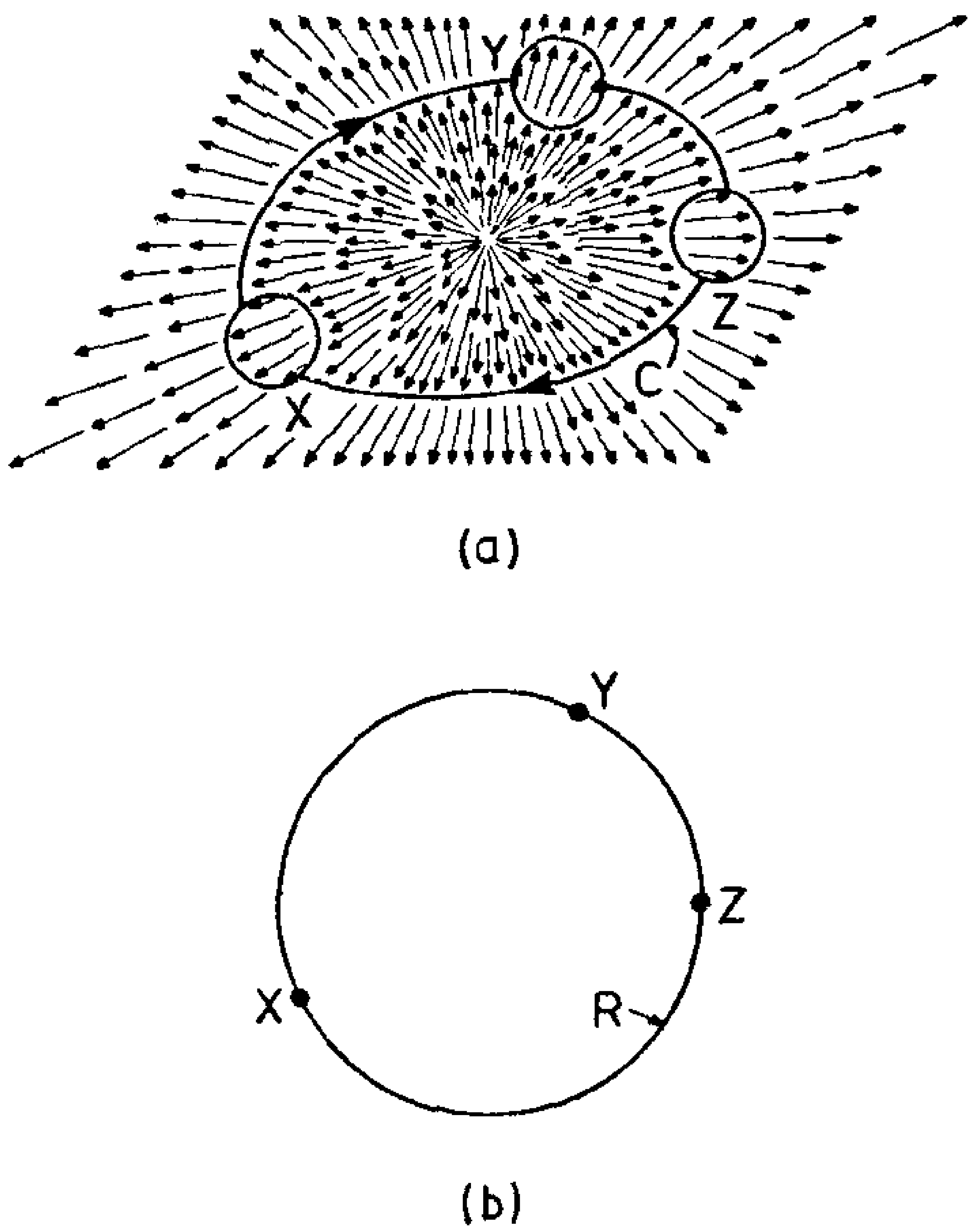

Figure 5. (a) shows schematically a topological defect in the planar magnet. As the contour C surrounding the defect is traversed, one sees that in local regions like X, Y and Z, it appears as if there is perfect order. The defect pattern can thus be characterized by sequentially describing the local scenario, using the language of perfect ordering, *i.e.* the OPMS *R* illustrated in (b).

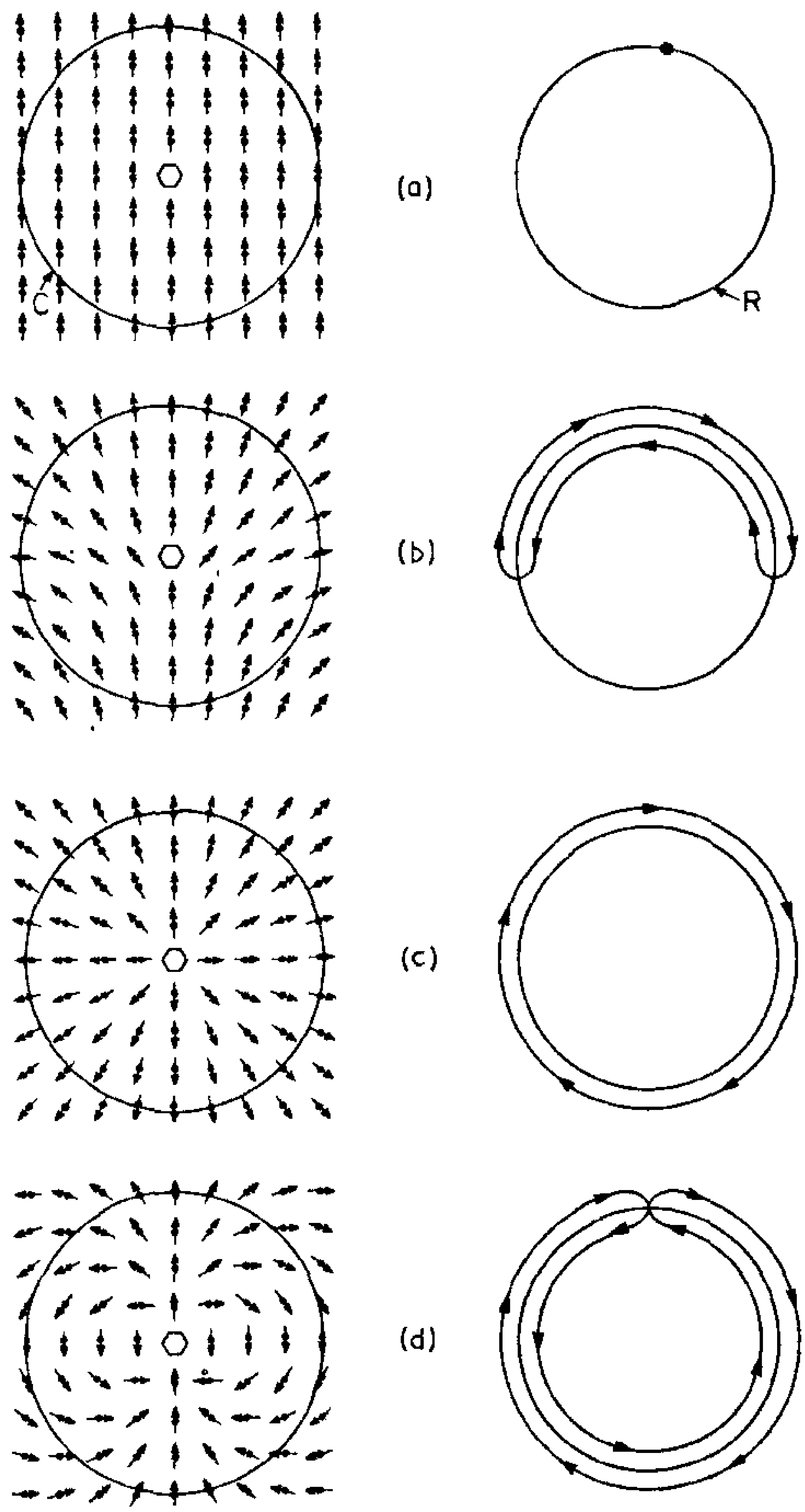

Figure 6. Illustrated here on the left are various spin configurations of the planar magnet. While that in (a) represents perfect ordering, all others represent states with defects. To assess the defect, one makes a round trip along contour *C* in real space. This leads to loops in the order parameter space *R* as shown on the right. If these loops can be continuously shrunk to a point, then the corresponding defects are topologically unstable. Thus defect (b) is a trivial one.

planar magnet and the corresponding loops in *R*. Two features are noteworthy. Firstly, even though one makes only one circuit along the real space contour *C*, the loops produced in *R* by the mapping process can have more than or even less than one turn. Further, while some loops can be continuously shrunk to a point (see figure 6), other loops cannot be so shrunk. This important point is amplified in figure 7 where, as an illustrative aid, the space *R* is depicted as a cylindrical former. If now we imagine the loops to be perfect elastic bands wrapped around the cylinder as shown, we can readily see that only the loop with less than one turn can be continuously shrunk to a point without breaking it. All other loops while deformable, *cannot* change their winding number (*i.e.* number of turns in the loop). From this we can deduce that defects corresponding to loops in *R* which can be continuously shrunk to a point can be eliminated by local adjustment of the spin orientations (also referred to as local surgery; compare figures 6a and b). On the other hand, defects with winding

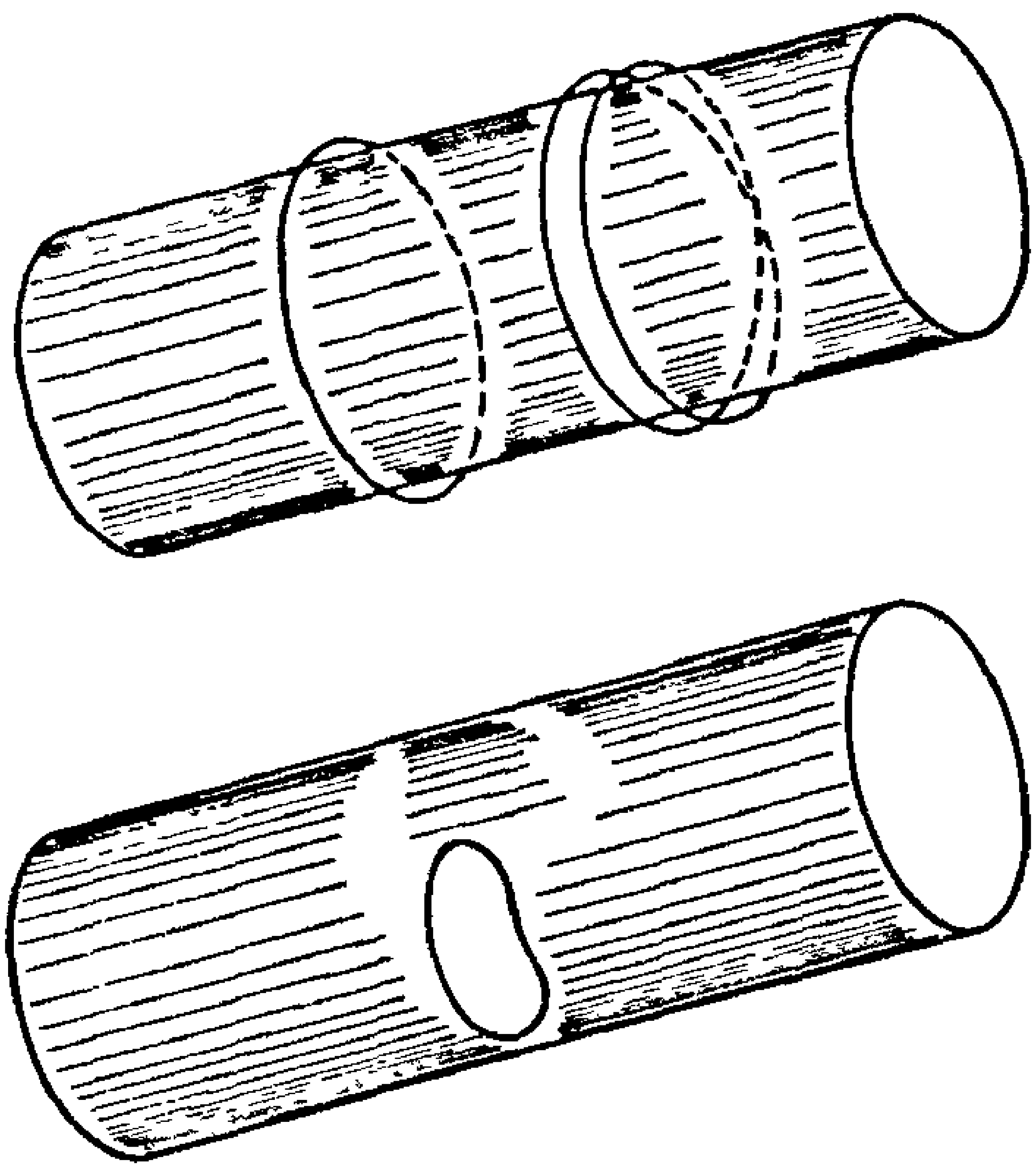

Figure 7. Pictorial aid to illustrate the shrinkability or otherwise of loops in order parameter space. For explanation, see text.

number $n \neq 0$ cannot be so eliminated. Their elimination requires readjustment of spins over the *entire* lattice which clearly will cost a lot of energy especially in the thermodynamic limit. This leads us on to the topic of stability of defects. Whereas defects with $n = 0$ are unstable, those with $n \neq 0$ are not, the stability being related to the properties of loops in R, in turn derived from the topological properties of the space R. The stability we are considering is therefore the topological stability. Notice also that we have quietly introduced a defect label called the winding number which is based on the number of loops in R produced by the mapping of $\psi(r)$. In a nutshell, the defects we are presently considering are related to the topological properties of R, and there is a labelling scheme possible based on these topological properties. For this reason such defects often are referred to as topological defects*. The entire qualitative reasoning given above can be formalized using homotopy theory which, hopefully, will be comforting to those who prefer rigour!

* A substitutional impurity in a crystal is not a topological defect. A dislocation however is.

HOMOTOPY AND DEFECT CLASSIFICATION

We can now generalize the above discussion. Existence of topological defects in condensed matter can be assessed by scanning over an appropriate Burger's circuit surrounding the suspect region[4]. For point defects in 2D and line defects in 3D, the circuit is a loop or circle (like in the planar magnet example). For point defects in 3D it is a sphere. Once again, one makes a round trip in real space along the Burger's circuit and studies the variation of the order parameter field. These field variations are then mapped into R whereupon one gets loops or spheres (as the case may be) in R. The classification of defects now boils down to a study of the property of the loops or spheres in R.

Directing attention to the loops first, one can regard each loop as an element of an abstract group, and, based on their homotopic properties, assign a group structure to the collection of loops. This group denoted $\pi_1(R)$ is referred to as the fundamental homotopy group of R or simply as the fundamental group of R. It can be shown that there are as many distinct defects as there are classes in π_1. For the planar magnet, $\pi_1 = Z$ the group of integers. The existence of winding numbers thus emerges from an analysis of the homotopy properties of loops in R. It is important to appreciate that this can be done *without* requiring a knowledge of the actual field patterns such as those shown in figure 3. All that needs to be known is the structure of R. The defect classification just described is rather similar to the classification of normal modes of vibration of a molecule using purely the symmetry of the molecule. To construct the field patterns (as in figure 4) one must appeal to physics even as in the molecular example, we must analyze the dynamical equations to explicitly construct the eigenvectors.

The group π_1 helps label point defects in 2D and line defects in 3D. Likewise, from a study of spheres mapped into R, one can construct the second homotopy group π_2 which comes in handy for classifying point defects in 3D. Table 1 summarizes the basic ideas.

Table 1 *Summary of homotopic classification of defects. For simplicity, we assume that the order parameter is a vector with n components. The OPMS is then the sphere S_n. One can associate a dimensionality d' with defects. Using the theorems*

$$\pi_i(S_j) = 0 \qquad \text{for } i < j$$
$$\pi_j(S_j) = Z,$$

where i, j are integers, π_i is the homotopy group of order i and Z is the group of integers, one finds that topologically stable defects have the dimensionality $d' = d - n$. To assess the defect one surrounds it by a Burgers' sphere of dimensionality r where r is defined by $(d' + r + 1) = d$. Shown below are the topologically stable defects possible for various (n, d) combinations. For $n > d$, there are no stable defects.

d \ n	1	2	3
1	point	–	–
2	line	point	–
3	wall	line	point

OF WHAT USE IN HOMOTOPY

Classifying defects using the homotopy groups π_n is just one of the uses of the homotopy theory. There are many other uses, and, as with classification, these other applications also have their analogues in the conventional applications of group theory, say to spectroscopy. One such application concerns the combination of defects[23]. In the case of the vortices of the planar magnet, one can intuitively see two vortices with winding numbers n_1 and n_2 can combine to give a composite one with winding number $(n_1 + n_2)$. More interesting is the case of the defects.

Consider the two shown in figure 8. When they move (which can happen in the presence of stress), they can have an encounter and the question is whether they will just cross each other as in 8b or get entangled as in 8c. This depends on whether or not π_1 is Abelian, and if π_1 is non-Abelian, rather specific statements can be made about scars produced by the entanglement, from an analysis of the class multiplication structure of π_1. This study of combination of defects is not

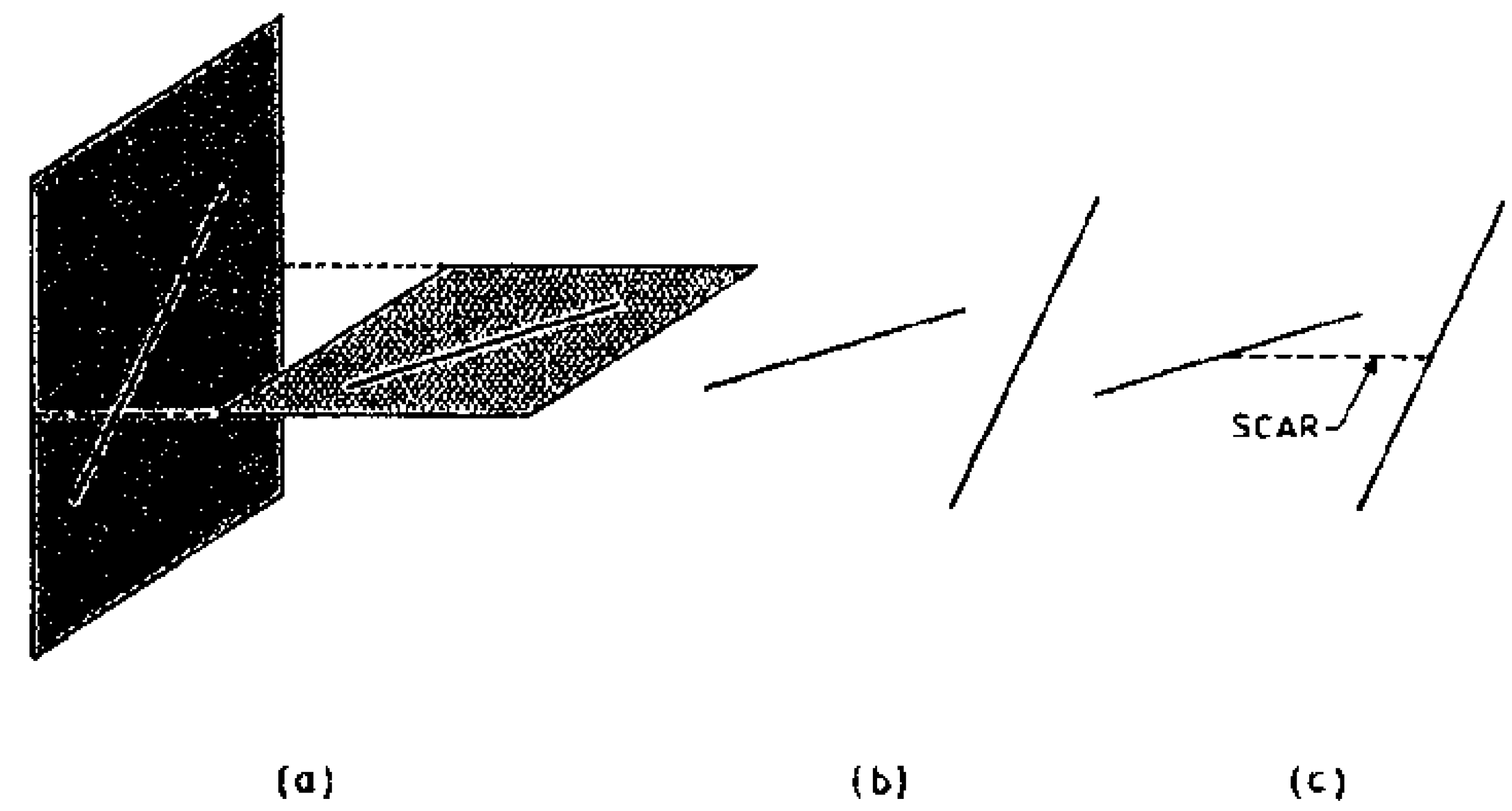

Figure 8. (a) shows two line defects. In (b) the two have crossed without a scar. This happens if π_1 is Abelian. If π_1 is non-Abelian, the situation is as in (c).

unlike the use of group theory to study selection rules.

Yet another application of homotopy concerns changes to defects during a phase transition. This is particularly interesting in the case of the A-B transition in superfluid ^{3}He, and thanks to the complexity of the order parameter, the problem cannot be tackled without resort to topological concepts[24]. The analogous conventional problem is crystal field splitting, where again one studies changes in classification arising from changes in symmetry.

In passing it is worth observing that homotopic analyses of defects in condensed matter have close parallels in particle physics[25]. It is not surprising therefore to find theorists working on polymers or liquid crystals and monopoles at the same time!

BEYOND SIMPLE HOMOTOPY

So far, we have restricted ourselves mainly to single defects and at best a combination of two of them. Such studies have yielded a wealth of information, particularly in the case of ^{3}He and certain phases of liquid crystals. In all the success stories thus far, the ordered system retains its continuous translational symmetry, the (continuous) symmetry broken during the ordering process being something else (often a rotational symmetry of some sort). Application of homotopy to systems with broken translational symmetry (*e.g.* crystals) poses some problems[6,7], and progress to the extent realized in ^3He, for example, is yet to be attained.

Moving from single to many defects, one now has the analogue of the familiar many-body problem. The many-defect problem is still in its infancy but it is already clear that as in the case of conventional many-body problem, field-theoretic techniques will be a *sine-qua non.* It is also likely that inputs derived from homotopic analysis of single defects may be necessary[26]. In addition, fresh ideas like gauge fields[27], fibre bundles[28] etc may also have to be imported.

What we have described is but the tip of the ice berg. In a broad sense, one is now trying to obtain a unified and sweeping perspective of the various phases of condensed matter with due regard to symmetry, in which defects find a natural place. This is best exemplified by the fascinating table prepared by Michel[9] which we reproduce here as table 2. The list is no doubt partial but one can see that one is trying to encompass other states of matter besides crystals into the symmetry scheme. The table raises many tantalizing questions. Where do the many-defect solids considered by Aubry[29] (whose description requires concepts related to chaos) fit in? Do they form a part of this Grand Design? And what about glass which, according to some, are really ordered in an appropriate curved space even though they may appear disordered in Euclidean space? and so on.

Table 2 *This table adapted from reference 9 deals with various mesomorphic states of matter. Here the parent group G is the Euclidean group E(3). Different states correspond to different isotropy subgroups H. In this case, all are compact.* H_o *is the largest connected subgroup of H while* $T_H = H \cap T$ *where T is the translational subgroup of E(3) R is the space of real numbers,* $R^2 = R \times R$ *and* $R^3 = R \times R \times R$. *Z is the group of integers,* $Z^2 = Z \times Z$ *and* $Z^3 = Z \times Z \times Z$. *U(1) is the unitary group.*

Family	T_H	H_o	Description
I_a	R^3	$R^3 \times U(1)$	Ordinary nematics
I_b	R^3	R^3	Exceptional nematics
II_a	$R^2 \times Z$	R^3	Cholesterics
II_b	$R^2 \times Z$	$R^2 \times U(1)$	Smectics A
$II_{c,d}$	$R^2 \times Z$	R^2	Smectics C
V	R^2	R^2	Chiral smectics
III	$R \times Z^2$	R	Rod lattices (*e.g.* lyotropics)
IV	Z^3	{1}	Crystals

CONCLUDING REMARKS

To conclude, we are moving away from the era when perfection and defects were studied in isolation. Not only have we come to recognize that defects have a deep connection with symmetry, but we also find that in contrast to its relative neglect in the past, the study of the defect state is now attracting the use of the most sophisticated tools physicists command at present, normally reserved for particle theory! More important, we might even uncover a Grand Design lurking behind the various apparently unrelated phases of condensed matter. The day is also not far off when attention will turn to the fundamental aspect of defect dynamics, especially as it is closely related to flow properties[30]. Here again a cross flow of ideas from elementary particle theory is highly likely[31].

It is heartening that Nature is after all not mundane at any level! If defects appeared dull and uninteresting in the past, it was largely the result of our own ignorance. Mercifully we are making up for our past neglect, almost with a vengence it seems!

29 October 1984

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ANNOUNCEMENTS

INTERNATIONAL SYMPOSIUM ON WHOLE-PLANT PHYSIOLOGY: CALL FOR PAPERS

The International Union of Forestry Research Organizations (IUFRO) is sponsoring a symposium on the "Coupling of carbon, water and nutrient interactions in woody plant soil systems" on October 6–11, 1985 at Knoxville, Tennessee, USA. The meeting will promote the synthesis of research on physiological processes at the whole-plant level. Four sessions of invited and contributed papers will address the linkages between water-nutrient, carbon-nutrient, carbon-water and carbon-water-nutrient interactions of forest, orchard and plantation tree or shrub species.

The scope of the symposium includes source-sink-storage relationships of carbon, water and nutrients; diurnal and annual cycles of physiological variables; photosynthesis, translocation, transpiration, nutrient and water uptake, and nutrient utilization; enzymatic and hormonal regulation; influence of soil and aerial environment and the rhizosphere on plant growth and development; physiological characteristics influencing the competition between individuals for resources from the environment; experimental and modeling methods of whole-plant research.

Contributed papers on the above themes are welcomed. Authors should submit an abstract of 200–300 words (four copies) to the Organizing Committee as soon as possible but no later than 15 May, 1985 for program planning. Please ensure that your name and full address for correspondence appears on the abstract and send to R. J. Luxmoore, Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 USA. Telephone contact at (615) 574-7357.

NATIONAL SEMINAR ON LINEAR FREE ENERGY RELATIONSHIP AT MADRAS

The above Seminar will be held at Anna University, Madras during February 27–March 1, 1985. For details please contact Prof. P. Ananthakrishna Nadar, Professor and Head of the Department of Chemistry, College of Engineering, Anna University, Guindy, Madras 600 025.