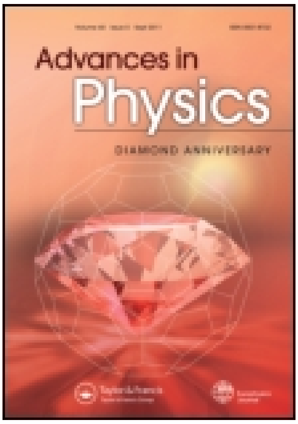


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# The topology of non-uniform media in condensed matter physics

H.-R. Trebin [a]

[a] Institut für Theoretische Physik der, Universität, D-8400, Regensburg, F.R. Germany

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# The topology of non-uniform media in condensed matter physics

By H.-R. Trebin
Institut für Theoretische Physik der Universität, D-8400 Regensburg, F.R. Germany

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Abstract

Methods of algebraic topology have been employed recently to classify defects and non-singular textures of condensed matter systems, and to describe two-defect processes. In this article a systematic review is presented of these methods and their applications. The non-uniform media are characterized by fields valued in a space of degeneracy, whose topological properties are investigated. Ways to represent such a space are reported. An introduction is given to the necessary mathematical tools, viz. the homotopy groups and exact sequences thereof. Combinations, entanglements and transformations of singularities are discussed. The connection between the homotopic defect classification and the description of many-defect systems is elaborated. The limitations and necessary modifications of the method for systems of broken translational symmetry are examined.

CONTENTS

## §1. Introduction

### 1.1. *General remarks*

The defects dealt with in this review are structural and are therefore also denoted topological or symmetry defects; this is in contrast to substitutional defects, like impurities or vacancies. Symmetry defects are responsible for many of the physical and chemical properties of solids and fluids. Dislocations in metals, for example, strongly influence the electrical and thermal resistivity (Seeger and Stehle 1956, Bross and Seeger 1958), and govern plastic flow by their motion (Taylor 1934, Polanyi 1934, Orowan 1934). Hysteresis in a ferromagnet occurs due to the displacement of Bloch walls. The quantum nature of vortices causes permanent currents in superconductors and superfluids. Symmetry defects mediate the nucleation in phase transitions: screw dislocations, for instance, direct the growth pattern of crystals (Burton *et al.* 1949). But symmetry defects also invoke new types of phase transitions, like the melting of crystals in two or three dimensions (Halperin and Nelson 1978, Kleinert 1982), and even give rise to entirely new phases, like the hexatic liquid crystals (Birgeneau and Litster 1978), or the blue phase of cholesteric liquid crystals (Meiboom *et al.* 1981, Hornreich and Shtrikman 1981, Stegemeyer and Bergmann 1980, Kleinert and Maki 1981.)

Although defects disturb order, their observation provides insight into order and structure. Texture observation is a most important means for the identification of liquid crystalline phases (Demus and Richter 1980). From the existence of focal conic textures, G. Friedel (1922) concluded that the smectic-A liquid crystals are layered systems.

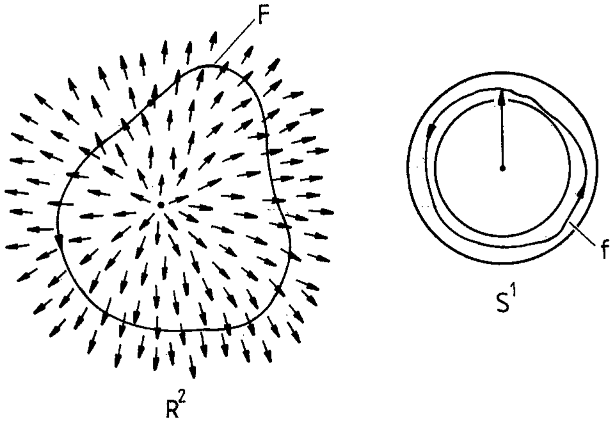
Because of the importance of symmetry defects, their exploration has a long history and there were early attempts to classify them. Standard methods were the Volterra construction and Burgers circuit characterization (for a review see Friedel 1979). But these approaches only allow one to catalogue point defects in two-dimensional, and certain line defects in three-dimensional, spaces. A major advance was made in 1976 when single defect states were first classified systematically by methods of algebraic topology (Rogula 1976, Toulouse and Kléman 1976, Volovik and Mineev 1976, 1977 a, b, Kléman *et al.* 1977). The new scheme amounts to a generalization of the Burgers circuit method to systems of arbitrary dimension $d$ and to defects of any dimension $d' < d$, with the circuit that probes the defect being replaced by a surface of dimension $r = d - d' - 1$. A fundamental algebraic structure was discovered in the form of homotopy groups. These groups are discrete. Their elements, in essence, label the defects and constitute a generalization of the index of a defect (like the vorticity in a superfluid) or of the triple of indices (like the Burgers vector of a dislocation in three dimensions). Physical processes involving defects were recognized to correspond to algebraic operations: defect coalescence to the group product, defect transformation (for instance in a phase transition) to a group homomorphism, the crossing of defect lines to the commutator of group elements, the motion of a point defect about a line defect to a group action.

A distorted (non-uniform) medium containing single defects is described by a field, which is either a displacement-, a vector- or a phase-field, or, generally, a 'field in the degeneracy parameter' valued in a 'space of degeneracy'. The homotopy groups express topological properties of the space degeneracy (§ 2). Since these properties are similar or identical for completely different physical systems, universality classes appear in the defect structures of ordered media. Moreover, the space of degeneracy is closely connected to the invariance group of the system. Thus, via the homotopy groups, a deep relation between the symmetry group of the uniform medium and the defects of its distorted states becomes manifest (§ 3).

### 1.2. *Principles of the classification*

The basic notions become evident through the simple standard example of fig. 1, which shows a source defect of a field of two-dimensional unit vectors in a plane. This might describe, for example, the magnetization of a two-dimensional ferromagnet, or the phase-field of a superconducting film. The range of values of the field (the space of degeneracy) is the unit circle or, if small variations of the vector length are admitted, an annulus. If the defect is probed by a closed loop $F$ and the vectors along the loop are plotted from a common origin, a closed loop $f$ is obtained in the annulus. It winds once around the annulus and cannot be contracted to a point. This property of the space of degeneracy of not being simply connected is crucial for the existence of stable defects. For, as the 'Burgers circuit' $F$ in physical space is shrunk to a point, the corresponding loop in the annulus cannot follow suit. Even

Fig. 1



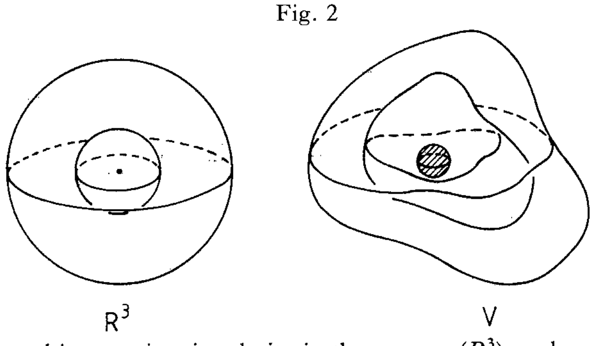

Burgers circuit $F$ probing a source defect of a vector field in the plane ($R^2$), and corresponding loop $f$ in the space of degeneracy ($S^1$).

for a very small diameter of $F$, the magnetization vectors along $F$ must perform a full 360°-turn, and there is necessarily at least one point inside $F$ where the field is undefined. All loops encircling the source, regardless of their extension, have a companion in the space of degeneracy that is non-contractable. The source is therefore noticeable arbitrarily far away and has a far field. Smoothing it out cannot be accomplished by a local field modification, but requires a global rearrangement which (in an infinite system) costs an infinite amount of energy. The source is separated by a topological barrier from the uniform ground state. Defects of this type are denoted as topologically stable, and topological stability implies energetic metastability.

To probe the source of a three-dimensional field of unit vectors in three-space the singular point is surrounded by a (Burgers-)sphere (fig. 2). The vectors on the sphere form a closed surface in the space of degeneracy (for unit vectors this space is also a sphere, which in general is covered more than once). Again, if this surface cannot be contracted to a point, the sphere in physical space necessarily contains at least one singular point, which is not removable by local surgery.

Hence the existence of topologically stable defects depends crucially on the connectivity properties of the space of degeneracy. Arguments of the preceding type were already presented by Feldtkeller (1965) and Döring (1966, 1968) in the case of

Fig. 2




Burgers spheres probing a point singularity in three-space ($R^3$), and corresponding closed surfaces in the space of degeneracy $V$.

special point singularities of ferromagnets, and by Saupe (1973) for line defects in nematic liquid crystals. Homotopy theory explores systematically loops, surfaces and hypersurfaces in spaces of degeneracy. These spaces are therefore central objects of investigation, and the ways to establish and represent them are studied in § 2. The loops (and surfaces) can be grouped into classes such that loops of different classes cannot be deformed continuously one into the other, and thus correspond to different, topologically inequivalent, defects.

§ 4 is dedicated to applications of the topological theory of defects: to defect coalescence, crossing of line defects, surface defects, defect transformation. Here also a new classification scheme is proposed, which corresponds to a generalized notion of defect equivalence.

The homotopic defect classification serves also to classify non-singular parameter fields which, due to boundary conditions, cannot relax to the uniform ground state and hence are known as 'topological solitons' (§ 5).

In special but representative cases the symmetry defects can be labelled by integers; these 'topological charges' can be expressed as analytical functionals of the degeneracy parameter field. The differential geometry of parameter fields, which is a prerequisite for many-defect theories, and for gauge theories for defect dynamics, is commented on in § 6.

### 1.3. *Prospects*

The topological defect classification has provided new insights and spectacular predictions but it suffers from the major deficiency that its full validity is limited to systems of continuous translational symmetry. Whenever this symmetry is broken, as in layered media or crystals, homotopy is restrained by compatibility and integrability conditions. No adequately developed mathematical theory is available to take account of these restrictions. Some first considerations are presented in § 7.

Not only mathematical but also energetic constraints have to be observed, if the homotopic defect classification is to be incorporated fully into physics. Hence, together with the space of degeneracy, one must study the free-energy functional of the system of interest. Indeed, elastic energy terms can seriously change the topology of the space of degeneracy (Kleinert 1979). Since homotopy has become 'the natural language of defect classification' (Mermin 1979), inclusion of compatibility and integrability conditions, and of energetic restrictions, warrants major attention in the future.

Short courses on the topological defect classification are presented by Shankar (1977), Michel (1978, 1981), Stein (1979 a) and Toulouse (1980 a). For a pedagogical, but none the less thorough, introductory review, Mermin's article (1979) is recommended. In the context of broken symmetry, Michel (1980) treats the subject in a deep and extensive way and with mathematical rigour. Poénaru (1979) emphasizes mathematical aspects. Some differential geometric aspects, and numerous applications to the superfluid phases of $^3$He, are contained in the review of Mineev (1980). Finally chapter 10 of Kléman's rich book on defects (1977 b) is to be mentioned.

In this article attention has been paid to various applications of the exact homotopy sequence which receive less emphasis in the other reviews, such as the classification of surface singularities and defect transformation (§ 4). Stress has been laid on the analytic determination of topological charges and the description of many-defect systems (§ 6). The chapter on defects in layer systems and crystals (§ 7) provides some answers to the questions posed in the corresponding section of Mermin's review (1979). Several previously unpublished studies by the author have been included.

This review is intended to be self-contained and mathematical preliminaries are therefore presented in some length (§ 3); an effort was made to support those paragraphs that appear technical and specialized with simple illustrative examples.

## § 2. Spaces of degeneracy

### 2.1. *Degeneracy parameter and London limit*

Any ordered medium in uniform equilibrium is characterized by a constant order parameter. In an *s*-type superconductor, or in superfluid $^4$He, for example, this parameter is a complex number $\psi_0$, which minimizes the Landau free-energy $F=\alpha|\psi|^2+\beta|\psi|^4$. $F$ depends only on the modulus of $\psi$, and not on its phase. Systems with an order parameter $\psi$ of the same modulus $|\psi_0|$ are energetically degenerate. The order parameter is separable into modulus and degeneracy parameter, the latter being valued in a space of degeneracy $V$, which here is the unit circle $S^1$. ($V$ is often named 'order parameter' or 'manifold of internal states', but I regard 'degeneracy parameter', as used by the Moscow school, more expressive).

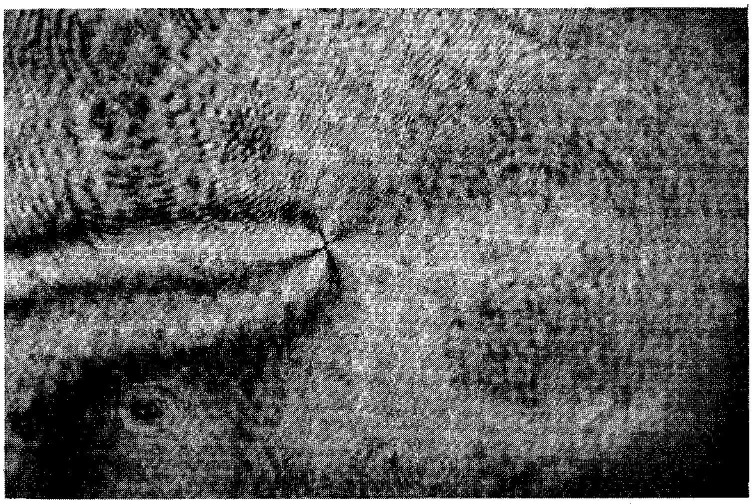
In non-uniform ordered media, the order parameter depends on position, and the free-energy density acquires an elastic term:

$$F=\tfrac{1}{2}K|\nabla\psi|^2+\alpha|\psi|^2+\beta|\psi|^4. \tag{2.1}$$

For making a comparison between the gradient and bulk energy terms the coherence length $\xi=(K/|\alpha|)^{1/2}$, which diverges at the transition to the isotropic phase, constitutes an important length scale. If the typical length over which there is a significant variation of the order parameter is much larger than $\xi$, the gradient energy is small compared to the bulk energy. The modulus of the order parameter deviates little from the bulk equilibrium value $|\psi_0|$ and only the phase will vary in space. In this London limit, locally the order parameter is represented by $\psi(\mathbf{r})=|\psi_0|\exp(i\phi(\mathbf{r}))$, and the distorted medium is described as a mapping from the domain $D$ of physical space $R^3$, which it occupies, to $V=S^1$. Only close to singularities (fig. 1), where the phase varies rapidly, is the modulus reduced and an increase in bulk energy accepted, since there is no other way to avoid the diverging gradient energy (Mermin 1978 a, Pokrovsky 1979).

The unit circle is the space of degeneracy also for planar layers of smectic-C liquid crystals. They consist of elongated molecules whose centres of gravity concentrate on equidistant planes. The long axes of the molecules possess a long-range orientational order, expressed by a unit vector $\hat{n}$, the director. In the smectic-A phase on the average the molecules stand perpendicular to the layers ('like corn on the field', Bragg 1934). In the uniform smectic-C phase they are tilted (like corn in the wind), with constant tilt angle $\theta$ and azimuthal angle $\phi$. It is possible to prepare smectic-C systems with thickness down to three layers. These are almost ideal realizations of a two-dimensional plane spin system; the spins are the projections of the molecule axes onto the plane. The order parameter is the solid angle $(\theta, \phi)$, where $\theta$ is the modulus and $\phi$ the degeneracy parameter. In fig. 3 a point defect in a smectic-C layer is presented as observed by Pindak *et al.* (1980).

Fig. 3



Source defect ($n=1$) in a smectic-C layer observed by Pindak *et al.* (1980) in reflection of polarized light. Polarizer and analyser are crossed. The bright bands are reflection minima (the image is a negative) for which the projection of the molecule axes onto the plane stands parallel to either polarizer or analyser.

For an isotropic three-dimensional ferromagnet the order parameter is the magnetization vector $\mathbf{m}$. The bulk free-energy depends only on the vector length $|\mathbf{m}|$, and the space of degeneracy is the two-sphere $S^2$.

In these examples the bulk free-energy is determined by one non-negative parameter, and only two phases exist: the isotropic phase, which is the normally-conducting ($|\psi_0|=0$), the smectic-A type ($\theta=0$), or the paramagnetic ($\mathbf{m}=0$) state, respectively, and the ordered phase. The separation of the order parameter into modulus and degeneracy parameter is an expression of a broken symmetry, and it is useful to resort to symmetry considerations in cases of more intricate order parameters.

### 2.2. *Group theoretic description of the space of degeneracy*

#### 2.2.1. *Spaces of degeneracy as coset spaces*

The following general formalism, which has been promoted by Michel (1980), is illustrated by the three-dimensional ferromagnet. The magnetization vector $\mathbf{m}$ can be turned by an element $g$ of the group SO(3) of proper rotations to a position denoted $g\mathbf{m}$. We say that $G=\mathrm{SO}(3)$ acts on the order parameter. The bulk free-energy of the isotropic ferromagnet is invariant under SO(3): $F(\mathbf{m})=F(g\mathbf{m})$ for any $g\in\mathrm{SO}(3)$. If $F$ is minimized by $\mathbf{m}$, it is also minimized by all values of the set $G\mathbf{m}=\{g\mathbf{m}|g\in G\}$, which is denoted an orbit of $\mathbf{m}$ under the group action. So the space of degeneracy is an orbit.

Our example provides two types of orbits ('strata'). One is represented by the set $\{\mathbf{m}=0\}$. It contains only the null-vector, which is invariant under $H=\mathrm{SO}(3)$, and represents the isotropic (paramagnetic) phase of unbroken symmetry. The orbits of the second type are spheres of radii $m\neq 0$. The symmetry (isotropy) group of a representative element of such an orbit, say $\mathbf{m}_0=(0,0,m)$, consists of the rotations about the $z$-axis and is denoted $H = C_\infty$ or $H = \mathrm{SO}(2)$. Hence, in the ferromagnetic phase, SO(3) is broken to SO(2).

An important theorem allows one to deduce the spaces of degeneracy from symmetry considerations. It states that an orbit and space of degeneracy $V$ stands in bijective (one-to-one) and continuous correspondence with the set of left cosets of $H$ in $G$. This is the set $\{gH \subset G | g \in G\}$ of subsets of $G$, denoted $G/H$ and named coset space. Take again $\mathbf{m}_0$ as representative of the orbit $V$, whose isotropy group is $H \subset G$. The correspondence between $V$ and $G/H$ amounts to associating the point $g\mathbf{m}_0$ in $V$, $g \in G$, with the coset $gH$ in $G/H$. This coset contains all those elements of $G$ that turn $\mathbf{m}_0$ into $g\mathbf{m}_0$. The two types of orbit of a ferromagnet are then represented by the trivial one SO(3)/SO(3), and the two-sphere $S^2 = \mathrm{SO}(3)/\mathrm{SO}(2)$†. The factorization does not depend on the representative $\mathbf{m}_0$. The coset space $G/H$ is a group only if $H$ is a normal divisor of $G$. A note on the factorization of general spaces via group actions is provided in Appendix 1.

### 2.2.2. *Nematic liquid crystals as an example*

The abstract formalism proves useful for the case of nematic liquid crystals which, like the smectic liquid crystals, are composed of anisotropic organic molecules. The molecules display long-range orientational order, but their centres of gravity are distributed statistically, as in a fluid. The anisotropy appears in the form of an anisotropic dielectric tensor (birefringence), or magnetic susceptibility tensor. Therefore the order parameter is assumed to be a second rank traceless symmetric tensor $Q$ with components $Q_{\alpha\beta}$. The bulk free-energy is constructed so as to be invariant under SO(3) (de Gennes 1975, Pokrovskii and Kats (1977):

$$F = \tfrac{1}{2}A \operatorname{tr} Q^2 - \tfrac{1}{3}B \operatorname{tr} Q^3 + \tfrac{1}{4}C(\operatorname{tr} Q^2)^2. \tag{2.2}$$

$Q$ can have, as isotropy subgroup of SO(3), either SO(3) itself (if $Q = 0$), $D_\infty$ (if two eigenvalues are equal), or, in general, $D_2$. ($D_\infty$ is generated by all rotations about an axis $c$ and by the 180°-rotations about all axes perpendicular to $c$; $D_2$ by 180°-rotations about three perpendicular axes $a, b, c$). Two nematic phases of broken symmetry may exist. In the uniaxial phase ($H = D_\infty$) the degeneracy parameter is the cylinder axis $c$, expressed by the director $\hat{n}$, which serves as local coordinate in the space of degeneracy. The order parameter has components $Q_{lk} = \sqrt{\tfrac{3}{2}}|Q|(n_l n_k - \tfrac{1}{3}\delta_{lk})$; $|Q|$ is the modulus. The space of degeneracy is a two-sphere, where opposite points are identified, and is denoted projective plane $P^2 = \mathrm{SO}(3)/D_\infty = S^2/Z_2$ (for this last notation see Appendix 1; $Z_2$ denotes the two-element group, here interpreted as identity and inversion). The other nematic phase is biaxial ($H = D_2$). The space of degeneracy consists of all possible orientations of the triple $(a, b, c)$ of axes, representing the eigenspaces of $Q$. A point in this space is depicted by a cross with bars of different lengths, or by a rectangular box. Local coordinates of $V = \mathrm{SO}(3)/D_2$ are the eulerian angles of the axes $(a, b, c)$ with respect to a fixed coordinate frame. Sets of angles differing by 180°-rotations about $a$, $b$ or $c$ describe the same degeneracy parameter.

### 2.2.3. *The unbroken symmetry group*

The unbroken symmetry group $G$, the type of the order parameter $x$ (phase, vector, tensor, etc.), and in consequence the orbits arise from the phenomenological

† The equality means continuous and bijective correspondence (an homeomorphism) between topological spaces.

model of a system, expressed by the Landau–Ginzburg free-energy. For the description of the orbits as coset spaces any other group $\tilde{G}$ is acceptable which acts on the order parameter $x$ and produces the same orbits: $Gx=\tilde{G}x$, for all $x\in X$, $X$ denoting the order parameter space. If $\tilde{H}$ is the subgroup of $\tilde{G}$ which leaves a representative point $x\in X$ invariant, then the space of degeneracy is $V=G/H$ as well as $V=\tilde{G}/\tilde{H}$. It is this fact why, for the three-dimensional ferromagnet and the nematic liquid crystals, we restricted ourselves to an unbroken group $G=\mathrm{SO}(3)$, although the free-energy is invariant even under O(3), the group of proper and improper rotations, or under E(3), the euclidean group, consisting of all translations, rotations and reflexions in three-space. In later applications it will be necessary to apply SU(2), the group of unitary $2\times 2$ matrices of determinant 1, with an action yet to be specified.

Physical circumstances may change the unbroken symmetry group so as to alter the orbit structure drastically. An example has been presented by Pokrovskii and Kats (1977) and Lyuksyutov (1978) for nematic liquid crystals. The quadrupole-type tensor order parameter $Q$ has five independent components and can be interpreted as vector of length $|Q|$ in a five-dimensional space, where $|Q|^2=\mathrm{tr}\,Q^2$. If at a certain temperature and pressure (or concentration) the coefficient $B$ of eqn. (2.2) vanishes, then $F$ depends only on this vector's length and is invariant under orthogonal rotations in five-dimensional space about the vector's direction. The unbroken symmetry group becomes $G=\mathrm{SO}(5)$, and the broken symmetry group $H=\mathrm{SO}(4)$. The system resembles a five-dimensional ferromagnet, the space of degeneracy a four-sphere $V=S^4=\mathrm{SO}(5)/\mathrm{SO}(4)$. As local coordinates on $S^4$ serve the three eulerian angles of the triple of axes $(a, b, c)$ and the normed value $\mathrm{tr}\,Q^3/|Q|^3$ (the two other traces are fixed: $\mathrm{tr}\,Q=0$, $\mathrm{tr}\,Q^2=|Q|^2=\mathrm{const}$). Only in the case $B=0$ does Landau theory allow biaxiality for uniform nematic liquid crystals, since otherwise the minimum of the free-energy is taken by uniaxial order parameters (Pokrovskii and Kats 1977).

However, biaxiality and a change of the unbroken symmetry group is also enforced in a strongly deformed nematic liquid crystal with suitable scale $\lambda$ of the order parameter variations. If $B$ is small, in addition to $\xi=(K/|A|)^{1/2}$ a second coherence length $\xi_B=(K/B|Q|)^{1/2}$, $\xi_B\gg\xi$, becomes active, where $K$ denotes an elastic constant (cp. with eqn. (2.17)). If $\lambda\gg\xi_B$, the order parameter is restricted to $P^2$, the space of degeneracy of the uniaxial nematic phase. If $\xi_B>\lambda\gg\xi$, the gradient energy surpasses the term $-B\,\mathrm{tr}\,Q^3/3$, and to diminish it, the order parameter moves from $P^2$ out to $S^4$. Finally, if $\lambda\cong\xi$, the order parameter can leave $S^4$ and even vanish. Strong deformations occur close to the singularities in the degeneracy parameter; so these scale considerations are important for the determination of the defect core structures (§ 4.4.1).

2.2.4. *The superfluid phases of* $^3$*He*

The superfluid phases of $^3$He also provide an order parameter, whose exploration requires group theoretic and topological methods (for an introduction see Mermin and Lee (1976) and Legget (1975)). The order parameter is a complex $3\times 3$ matrix $A_{\mu j}$ (Mermin 1978 a), which expands the spinor $\psi=\Sigma_{\mu j}A_{\mu j}|\mu\rangle|_j\rangle$ into $S=1$ spin states $|\mu\rangle$ and orbital $p$-states $|j\rangle$. $\psi$ transforms as the two-particle wavefunction of the $p$-wave Cooper pairs of spin 1. If—in a certain range of $\lambda$—the dipolar spin–orbit interaction is negligible, then the bulk free-energy remains invariant under separate rotations of the spin and orbital part of $\psi$, and under a change of its phase. Therefore, if $A^0_{\mu j}$ minimizes $F$, then also $\tilde{A}^0_{\mu j}=R^{(1)}_{\mu\mu'}R^{(2)}_{jj'}A^0_{\mu' j'}\exp(i\varphi)$, where $R^{(1)}$ and $R^{(2)}$ are different rotation matrices (summation over repeated indices is assumed here and in the following). The unbroken symmetry group is $G=\mathrm{SO}(3)\times\mathrm{SO}(3)\times\mathrm{U}(1)$ (U(1) denotes the group of rotations in the complex plane). The infinitesimal generators of $G$ (forming a basis of the corresponding Lie-algebra) are the spin-1 operators $S_1$, $S_2$, $S_3$, the orbital angular momentum operators $L_1$, $L_2$, $L_3$, and the differential operator $-id/d\varphi$. Out of the variety of possible isotropy subgroups two have physical significance: $H_{\mathrm{A}}$ and $H_{\mathrm{B}}$, which describe the symmetry of the superfluid A- and B-phase, respectively. The representative order parameter for the A-phase is invariant under separate rotations about the 3-axis in spin–space (of generator $S_3$) and orbital space. The orbital rotation, however, is coupled to a simultaneous change of the phase by the same angle, so that the corresponding generator is $L_3-id/d\varphi$. The incident, that an isotropy group is based on a linear combination of the unbroken group's generators is known as 'broken relative symmetry' (Liu 1982). From the generators the form of the A-phase degeneracy parameter is deduced as $A_{\mu j}=d_\mu(e_{1j}+ie_{2j})$ (Mineev 1980). $\hat{d}$ is a unit vector, and $\hat{e}_1, \hat{e}_2$ denote two orthogonal unit vectors, which together with $\hat{l}=\hat{e}_1\times\hat{e}_2$ define a tripod. A transformation $\hat{d}\to-\hat{d}$ and $\hat{e}_1\to-\hat{e}_1$, $\hat{e}_2\to-\hat{e}_2$, does not change $A_{\mu j}$. Therefore the space of degeneracy is the product of $S^2$ (representing the positions of $\hat{d}$) with SO(3) (the positions of the tripod), factorized to take into account that points $(\hat{d}, \hat{e}_1, \hat{e}_2)$ and $(-\hat{d}, -\hat{e}_1, -\hat{e}_2)$ in this space are to be identified: $V_{\mathrm{A}}=S^2\times\mathrm{SO}(3)/Z_2=G/H_{\mathrm{A}}$, where $H_{\mathrm{A}}=\mathrm{SO}(2)\times\mathrm{U}(1)\times Z_2$.

The representative order parameter for the B-phase is invariant under coupled rotations in spin and orbital space. The broken relative symmetry is characterized by an isotropy group $H_{\mathrm{B}}=\mathrm{SO}(3)$, generated by the linear combinations $S_j+L_j$, $j=1, 2, 3$. The degeneracy parameter assumes the form $A_{\mu j}=\exp(i\varphi)R_{\mu j}$, where $R$ is a real orthogonal $3\times3$ matrix. The space of degeneracy is $V_{\mathrm{B}}=G/H_{\mathrm{B}}=\mathrm{SO}(3)\times\mathrm{U}(1)$.

If the typical length $\lambda$ for order parameter variations increases, or in a certain temperature range, the dipolar spin–orbit interaction reduces both $V_{\mathrm{A}}$ and $V_{\mathrm{B}}$, similarly as for a nematic liquid crystal the term $\mathrm{tr}\,Q^3$ reduces $S^4$ to $P^2$. In the A-phase the vector $\hat{d}$ is locked parallel or antiparallel to $\hat{l}$, so that the space of degeneracy becomes $V'_{\mathrm{A}}=\mathrm{O}(3)/Z_2=\mathrm{SO}(3)$. In the B-phase the angle of the rotation described by the orthogonal matrix $R$ is fixed to the magic value $\arccos(-\frac{1}{4})\cong104°$. The degeneracy parameter is characterized by the unit vector $\hat{\omega}$ for the rotation axis, and by the phase, and the reduced space of degeneracy is $V'_{\mathrm{B}}=S^2\times\mathrm{U}(1)$.

### 2.2.5. *Ordered media of broken translational symmetry*

Until now only systems were considered which in uniform equilibrium possess continuous translational symmetry. As unbroken symmetry group $G$ we could therefore choose a geometric group of pure rotations (for nematics) or a gauge group (for superfluids). For distorted media of discrete translational symmetry, like layer systems or crystals, the degeneracy parameter at a point $P$ is found in the following way: a copy of the uniform medium is placed at $P$ such that its local structure coincides with that of the non-uniform medium. Degeneracy parameter is the set of rigid-body operations (translations plus rotations and reflexions) which move a uniform reference system to the position of the adjusted one. If $g$ is one of these operations, the set of all of them is the coset $gH$, where $H$ is the space group of the reference system. Space of degeneracy is $\mathrm{E}(d)/H$, $\mathrm{E}(d)$ denoting the euclidean group in $d$ dimensions. However, as we shall discuss in § 7, rotations and translations are not independent and not all fields in the degeneracy parameter describe a reasonable system.

In three-dimensional crystals with a finite number of dislocations, locally the deformation is described by translational displacements only. The displacements are vectors of the unit cell, where points differing by a primitive lattice vector are identified. This space, like a Brillouin zone, is identical with the direct product of three circles and corresponds to the three-dimensional torus $T^3 = S^1 \times S^1 \times S^1$.

Generally the spaces of degeneracy for systems of broken translational symmetry are intricate. A simple medium like the striped plane, which in its uniform state consists of equidistant parallel lines, has such an involved space of degeneracy as the 'Klein bottle' (Poénaru and Toulouse 1977).

In three dimensions, by a search for subgroups $H$ of E(3) satisfying certain requirements of statistical mechanics (essentially that E(3)/$H$ be compact), all the mesomorphic phases have been classified (Kastler *et al.* 1972, Kléman and Michel 1978, Michel 1980). Apart from the nematics and the crystals, which are of unbroken or completely broken translational symmetry, respectively, there are the media of partially periodic space groups, whose translational subgroup is discrete in only one or two directions.

Representatives for one-dimensional periodicity are the smectic and cholesteric liquid crystals. Whereas the smectics are layer systems, the mass density of the cholesterics, which also consist of elongated molecules with long-range orientational order, is constant. The director field of cholesteric liquid crystals in uniform equilibrium is helicoidal, described by $\hat{n}(\mathbf{r}) = \hat{e}_1 \cos q\hat{l}\cdot\mathbf{r} + \hat{e}_2 \sin q\hat{l}\cdot\mathbf{r}$. As in superfluid $^3$He-A, $\hat{e}_1, \hat{e}_2$ and $\hat{l} = \hat{e}_1 \times \hat{e}_2$ form an orthonormal tripod. Since $\hat{n}$ and $-\hat{n}$ are equivalent, the periodicity length along the twist axis $\hat{l}$ (the 'pitch') is $\pi/q$. The symmetry group is $\mathrm{T}(2) \wedge (R_\mathrm{h} \wedge D_2)$. $\wedge$ denotes the semidirect product (see, for example, Lax 1974), T(2) the group of continuous translations in two dimensions. $R_\mathrm{h}$ is the helicoidal group of coupled translations and rotations about the twist axis. If this is the 3-axis, $R_\mathrm{h}$ is generated by the linear combination $P_3 + qL_3$ of the operators for infinitesimal translations ($P_3$) and rotations ($L_3$) and as such represents a special type of broken relative symmetry. The dihedral group $D_2$ takes account of the fact that director, pitch axis and binormal are non-polar.

Representatives for periodicity along two directions are the rod lattices. They occur in discotic liquid crystals (Chandrasekhar *et al.* 1977), which are composed of flat molecules piled to columns, or in superconductors as vortex lattices (Träuble and Essman 1968). The intersection of the columns with a transverse plane forms a two-dimensional lattice.

The group theoretic description is not only of use in constructing the spaces of degeneracy, but also in the study of their topology. In the next section powerful theorems will be stated, which allow the deduction of homotopy groups of the spaces of degeneracy directly from their representation as homogeneous spaces.

## § 3. The topological defect classification

In this section the principles of the defect classification, which were sketched in § 1.2, are cast into a mathematical form. In § 3.1 loops and closed surfaces in degeneracy parameter space are arranged into classes. The classes are identified with defect types, and the set of classes is given an algebraic structure via the notion of homotopy groups. After some examples in § 3.2, theorems to determine these groups are stated in § 3.3. The central result, the exact sequence of homotopy groups, is derived in detail because of its importance. The theorems are applied to the degeneracy parameter spaces of several liquid crystalline and suprafluid phases in § 3.4. Mostly the theorems are not proved but illustrated. For a rigorous exposition of homotopy theory the books of Steenrod (1951), §§ 15–17, Hilton (1953), Hu (1959) and Whitehead (1978) are recommended.

### 3.1. *An algebraic structure for defect classes*

#### 3.1.1. *Free homotopy and defects*



We saw in § 2.1, that a non-uniform medium is described by a continuous mapping $\phi$: $D\backslash\Delta \to V$ valued in the space of degeneracy $V$. From the domain $D$ of the medium the set $\Delta$ of points has been excluded, where the degeneracy parameter is not defined. For a state of uniform equilibrium $\phi$ is constant and $\Delta$ empty. The singularity is denoted *topologically unstable*, if the mapping can be extended continuously over $\Delta$, otherwise it is *topologically stable*. Thus a topologically unstable defect can be eliminated by a fluctuation of the degeneracy parameter in a neighbourhood of $\Delta$. Defects probed by a Burgers circuit $B$ (point defects in two-dimensional, line defects in three-dimensional space) are topologically stable, if (and only if) the field values along $B$ form a loop $f$ in $V$ which cannot be contracted to a point. For a proof of this statement, several terms hitherto used must be given a precise definition.

A *loop* in the space of degeneracy is a continuous mapping $f$ from the unit interval $I=[0, 1]$ into $V$, so that $f(0)=f(1)$.

A loop $f$ in $V$ is *continuously deformable into* or *homotopic to* another loop $g$ (notation: $f \sim g$), if there is a family of loops $h_s$, $s\in[0, 1]$, connecting both, i.e. where $f=h_0$, $g=h_1$, and where the mapping

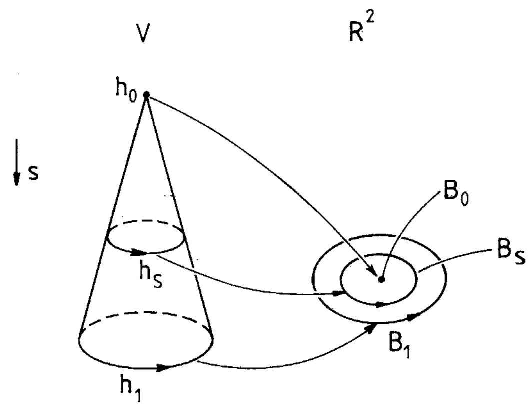
$$\left.\begin{array}{l} I\times I\to V \\ (s, t)\mapsto h_s(t) \end{array}\right\} \tag{3.1}$$

is continuous in $s$ and $t$. A loop $f$ is contractable to a point $x$ in $V$, if it is homotopic to the constant loop $g$ with $g(t)\equiv x$ for all $t$ in $I$.

Now let us specify $D$ as the $x$–$y$-plane, and $\Delta$ as the origin. As Burgers circuit we choose the circle $B_1$ of radius $\rho$ whose points are $\mathbf{r}_1(t)=(\rho\cos 2\pi t, \rho \sin 2\pi t)$. The loop $h_1$ in $V$ corresponding to $B_1$ is $h_1$ with $h_1(t)=\phi(\mathbf{r}_1(t))$. If $h_1$ is contractable to a point, then the field $\phi$ can be extended continuously over $\Delta$ on the disk bounded by $B_1$. This is done by 'spreading the homotopy out in space' (Mermin 1979). Thereby the values of $h_s$, $s\in[0, 1]$, are placed on the circle $B_s$ of radius $\rho_s=\rho s$, whose points are $\mathbf{r}_s(t)=(\rho_s\cos 2\pi t, \rho_s \sin 2\pi t)$, according to the prescription $\phi(\mathbf{r}_s(t))=h_s(t)$ (fig. 4). The constant loop $h_0$ in $V$ is then associated with the constant loop $B_0$, $\mathbf{r}_0(t)\equiv\mathbf{0}$, in the plane. Conversely, if $\phi$ can be continued over the singularity, a homotopy between $h_1$ and $h_0$ is provided by the same prescription. This argument is easily generalized to arbitrarily shaped Burgers circuits and to the case of defects of dimension $d'=d-2$ in $d$-dimensional space.

Yet there is a finer classification of closed loops available than just into those which are contractable and those which are not. The homotopy relation $\sim$ is an equivalence relation. The loops in $V$ can be grouped into homotopy classes, which are the corresponding disjoint equivalence classes. The respective loops in $V$ of all

Fig. 4

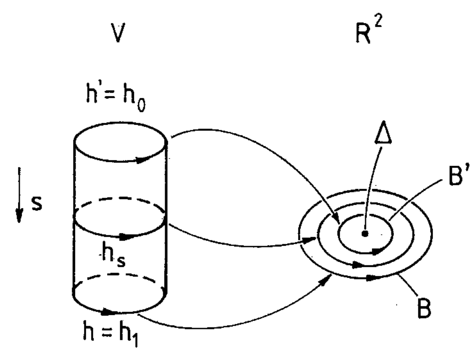



The homotopy between loops $h_0$ and $h_1$ in $V$ is spread out on a disk in two-dimensional physical space to smooth out an unstable point singularity.

Burgers circuits encircling a single defect belong to one and the same homotopy class. Hence the class characterizes the defect. If this class is identical for a singularity at $\Delta$ of two fields $\phi$ and $\phi'$, then by a local modification the structure of $\phi$ can be replaced by that of $\phi'$ in a neighbourhood of $\Delta$, in the following way: take for $D$ again the $x$–$y$-plane, and for $\Delta$ the origin, and choose as Burgers circuits $B$, $B'$ two concentric circles about the origin of radii $\rho$ and $\rho'$, respectively, $\rho > \rho' > 0$. Outside the radius $\rho$, $\phi$ is left unchanged, inside $\rho'$ it is replaced by $\phi'$. By assumption the loops $h'$ and $h$ in $V$ representing the field values of $\phi'$ and $\phi$ along $B'$ and $B$, respectively, are homotopic. An interpolating field $\phi''$ is constructed by spreading the homotopy $h_s$, $s \in [0, 1]$ between $h' = h_0$, and $h = h_1$ out in the annulus $\rho > |\mathbf{r}| > \rho'$ according to the rule $\phi''\ (\mathbf{r}_s(t)) = h_s(t)$, where $\mathbf{r}_s(t) = \rho_s \cos 2\pi t,\ \rho_s \sin 2\pi t)$, $\rho_s = \rho' + s(\rho - \rho')$(fig. 5).

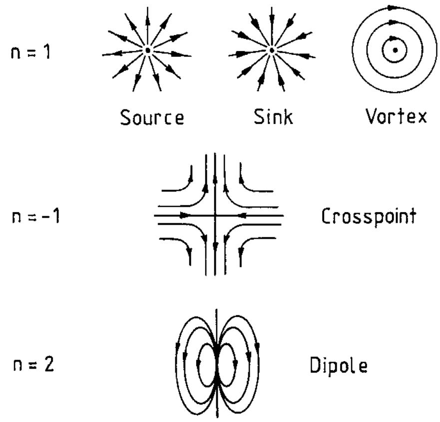
For the two-dimensional ferromagnet in the plane, the homotopy classes are labelled by an index (winding number) $n$, which counts how often the unit vector runs around the unit circle as one moves once about the singular point. Representatives for several indices and a source ($n = 1$) whose core has been replaced by a sink (also $n = 1$) are presented in figs. 6 and 7.

Fig. 5



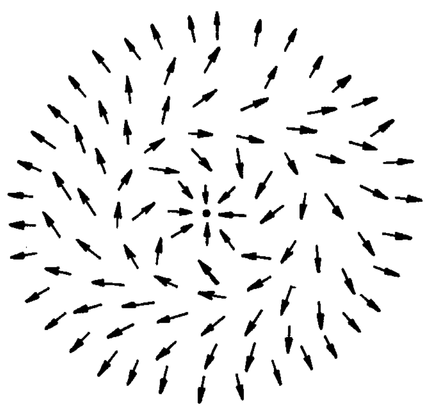

The homotopy between loops $h'$ and $h$ in $V$ is spread out in an annulus to replace the core of a defect by that of another defect.

Fig. 6




Point singularities of the two-dimensional ferromagnet in the plane for various winding numbers.

Fig. 7



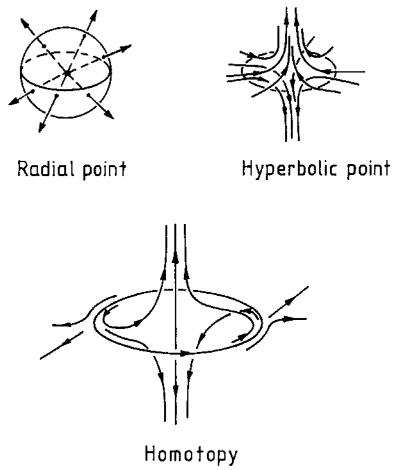
Source defect, whose core is replaced by that of a sink.

Defects of dimension $d' = d-3$ in $d$-dimensional space (point defects in three dimensions) are surrounded by a Burgers two-sphere $S^2$. Following the field values along the sphere amounts to mapping $S^2$ into the space of degeneracy. Homotopy classes of such mappings label the defects. Point defects of a three-dimensional ferromagnet in three-space also carry an integer index, which is interpreted in § 6. Two representatives of index $n=1$, the radial and the hyperbolic point, and a homotopy of both in space are depicted in fig. 8.

Generally defects of dimension $d'$ in $d$-space are classified by the homotopy classes of mappings from $r$-dimensional spheres, $r = d - d' - 1$, into the space of degeneracy. (The case of wall defects, $d' = d - 1$, is commented on later).

We already know that the homotopy classes of loops in $V = S^1$ and spheres in $V = S^2$ are in correspondence with the set $Z$ of integers and thus are endowed with a group structure. To impose an algebraic structure on homotopy classes in general, we have—as an interlude—to consider classes of based loops and spheres.

Fig. 8




Radial and hyperbolic point of a three-dimensional ferromagnet, and homotopy of both spread out in physical space.

3.1.2. *Based homotopy*

In $V$ one point is selected and marked as base point $x_0$. We now consider only those loops in $V$ which start and terminate at $x_0$, and denote them as 'loops based at $x_0$'. They are arranged into based homotopy classes. Loops $f$ and $g$ belong to the same class, if they can be continuously deformed into one another, and if all the interpolating loops $h_s$, $s\in[0, 1]$, are based at $x_0$. The notation $[f]$ is used for that based class to which a loop $f$ belongs. In contrast to the based homotopy classes those defined in § 3.1.1. are termed free.

For based loops $f$ and $g$ the product $fg$ is defined as the loop obtained, if first $f$ and then $g$ is traversed, but with doubled speed:

$$(fg)(t)=\begin{cases} f(2t) & \text{for } 0\leqslant t\leqslant \frac{1}{2}; \\ g(2t-1) & \text{for } \frac{1}{2}\leqslant t\leqslant 1. \end{cases} \tag{3.2}$$

Although $fg$ passes through $x_0$ at $t=\frac{1}{2}$, a general representative of $[fg]$ does not.

By the loop product a multiplication law for based homotopy classes is defined as $[f][g]:=[fg]$. It is independent of the representatives $f$ and $g$ and thus unique.

The product induces a group structure on the set of based homotopy classes, because (stated without proof)

(i) it is associative: $([f][g])[h]=[f]([g][h])$;
(ii) a unit element exists, namely $[e]$, where $e$ is the constant loop at $x_0$;
(iii) for each class $[f]$ an inverse exists, namely $[f]^{-1}:=[f^{-1}]$, where $f^{-1}$ is the loop $f$ traversed in the opposite direction: $f^{-1}(t)=f(1-t)$.

The resulting group is the fundamental group of $V$, or the first homotopy group $\pi_1(V, x_0)$.

For the definition of higher (based) homotopy groups a special parametrization of the $r$-sphere is opportune. A two-sphere ($r$-sphere) is topologically equivalent to the square ($r$-cube) whose boundary is pinched to a point. Based mappings of the two-sphere into $V$ are then viewed as mappings of the unit square $I^2=[0, 1]\times[0, 1]$ into $V$ where all points at the boundary go into $x_0$: $f$: $I^2\to V$, $f(t_1, t_2)=x_0$ for $t_1$ or $t_2$ equal 0 or

1. The product $fg$ is formed by redefining the domain of $t_1$ and glueing the domains of $f$ and $g$ together (fig. 9):

$$(fg)(t_1, t_2) = \begin{cases} f(2t_1, t_2) & \text{for } 0 \leqslant t_1 \leqslant \frac{1}{2}; \\ f(2t_1 - 1, t_2) & \text{for } \frac{1}{2} \leqslant t \leqslant 1. \end{cases} \tag{3.3}$$

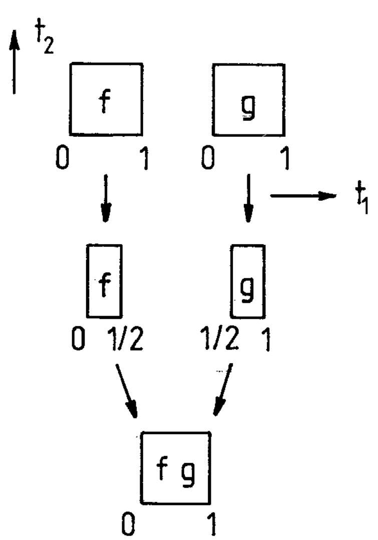
The based homotopy classes of these mappings, together with the product $[f][g] := [fg]$, form the second homotopy group $\pi_2(V, x_0)$ of $V$ at $x_0$.

Similarly mappings of higher-dimensional spheres $S^r$ (or unit cubes of dimension $r$ with the points at the boundary being identified) into $V$ are grouped into based homotopy classes, and a product is defined by rescaling two cubes and glueing them together on one face. The result is the $r$th homotopy group $\pi_r(V, x_0)$.

In general $V$ consists of different components $V_0, V_1, \ldots, V_k, \ldots$, where only points of the same component are arcwise connected. Two points $x, y$ are arcwise connected if a path $c$ exists (a continuous mapping $c$: $[0, 1] \to V$) with $c(0) = x$, $c(1) = y$. We denote by $V_0$ the component containing the base-point $x_0$. For $r \geqslant 1$ the loops and surfaces at $x_0$ reside only in $V_0$, so that $\pi_r(V, x_0) = \pi_r(V_0, x_0)$. For homogeneous spaces $V_0$ equals $G_p/H'$, where $G_0$ is the component of $G$ connected to the unit element $e$, and $H'$ the invariance group of $x_0$ in $G_0$. Therefore we can use $G_0$ for $G$ and assume in the following that the unbroken symmetry group is arcwise connected.

The representatives of the elements of $\pi_0(V, x_0)$ are mappings from the zero-sphere (two points) into $V$. While one point is tied to $x_0$, the other one may be placed into any other component of $V$. Therefore $\pi_0(V, x_0)$ is the set of components of $V$. It classifies defects of dimension $d' = d - 1$, which are walls in three dimensions. $\pi_0$ does not have a natural group structure. If, however, $V = H$ is a subgroup of a topological group $G$ of base point $e$ (the unit element), and if $H_0$ is the component of $H$ connected to $e$, the set of components of $H$ is the set of left cosets $H/H_0$ of $H_0$ in $H$. Because $H_0$ is a normal divisor of $H$ (which is readily proved), this is a group.

Fig. 9




How to form the product $fg$ of two mappings $f$ and $g$ from the two-sphere into the space of degeneracy.

If, for $r \geq 1$, the base point $x_0$ is shifted along a path to a point $y_0$, $\pi_r(V, x_0)$ and $\pi_r(V, y_0)$ are isomorphic due to a 'path isomorphism' (see, for example, Mermin 1979, p. 604). For this reason, the base point is often omitted in the notation.

Even so, to obtain the classes of freely homotopic loops, we have to get rid of the base point. Thereby, however, the group structure is partially lost, which turns out to be not only a complication but also an enrichment in applications of the theory to defect processes.

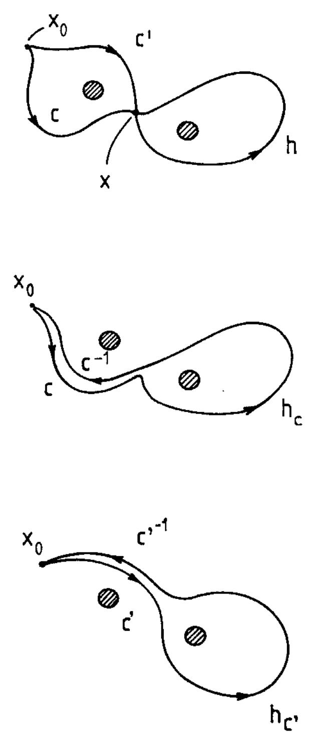
3.1.3. *Algebraic structure for free homotopy classes*

We assume that $V$ is arcwise connected. For an illustration of the following thoughts imagine $V$ to be the plane with two holes (fig. 10). On an unbased loop $h$ we choose a point $x$ and connect the base point $x_0$ with $x$ by a path $c$. The loop $h_c = chc^{-1}$ (fig. 10, the notation is evident) is based at $x_0$ and simultaneously freely homotopic to $h$ (for the homotopy simply retract the connecting string from $x_0$ to $x$). We would like to identify the free homotopy class of $h$ with the based one $[h_c]$. However, this attachment of $h$ to $x_0$ does not lead to a unique class $[h_c]$. Choose another path $c'$ from $x_0$ to $x$. Then $h_{c'} = c'hc'^{-1}$ is freely homotopic to $h$ and $h_c$, but the based class $[h_{c'}]$ is not necessarily equal to $[h_c]$. This can be seen from fig. 10 and also from the relations

$$[h_{c'}] = [c'hc'^{-1}] = [c'c^{-1}chc^{-1}cc'^{-1}] = [a][h_c][a]^{-1}, \tag{3.4}$$

where $a = c'c^{-1}$ is a loop at $x_0$. $[h_{c'}]$ and $[h_c]$ are conjugate elements in $\pi_1(V, x_0)$, and in

Fig. 10



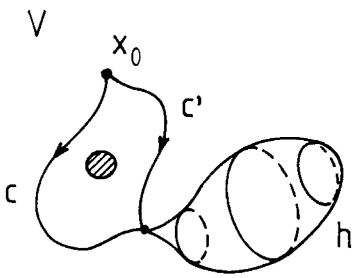

A loop $h$ in $V$ is attached to a base point $x_0$ by two different paths $c$ and $c'$. The resulting loops $h_c$ and $h_{c'}$ are freely homotopic, but are not elements of the same based homotopy class.

general not identical. By connecting $h$ to $x_0$ in all possible ways, representatives from all based classes conjugate to $[h_c]$, but not from others, are formed. So $h$, and as is quickly proved, all loops freely homotopic to $h$, must be associated with an entire conjugation class of $\pi_1(V, x_0)$. Conversely conjugate based classes merge into the same free homotopy class, if their loops are liberated from the base point. With the free homotopy classes the defect types also stand in one-to-one correspondence to the conjugation classes of the fundamental group. If this group is abelian, each conjugation class consists of one element, and the defects are labelled directly by the group elements.

The transformation of the class $[h_c]$ into $[h_{c'}]=[a][h_c][a]^{-1}$ may also be interpreted as resulting from the motion of the base point along the closed loop $a$. This motion transforms each element $\gamma\in\pi_1(V, x_0)$ into its conjugate $[a]\gamma[a]^{-1}$ and amounts to a group action of the elements of $\pi_1(V, x_0)$ (here of $[a]$) on the fundamental group itself. The conjugation classes are the orbits, into which $\pi_1(V, x_0)$ is divided under this action. The orbits are the smallest subentities of the fundamental group invariant under all path isomorphisms, i.e. under the displacements of the base point along paths in $V$.

The notion of group action is of special value, if the relation between free and based homotopy classes is established for mappings of $r$-spheres into $V$, $r>1$. An unbased sphere $h$ in $V$ can be connected to the base point by a path $c$ resulting in a based sphere $h_c$ (the points along the path being degenerate). Another path $c'$ yields a sphere $h_{c'}$, in general of a different based class, but freely homotopic to $h$ and $h_c$ (fig. 11). Passing from $h_c$ to $h_{c'}$ amounts to attaching a loop $a=c'c^{-1}$ to $h_c$ and as such to the action of the element $[a]\in\pi_1(V, x_0)$ on an element $[h_c]\in\pi_r(V, x_0)$. The elements of $\pi_r(V, x_0)$, which are obtained if all members of $\pi_1(V, x_0)$ act on a single element $\chi\in\pi_r(V, x_0)$, form an orbit under this action, denoted $\hat{\chi}$. The representatives of the based homotopy classes of an orbit are freely homotopic. Orbits label the defects. A recipe for computing action and orbits is presented in § 3.3.3.

Fig. 11




A sphere in $V$ being connected with the base point by two different paths $c$ and $c'$.

## 3.2. *Some examples for homotopy groups*

The $r$th homotopy group of the $k$-sphere is

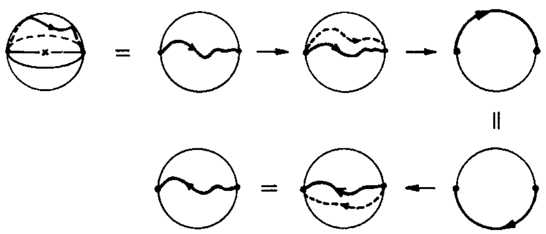
$$\pi_r(S^k)=\begin{cases} 0 \ \text{(the trivial group)} & \text{for } r<k \\ Z \ \text{(the set of integers)} & \text{for } r=k, \end{cases}$$

while no general rule exists yet for $r>k$ (Whitehead 1978). Accordingly for a three-dimensional medium with the unit circle as space of degeneracy (superfluid $^4$He, s-type superconductors) the line defects carry an integer index ($r = k = 1$). The point defects are not stable, because $\pi_2(S^1) = 0$. Every closed loop on a two-sphere is contractable to a point. Therefore $\pi_1(S^2) = 0$, and line defects of three-dimensional ferromagnets in three-space are unstable; their point defects, however, are stable, since $\pi_2(S^2) = Z$. Note, that the index $n$ of these point defects changes sign, if at each point in space the unit vector is reversed (for a source: $n = 1$; for a sink: $n = -1$), in contrast to the case of a two-dimensional unit vector field in the plane.

The space of degeneracy of uniaxial nematic liquid crystals is the sphere with opposite points being identified: $P^2 = S^2/Z_2$. In drawing loops we only require the upper hemisphere, which, by a typical topological manipulation, is compressed to a disk (fig. 12). Opposite points on the disk's boundary describe the same point of $V$. There is only one homotopy class of non-contractable based (and free) loops, whose representatives connect a point on the boundary with its counterpart. Figure 12 displays a sequence where a non-contractable loop is deformed into its inverse. Hence the fundamental group of $P^2$ is the two-element group $Z_2$. The only topologically stable line defect of uniaxial nematic liquid crystals is a 180°-disclination (fig. 13). Along a loop about the disclination the director changes sign.

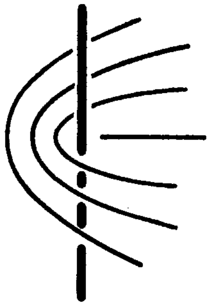
Around a nematic point singularity the director field constitutes a unique vector field. Just as for a three-dimensional ferromagnet we find $\pi_2(P^2) = Z$. A sign reversal of each vector describes the same degeneracy parameter field but alters the index $n$ of the singular point to $-n$. Therefore a single point defect is labelled by the set (orbit) $\{n, -n\}$. The sign is reversed, for instance, if the singular point is moved around a 180°-disclination. This process amounts to an action of the non-trivial element of the fundamental group on an element of the second homotopy group.

Fig. 12



Continuous deformation of a closed loop in the projective plane into its inverse.

Fig. 13



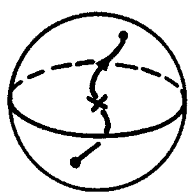
180°-disclination line of a uniaxial nematic liquid crystal.

The space of degeneracy of the dipole-locked $^3$He-A phase, $V = SO(3)$, is depicted by a solid three-dimensional ball of radius $\pi$ (fig. 14). Each point of the ball stands for an orthogonal rotation. The vector drawn from the centre to a certain point denotes the rotation axis, its length the rotation angle. Since rotations of angles $\pi$ and $-\pi$ are identical, opposite points on the surface of the ball must be identified, and SO(3) is recognized as the higher dimensional analogue of the nematic space of degeneracy, namely, as projective space $P^3$. As for $P^2$ there is only one stable line defect, whose homotopy class is represented by a path connecting antipodal points on the surface of the ball, and $\pi_1(SO(3))$ equals $Z_2$. The point defects are unstable.

If the space of degeneracy is a product space, for example $V_B = S^1 \times SO(3)$ for dipole-free $^3$He-B (§ 2.2.4), the homotopy group is the direct product of each factor's homotopy group: $\pi_1(S^1 \times SO(3)) = \pi_1(S^1) \times \pi_1(SO(3)) = Z \times Z_2$, $\pi_2(S^1 \times SO(3)) = 0$. Line defects in dipole free $^3$He–B can be formed independently in the phase field and the rotation field.

As a rule topological spaces are complicated if they have been obtained by factorization of others (Appendix 1). To derive the homotopy groups of biaxial nematic liquid crystals ($V = SO(3)/D_2$) or of dipole-free $^3$He-A ($V = S^2 \times SO(3)/Z_2$), we resort to a calculus developed in the next section.

Fig. 14



Non-contractable loop in SO(3). SO(3) is depicted as a solid ball with antipodal points on the surface being identified.

### 3.3. *Relative homotopy groups, exact sequences and homotopy groups of homogeneous spaces*

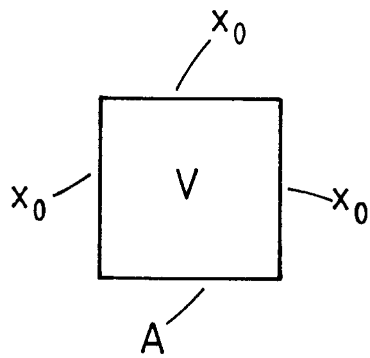
In this section an important relation between homotopy groups is introduced: the exact sequence. It is required for the applications in §§ 4 and 5, and for the calculation of homotopy groups, in particular of factorized spaces. Its exposition reveals many useful properties of homotopy groups, but necessarily must be somewhat technical. On first reading, one should concentrate on the definition of relative homotopy groups, and on the central eqns. (3.11)–(3.14).

#### 3.3.1. *Relative homotopy groups*

Homotopy groups $\pi_r(V, x_0)$ are special cases of relative homotopy groups and, in distinction from these, are also called 'absolute' homotopy groups. For the definition of relative homotopy groups we need a subset $A$ of $V$ which contains the base point $x_0$.

The relative homotopy group $\pi_2(V, A, x_0)$ consists of equivalence classes $[f]$ of mappings $f$ from the unit square into $V$ (fig. 15), which carry the base edge (points with $t_2 = 0$) into $A$, and the remaining edges into $x_0$. Two such mappings, $f$ and $g$, are equivalent, if one is deformed into the other via a continuous family of mappings of

Fig. 15




Mapping of the square into $V$, with the base going into a subset $A \subset V$, and the other edges into the base point $x_0$.

the same type. The product $fg$, and consequently the product $[f][g] := [fg]$ is formed in analogy to the procedure applied for absolute homotopy groups (fig. 9). If $A$ contains only the base point $x_0$, we retrieve $\pi_2(V, x_0)$.

Higher relative homotopy groups $\pi_r(V, A, x_0)$ consist of equivalence classes of continuous mappings from the $r$-cube $I^r$ into $V$, which take the base face ($t_r = 0$) into $A$, and the remaining boundary into $x_0$. The relative homotopy groups are abelian for $r \geqslant 3$; $\pi_2(V, A, x_0)$ is not abelian in general.

The representatives of the elements of $\pi_1(V, A, x_0)$ are mappings from the unit interval into $V$, where $t=0$ goes into $A$, and $t=1$ into $x_0$. The product $f_1 f_2$ of mappings (and a group structure of $\pi_1(V, A, x_0)$) is defined only in two cases:

(i) The set $A$ is arcwise connected. Then the point $f_2(t=0)$ is guided along a path to $x_0$ and attached to $f_1(t=1) = x_0$.

(ii) $V = G$ is a group, $A = H \subset G$ a subgroup, and $x_0 = e$ the unit element. If $f_1$ is a path from $h_1 \in H$ to $e$, and $f_2$ from $h_2 \in H$ to $e$, then one translates the points of $f_1$ from the right by $h_2$ and obtains a path of points $f_1(t) \cdot h_2$ (the dot denotes the product in $G$). On this path, which runs from $h_1 \cdot h_2$ to $h_2$, $f_2$ is attached. By definition $f_1 f_2$ is the path connecting $h_1 \cdot h_2$ via $h_2$ with $e$.

What are relative homotopy groups good for? First, they are applied, if in part of the domain the degeneracy parameter is restricted to a subset $A$ of $V$, for instance on surfaces, or in regions of small parameter variations. Thus one needs them to classify surface defects (§4.3) or to study the cores of defects (§4.4). Second, in connection with the exact sequence of relative homotopy groups, they allow the calculation of absolute homotopy groups.

3.3.2. *The exact sequence of relative homotopy groups*

Continuous mappings between topological spaces induce homomorphisms between their homotopy groups ($\pi_r$ is a 'functor' (Michel 1980)). Take another space $W$, a subset $B \subset W$ and a base point $y_0 \in B$, and a continuous mapping $k$ from $V$ to $W$, which carries $A$ into $B$, and $x_0$ into $y_0$ (notation: $k$: $(V, A, x_0) \to (W, B, y_0)$). If $f$ is a representative of an element of $\pi_r(V, A, x_0)$, then the composed mapping $k \circ f$ (defined by $(k \circ f)(x) = k(f(x))$ for all $x \in V$) represents an element of $\pi_r(W, B, y_0)$. The association $[f] \to [k \circ f]$ establishes a homomorphism between both relative homotopy groups, which is denoted

$$k_*: \pi_r(V, A, x_0) \to \pi_r(W, B, y_0). \tag{3.5}$$

Simple examples are the inclusions

$$j: (V, x_0) \equiv (V, x_0, x_0) \to (V, A, x_0) \tag{3.6}$$

with $j(x) = x$, $x \in V$, and

$$i: (A, x_0) \to (V, x_0) \tag{3.7}$$

with $i(x) = x$, $x \in A$. They induce homomorphisms

$$j_*^{(r)}: \pi_r(V, x_0) \to \pi_r(V, A, x_0) \tag{3.8}$$

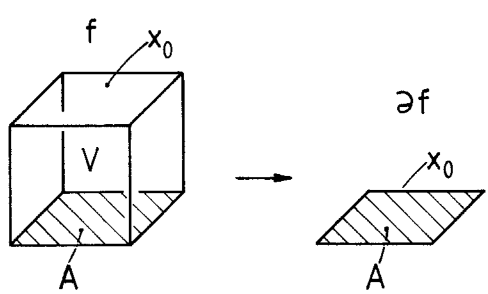
and

$$i_*^{(r)}: \pi_r(A, x_0) \to \pi_r(V, x_0). \tag{3.9}$$

Now take a mapping $f$ which represents an element of $\pi_r(V, A, x_0)$. The restriction of $f$ to the base face (fig. 16), denoted $\partial f$, maps the $(r-1)$-cube into $A$, and its boundary into $x_0$. Associating $[f]$ with $[\partial f]$ leads to homomorphisms

$$\partial^{(r)}: \pi_r(V, A, x_0) \to \pi_{r-1}(A, x_0). \tag{3.10}$$

Fig. 16




Domain of the mapping $f$, representing an element of $\pi_2(V, A, x_0)$, and domain of $\partial f$, which is the restriction of $f$ to the base face.

Homomorphisms (3.8)–(3.10) establish the following sequence:

$$\left.\begin{aligned}
&\ldots \to \pi_r(A, x_0) \xrightarrow{i_*^{(r)}} \pi_r(V, x_0) \xrightarrow{j_*^{(r)}} \pi_r(V, A, x_0) \xrightarrow{\partial^{(r)}} \\
&\quad \to \pi_{r-1}(A, x_0) \to \ldots \\
&\ldots \to \pi_2(A, x_0) \to \pi_2(V, x_0) \to \pi_2(V, A, x_0) \\
&\quad \to \pi_1(A, x_0) \to \pi_1(V, x_0) \to \pi_1(V, A, x_0) \\
&\quad \to \pi_0(A, x_0) \to \pi_0(V, x_0).
\end{aligned}\right\} \tag{3.11}$$

The last three members of the sequence are homomorphisms only, if domain and range have group structure. Otherwise they are just mappings of pointed spaces.

The sequence is exact (see, for example, Steenrod 1951, Mermin 1979). Exactness of a sequence of homomorphisms

$$\ldots \rightarrow \mathrm{F} \xrightarrow{\alpha} \mathrm{G} \xrightarrow{\beta} \mathrm{H} \xrightarrow{\gamma} \ldots$$

means that the image of one homomorphism is the kernel of the next one (the image of $\alpha$, written im $\alpha$, consists of all points in $G$ which are mapped upon, the kernel of $\alpha$ of all those elements of $F$ which are mapped into the unit element or the base point of $G$).

For exact sequences

(i) $0 \rightarrow F \xrightarrow{\alpha} G$

(ii) $F \rightarrow G \xrightarrow{\beta} 0$

(iii) $0 \rightarrow F \xrightarrow{\gamma} G \rightarrow 0$

involving the trivial group 0, the following statements hold: $\alpha$ is injective (one-to-one), $\beta$ is surjective (onto) and $\gamma$ is bijective (one-to-one and onto), i.e. $\gamma$ is an isomorphism. To compute homotopy groups of homogeneous spaces, it is attempted to convert the exact sequence (3.11) into sections of type (iii). But first the homotopy group of a homogeneous space must be identified with a relative homotopy group.

3.3.3. *Homotopy groups of homogeneous spaces*

We start out from a representation of the space of degeneracy $V$ as coset space $G/H$ of base point $x_0 = H$. A loop $f$ in $V$ may be described by a path $g$ in the unbroken symmetry group $G$, whose points pilot $x_0$ through $V$: $f(t) = g(t)x_0$. The path $g$ must depart and terminate in the isotropy group $H$ of $x_0$ because of the equalities $f(0) = f(1) = x_0 = g(0)x_0 = g(1)x_0$. It can always be chosen to end at the unit element $e$; should it not, then we use the path $g'$ with $g'(t) = g(t)g(1)^{-1}$, which generates the same loop $f$. The path $g$ represents an element of the relative homotopy group $\pi_1(G, H, e)$. In associating $[f] \in \pi_1(V, x_0)$ with $[g] \in \pi_1(G, H, e)$ we obtain an isomorphism $\pi_1(V, x_0) = \pi_1(G, H, e)$. The same isomorphism holds for any integer $r > 1$ (Steenrod 1951): $\pi_r(V, x_0) = \pi_r(G, H, e)$.

Given this identity, the exact sequence of relative homotopy groups is transferred into an exact sequence of absolute homotopy groups:

$$\left.\begin{array}{l} \rightarrow \pi_r(H) \rightarrow \pi_r(G) \rightarrow \pi_r(G/H) \\ \rightarrow \pi_{r-1}(H) \rightarrow \ldots \\ \rightarrow \pi_2(H) \rightarrow \pi_2(G) \rightarrow \pi_2(G/H) \\ \rightarrow \pi_1(H) \rightarrow \pi_1(G) \rightarrow \pi_1(G/H) \\ \rightarrow \pi_0(H) \rightarrow \pi_0(G). \end{array}\right\} \tag{3.12}$$

(The same sequence applies to factorized spaces under special conditions; see Appendix 1).

In all applications $G$ is arcwise connected ($\pi_0(G) = 0$, see § 3.1.2) and either a compact Lie group or a product of a compact Lie group with a group of continuous translations in $d$ dimensions. In both cases $\pi_2(G)$ is trivial (Cartan 1936, Whitehead

1978). If in addition $G$ is simply connected ($\pi_1(G)=0$), then from the exact sequence follow the isomorphisms

$$\pi_2(G/H)=\pi_1(H)=\pi_1(H_0), \tag{3.13}$$

$$\pi_1(G/H)=\pi_0(H)=H/H_0. \tag{3.14}$$

All we have to do to exploit these equations is to choose a simply connected unbroken symmetry group. Now for each arcwise connected group $G$ a universal covering group $\bar{G}$ exists which has this property (Hamermesh 1964). $\bar{G}$ is related to $G$ by a surjective homomorphism $\varphi$: $\bar{G}\to G$. It is decisive that the set of elements of $\bar{G}$ which map on a single element $g\in G$ (the 'inverse image of $g$', denoted $\varphi^{-1}(g)$) is discrete. The group action of $G$ on $V$ is transferred to an action of $\bar{G}$ on $V$ by the prescription: $\bar{g}x := \varphi(\bar{g})x$ for all $\bar{g}\in\bar{G}$. So $\bar{G}$ replaces $G$ as unbroken group, and $V$ is expressed by $V=G/H=\bar{G}/\bar{H}$. $\bar{H}$ is the subgroup of $\bar{G}$ which leaves $x_0$ invariant, consisting of the elements of $\bar{G}$ which are mapped by $\varphi$ on $H$ ($\bar{H}=\varphi^{-1}(H)$ is the 'lift' of $H$ into $\bar{G}$).

The groups SO(2) and SO(3) of two- and three-dimensional rotations, for example, are not simply connected. For SO(2), which is topologically equivalent to U(1) and the unit circle in the complex plane, the universal covering group is the group T(1) of one-dimensional translations, equivalent to the set $R$ of real numbers. Homomorphism $\varphi$ associates with a real number $\theta$ the complex number $\exp(i\theta)$ of unit modulus. The universal covering group of SO(3) is SU(2), the group of complex unitary $2\times 2$ matrices of determinant 1. An element of SU(2) is represented by the matrix

$$u(\hat{\omega},\theta)=\exp(i\theta\hat{\omega}\cdot\boldsymbol{\sigma}/2)=\cos\tfrac{1}{2}\theta+i(\hat{\omega}\cdot\boldsymbol{\sigma})\sin\tfrac{1}{2}\theta. \tag{3.15}$$

$\boldsymbol{\sigma}$ is the vector $(\sigma_1,\sigma_2,\sigma_3)$ of Pauli matrices, $\hat{\omega}$ a unit vector, $\theta\in[0,4\pi]$. Homomorphism $\varphi$ associates with $u(\hat{\omega},\theta)$ the orthogonal rotation about the $\hat{\omega}$-axis of angle $\theta$ (modulo $2\pi$). $\varphi$ describes a double covering, since $u(\hat{\omega},\theta)$ and $u(\hat{\omega},\theta+2\pi)=-u(\hat{\omega},\theta)$ are mapped on the same element of SO(3), and gives rise to double valued representations of SO(3). This fact is the deep origin for the existence of half-integer spin. From eqn. (3.15) it follows that the elements of SU(2) are parametrized as $u=a_0+a_1\sigma_1+a_2\sigma_2+a_3\sigma_3$, where $a_0^2+a_1^2+a_2^2+a_3^2=1$, i.e. by a four-component unit vector. Thus SU(2) is recognized as topologically equivalent to the three-sphere $S^3$.

A first conclusion can be drawn from eqns. (3.13) and (3.14) for the homotopy groups of a wide class of ordered media: if the symmetry group $H$ is discrete, then its lift $\bar{H}$ into the universal covering group is also discrete, and $\bar{H}_0=\{e\}$ is the trivial subgroup of $\bar{H}$. Hence $\pi_1(V)=\bar{H}/\bar{H}_0=\bar{H}$ is equal to this lift. Furthermore, $\pi_2(V)=\pi_1(\bar{H}_0)=0$: such media have no stable point defects in three dimensions.

Given a simply connected group $G$, then via eqns. (3.13) and (3.14) the action of $\pi_1(G/H)$ on $\pi_2(G/H)$ must be interpreted as action of $H/H_0$ on $\pi_1(H_0)$. This action is computed according to the following rule (see, for example, Mermin 1978 b): if an element of $\pi_1(H_0)$ is represented by a loop $g$ in $H_0$, and a coset of $H/H_0$ by an element $h$ of $H$, the class of $\pi_1(H_0)$ resulting from the action of this coset on $[g]$ is $[g_h]$, where the loop $g_h$ is related to $g$ by $g_h(t)=h\cdot g(t)\cdot h^{-1}$.

### 3.4. *Further examples*

The unbroken symmetry group $G$ for the system of two-dimensional unit vectors is SO(2), the isotropy group $H$ of a representative vector consists of the identity.

When SO(2) is lifted to $T(1)=R$, the identity is lifted to the translations by integer multiples of $2\pi$. Hence $\bar{H}$ is isomorphic to the group $Z$ of integers, and the space of degeneracy, the circle, is expressed as homogeneous space $V=R/Z$. We recover from eqns. (3.13) and (3.14) that $\pi_1(V)=Z$ and $\pi_2(V)=0$.

For biaxial nematic liquid crystals the space of degeneracy is $V=SO(3)/D_2$ (§ 2.2.2). Since the dihedral group $D_2$ is discrete, point defects are not stable. The lift of $D_2$ into SU(2), isomorphic to the fundamental group, is the eight element quaternion group $Q=\{1, -1, \pm i\sigma_1, \pm i\sigma_2, \pm i\sigma_3\}$ (Toulouse 1977). This group is non-abelian. The conjugation classes of $Q$, which label the line defects, are: $\{1\}$, $\{-1\}$, $\{\pm i\sigma_k\}$, $k=1,2,3$. So there are four stable line defects. On a contour encircling these singularities, the degeneracy parameter rotates by 360° about an arbitrary axis, and by $\pm 180°$ about the three main axes, respectively.

The symmetry group of cholesteric liquid crystals, $H=T(2)\wedge(R_h\wedge D_2)$, is broken from the group $E_0(3)=T(3)\wedge SO(3)$ of rigid motions in three-space (reflections not being included). Since the connected part $H_0$ of $H$ equals $T(2)\wedge R_h$, the different arcwise connected components of $H$ are labelled by the elements of $D_2$. Therefore the line defect structure is similar to that of the biaxial nematic phase: $\pi_1(V)=Q$, $\pi_2(V)=0$ (Kukula 1977, Volovik and Mineev 1977 a). The defect lines are denoted to be of type $\chi$, $\lambda$ and $\tau$, if along the Burgers circuit the degeneracy parameter rotates about the helix-axis, the director and the binormal, respectively (Kléman and Friedel 1969). Those of type $\lambda$ are not singular in the director. Therefore, the associated elastic energy is assumed to be less for the $\lambda$-type than for the others. Since, due to the helicoidal nature of the degeneracy parameter, rotations and translations are coupled, the singularities of type $\chi$ can also be interpreted as translational defects (dislocations).

The defect topology of the dipole-free superfluid $^3$He-A phase is a mixture of that of the uniaxial nematic and of the dipole-locked $^3$He-A phases. The connected components of the lift of the isotropy group $H$ form the cyclic four-element group $Z_4=\{1, \alpha, \alpha^2, \alpha^3\}$ (Volovik and Mineev 1977 a, Mermin 1979). $\alpha^2$ describes a 360°-disclination in the tripod $(\hat{e}_1, \hat{e}_2, \hat{l})$. Defects of type $\alpha$ and $\alpha^3$ are 180°-disclinations in the vector $\hat{d}$ combined with a rotation of the tripod about $\hat{l}$ by 180° and $-180°$, respectively. Point defects are formed only in the $\hat{d}$-field. They are labelled by pairs $\{n, -n\}$ of integers, since on going around a singular line of type $\alpha$ or $\alpha^3$ the sign of $\hat{d}$ is changed, similarly as the sign of the director alters on moving about a 180°-disclination in a uniaxial nematic liquid crystal.

Detailed derivations of the homotomy groups in all superfluid phases of He are found in the articles of Toulouse and Kléman (1976), Volovik and Mineev (1977 a, b), Cross and Brinkman (1977), Bailin and Love (1978 a–d) and Mermin (1978 b, 1979).

Kléman and Michel (1978) and Michel (1980) have calculated and listed the homotopy groups of the mesomorphous phases. The defect structure for thin layers of liquid crystals has been discussed by Rosciszewski (1980).

## § 4. Applications

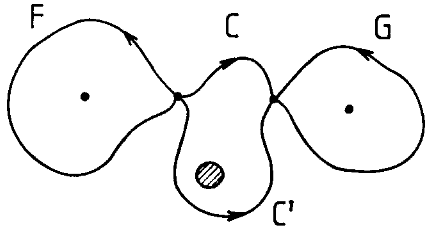
With the mathematical tools developed in the preceding sections, the defects not only can be placed into categories but due to the algebraic structure of the labelling scheme, interactions of singularities can be described by group operations. In § 4.1 the coalescence of defects is studied. Thereby we shall see that stable defects can decay in the presence of other line singularities. To take account of this phenomenon a more rigorous conception of stability is introduced, which leads to a classification in the form of 'orbit groups'. In § 4.2 we discuss entanglement problems of line defects. The relative homotopy groups are applied in §§ 4.3 and 4.4 to classify surface defects and to investigate how defects transform when the space of degeneracy is changed. Finally, in § 4.5, we examine ensembles of point singularities and loops of line defects by mappings of tori into the space of degeneracy.

## 4.1. *Defect coalescence*

### 4.1.1. *The combination process*

If two defect lines, which are encircled by contours $F$ and $G$, are combined, the type of resulting defect is determined by probing the degeneracy parameter field along a loop surrounding both (fig. 17). A candidate is the loop $FCGC^{-1}$ obtained when the initial points of $F$ and $G$ are connected by a path $C$. The corresponding free loops in $V$ are denoted $f$, $g$ and $h=fcgc^{-1}$. To apply the homotopic classification scheme, we choose $x_0=f(0)$ as base point in $V$. The loops $f$ and $h$ already adhere to $x_0$. $g$ is tied to the base point by the path $c$ and becomes a based loop $g_c=cgc^{-1}$. If the fundamental group is abelian, the single defect equivalent to the two lines is uniquely labelled by the based homotopy class $[h]=[f][g_c]$. Combination law is the group multiplication. In case $\pi_1(V)$ is non-abelian, each of the original line singularities is characterized by an entire conjugation class of $\pi_1(V)$. We denote the set of elements conjugate to $[f]$ and $[g_c]$ by $\hat{\alpha}_f$ and $\hat{\alpha}_g$, respectively. The pair of defects corresponds to the product $\hat{\alpha}_f\hat{\alpha}_g$ of the conjugation classes (the set of elements of $\pi_1(V)$ resulting if each element of $\hat{\alpha}_f$ is multiplied with each element of $\hat{\alpha}_g$). But this product in general yields a disjoint union of several conjugation classes. For example, in biaxial nematic liquid crystals, the class $\{\pm i\sigma_3\}$ describes a 180°-disclination line, $\sigma_3$ denoting one of the $2\times 2$ Pauli matrices. Multiplication of the class with itself leads to the conjugation classes $\{1\}$ and $\{-1\}$, which characterize the unstable defect and the 360°-disclination, respectively. To make the combination process unique, we have to provide more information than just the conjugation classes. The ambiguity rests in the choice of path $c$. For, take a representative of a based homotopy class conjugate to $[f]$ in $\pi_1(V)$, say $f'=kfk^{-1}$, which arises if the base point for $f$ is moved along a loop $k$ at $x_0$. The product loop $f'g_c=kfk^{-1}cgc^{-1}$ is homotopic to $kf(k^{-1}c)g(k^{-1}c)^{-1}k^{-1} \doteq k(fg_{c'})k^{-1}$, $c'=k^{-1}c$, and represents a group element conjugate to $[fg_{c'}]$. Alternatively we could have tied $g$ to $x_0$ along path $c'$. The conjugation class to which $[fg_{c'}]$ belongs describes the single defect resulting from the combination process along path $c'=k^{-1}c$. If the based homotopy class $[f]$ differs from $[kfk^{-1}]$, and

Fig. 17




Combination of two defects along paths $C$ and $C'$ in physical space.

$[k^{-1}g_ck]$ from $[g_c]$, then $[fg_c]$ is not conjugate to $[fg_{c'}]$, and merging the defects along $c$ and $c'$ leads to topologically inequivalent singularities. When in real space the defects are moved together along a path $C'$ instead of $C$, the ambiguity may occur only if the contour $CC'^{-1}$ surrounds a defect line of different type than the two other lines. Thus the uniqueness of the combination process is destroyed only in the presence of a third line singularity.

Similarly the combination of point defects in three-dimensional space is expressed by an orbit product which in general contains several disjoint orbits. Again, in the presence of a line defect, the combination of point singularities is ambiguous. As an example consider radial point defects of a nematic liquid crystal (hedgehogs). For a single hedgehog it cannot be decided whether it carries the index $+1$ or $-1$. For two hedgehogs the relative sign is fixed. But a 180°-line disclination destroys the well-defined orientation (fig. 18). The field lines above the defect line are those of charges of opposite sign, and, if merged along there, the point singularities annihilate. Beneath, the field lines look like those between equal charges, and the combination below the line doubles the topological index. In fig. 19 it is shown how two point defects move together and annihilate (from Saupe (1973)). One the indeterminate relative sign in the presence of defect lines no experiment exist.

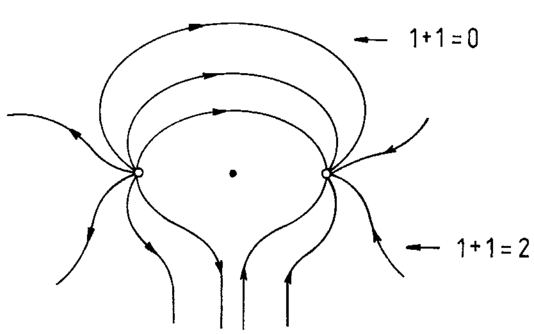
### 4.1.2. *Defect classification by orbit groups*

The example of fig. 18 displays a mechanism for the decay of a stable nematic point defect of even index $n$. The singularity is split into two, each of index $n/2$, which are then combined beyond a 180°-disclination line and annihilate. In a more general notion of stability even-indexed point defects are unstable. We shall introduce a classification scheme which takes account of this observation and inherits other useful properties.

Let us denote by $\alpha, \beta, \gamma, \ldots,$ elements of the fundamental group, represented by loops $a, b, c, \ldots,$ in $V$, which act on elements $\rho, \sigma, \tau, \ldots,$ of $\pi_1(V, x_0)$ or $\pi_2(V, x_0)$, represented by loops or spheres $r, s, t, \ldots$ When the base point of loop or sphere $r$ is moved along loop $a$, the result represents a homotopy class which we term $\alpha(\rho)$. In case $r$ is a loop, then both $\alpha$ and $\rho$ belong to the fundamental group, and $\alpha(\rho)$ equals $\alpha\rho\alpha^{-1}$. Now we form all possible 'generalized commutators' $\alpha(\rho)\rho^{-1}$, and denote the subgroup of $\pi_k(V)$, $k=1, 2$, generated by these as

$$D_k = \langle \alpha(\rho)\rho^{-1} | \alpha \in \pi_1(V), \rho \in \pi_k(V) \rangle. \tag{4.1}$$

Fig. 18



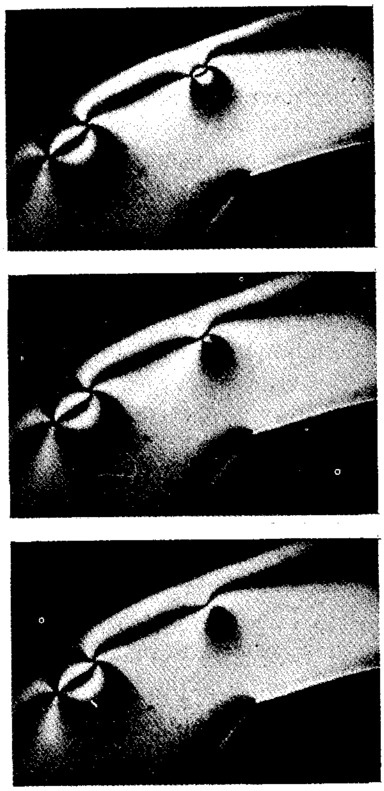

Point singularities (open circles) of a uniaxial nematic liquid crystal in the presence of a 180°-defect line (solid circle).

Fig. 19

(a)

(b)

(c)



Annihilation of nematic point singularities (from Saupe 1973).

$D_k$ is a normal subgroup. Therefore the quotient $\pi_k(V)/D_k$ is a group. This factor group has the following properties (proved only in part here):

(i) $\pi_k(V)/D_k$ is an abelian group. For $k=1$ this is true, because $D_1$ is the 'commutator subgroup' of $\pi_1(V)$, and $\pi_1(V)/D_1$ is the first homology group of $V$ (Spanier 1966, pp. 391, 394). $\pi_2(V)$ and $D_2$ are abelian anyhow.

(ii) The cosets of $D_k$ in $\pi_k(V)$ contain entire orbits. So we have grouped the orbits into larger units. Any other rearrangement of the orbits into sets which form a group is coarser. Therefore the name 'orbit group' is proposed for $\pi_k(V)/D_k$.

(iii) If $\hat{\rho}$ and $\hat{\sigma}$ are orbits contained in the cosets $\rho D_k$ and $\sigma D_k$, respectively, all the orbits of the product $\hat{\rho}\hat{\sigma}$ are contained in the group product $(\rho D_k)(\sigma D_k) = \rho\sigma D_k$. The group product in $\pi_k(V)/D_k$ limits the ambiguity of defect combination.

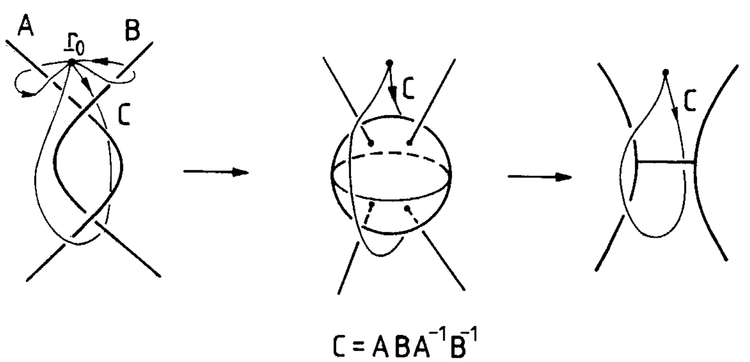
(iv) In the presence of suitable line singularities two defects which are described by homotopy classes $\rho$ and $\sigma$, respectively, can be transformed into one another, if and only if $\rho$ and $\sigma$ belong to the same coset of $D_k$ in $\pi_k(V)$. Transformation means continuous deformation, but also splitting and recombination beyond a line defect. The statement is valid also for the orbits $\hat{\rho}$ and $\hat{\sigma}$ which are the proper labels of the defects. For a proof write $\rho = \tau(\tau^{-1}\rho)$, where $\tau$ is an arbitrary element of $\pi_k(V)$. This operation describes the splitting of the defect into two of types $\tau$ and $\tau^{-1}\rho$. Moving the first about a singular line of type $\alpha\in\pi_1(V)$ and recombining it with the latter amounts to a transformation of $\rho$ into $\rho'=(\alpha(\tau)\tau^{-1})\rho$. The prefactor is an element of $D_k$. By repeating the process with other singular lines, $\rho$ can be changed into $\varphi\rho$, where $\varphi$ is an arbitrary element of $D_k$. The desired defect conversion is performed by choosing $\varphi=\sigma\rho^{-1}\in D_k$. But it is not possible to move $\rho$ out of the coset $\rho D_k$.

(v) A corollary of the preceding statement is that every singularity labelled by an element $\rho\in D_k$ can decay to the non-defect. For point defects of uniaxial nematic liquid crystals $D_2$ is the set of even integers, and $\pi_2(V)/D_2$ is the two element group $Z_2$. For line-defects in biaxial nematic liquid crystals, where $\pi_1(V)=Q$, $D_1$ is the group $\{1, -1\}$. The decay of a 360°-disclination (corresponding to the element $-1$) is catalysed by any 180°-disclination line.

### 4.2. *Entanglement of line defects*

The commutators of the fundamental group also play an important part in the crossing process of two line defects. It has been recognized by Toulouse and Poénaru (Toulouse 1977, Poénaru and Toulouse 1977), that there may be a topological obstruction to the crossing in media of non-abelian fundamental group. In fig. 20 two entangled line singularities are shown, which are probed by based Burgers circuits $A$, $B$ and $C$. The homotopy classes of the corresponding based loops in $V$ we denote by $\alpha$, $\beta$ and $\gamma$. Can one make the two singularities pass through each other by merely local fluctuations, i.e. by modifying the degeneracy parameter field only within a small ball at the meeting point? Apparently this can be achieved only if $\gamma$ is the unit element of $\pi_1(V)$. Otherwise a stable line defect must connect the two singularities. Moving the base point of $B$ along $A$ and attaching $B^{-1}$, one arrives at a loop $ABA^{-1}B^{-1}$ homotopic to $C$. Hence, class $\gamma$ is the commutator $\alpha\beta\alpha^{-1}\beta^{-1}$ of $\alpha$ and $\beta$. This identity is not easy to visualize and therefore illustrated in great detail in the articles of Kléman (1977 a), Mermin (1979) and of Jänich and Trebin (1981). In the latter it is derived that two $n$-fold twisted lines disentangle only if $\alpha^n$ and $\beta^n$ commute (i.e. $\alpha^n\beta^n=\beta^n\alpha^n$).

Fig. 20




Investigation of entangled line singularities by loops $A$, $B$ and $C$. If the loop in $V$ corresponding to $C=ABA^{-1}B^{-1}$ is non-contractable, after the crossing process the lines are connected by a third line defect.

The line singularities, which may prevent the crossing, are represented by elements of the commutator subgroup $D_1$. They act like rubber strings, since an increase of their length costs energy. The simplest substances of non-abelian fundamental group are the biaxial nematic liquid crystals. As Toulouse (1977) has speculated, such a biaxial phase with many defects may hold a polymer-type structure and 'topological rigidity' observable in elastic and flow properties. Yu and Saupe (1980) have discovered a biaxial nematic phase in a lyotropic system, but the defect structure has not been examined closer.

When, in general, an $n-p-1$- and an $n-q-1$-dimensional defect, represented by $\alpha \in \pi_p(V)$ and $\beta \in \pi_q(V)$, meet in an $n$-dimensional space, $n=p+q+1$, a singularity of dimension $n-2$, represented by $\gamma \in \pi_{n-2}(V)$, obstructs their crossing (Poénaru and Toulouse 1979). $\gamma$ is the Whitehead product $[\alpha, \beta]$ (Whitehead 1978). For $q=1$ and $q=1$ or 2, this product is identical to the 'generalized commutator' defined in §4.1.2.

### 4.3. *Surface defects*

For experimental observation usually a thin liquid crystalline layer is placed between two parallel glass plates. The orientation of the molecules on the surface can be well defined by rubbing the glass (de Gennes 1975, p. 70). This 'selective anchoring' is a prerequisite for the application of liquid crystals as display devices (Schadt and Helfrich 1971). Often the molecules of a uniaxial nematic liquid crystal assume all directions parallel to the surface or at a constant angle to it (i.e. on a cone). The possible positions of the director then form a subset $A$ of the bulk space of degeneracy $V$. Typical surface defects appear on the cover glass, which are known as 'Schlieren texture' (see fig. 21, taken from Demus and Richter 1980).

To classify these singularities, one regards the surface as a two-dimensional degeneracy parameter field valued in $A$ (Stein *et al.* 1978). The point singularities are tested by closed contours and labelled by the conjugation classes of $\pi_1(A)$. But this classification includes singular points that are the ends of stable defect lines in the volume. To separate volume from pure surface defects, Volovik (1978) proposed surrounding the point by a hemisphere in the bulk whose boundary lies in the surface. The mappings from the hemisphere to the space of degeneracy, where the values on the boundary are restricted to $A$, represent elements of the second relative homotopy group $\pi_2(V, A)$. The exact sequence of homotopy groups (eqn. (3.11))

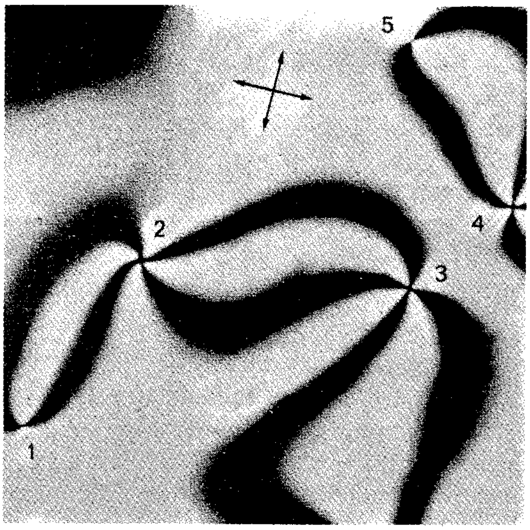
$$\ldots \to \pi_2(A) \xrightarrow{\rho} \pi_2(V) \xrightarrow{\sigma} \pi_2(V, A) \xrightarrow{\tau} \pi_1(A) \xrightarrow{\xi} \pi_1(V) \to \ldots$$

provides the following interpretation of the defect structure: according to a well-known theorem the kernel of $\tau$ (notation $\ker \tau$) is a normal subgroup of $\pi_2(V, A)$, and the factor group $\pi_2(V, A)/\ker \tau$ is isomorphic to the image of $\tau$ (notation $\operatorname{im} \tau$). Since the sequence is exact, $\ker \tau$ is equal to $\operatorname{im} \sigma$, and $\operatorname{im} \tau$ equal to $\ker \xi$, so that

$$\pi_2(V, A)/\operatorname{im} \sigma = \ker \xi. \tag{4.2}$$

To determine $\pi_2(V, A)$ is a matter of extending the group $\ker \xi$ by $\operatorname{im} \sigma$ (see, for example, Michel 1964). As Volovik (1978) remarks, $\pi_2(V, A)$ is for relevant cases simply the direct product $\operatorname{im} \sigma \times \ker \xi$. Accordingly an element of $\pi_2(V, A)$ is a pair $(\alpha, \beta)$; $\alpha \in \operatorname{im} \sigma$ characterizes a bulk point singularity transferred to the surface, $\beta \in \ker \xi$ a contour in $A$, which is contractable in $V$ and informs how the singularity $\alpha$ is glued to the boundary. To establish $\operatorname{im} \sigma$ one uses the relation $\operatorname{im} \sigma = \pi_2(V)/\ker \sigma = \pi_2(V)/\operatorname{im} \rho$. Similarly as $\pi_1(V)$ acts on $\pi_2(V)$, $\pi_1(A)$ also acts on $\pi_2(V, A)$ by 'path

Fig. 21




Surface point singularities of a nematic liquid crystal with tangential boundary conditions (from Demus and Richter 1980). The photo is taken in reflection of polarized light, with crossed polarizers (indicated by the arrows). Singularities 1 and 5 are the ends of 180°-line singularities, since only two black (and two white) bands emanate from them. The winding numbers $n$ of 2, 3 and 4 are $-1$, 1 and 1, respectively. Whereas the number of bands indicates the absolute value of the winding number, its sign is found by rotating the polarizers. For positive $n$, the cross of dark and bright bands rotate in the same direction, for negative $n$ they rotate in the opposite direction.

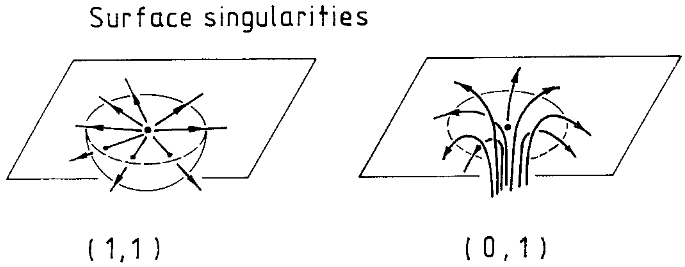


isomorphisms' along loops in $A$. The pure surface singularities are labelled by the orbits of $\pi_2(V, A)$ under this action.

For a uniaxial nematic liquid crystal, whose surface director lies in a plane, we find the following situation: $A = S^1/Z_2 = P^1$ (the set of straight lines in the plane passing through the origin); $\pi_1(A) = Z/2 = \{0, \pm\frac{1}{2}, \pm 1, \ldots\}$, $\pi_2(A) = 0$; $V = P^2$, $\pi_1(V) = Z_2$, $\pi_2(V) = Z$. Hence $\mathrm{im}\,\sigma$ is the entire group $\pi_2(V)$, $\ker \xi = Z$ describes the disclinations of the integer index and $\pi_2(V, A)$ equals $Z \times Z$. The surface point singularities correspond to the orbits $\{(\pm m, n)\}$, $m$, $n$ being integers. While $n$ is well explained as a winding number of the surface director, for the definition of $m$ the mapping from the hemisphere must be completed to the whole sphere. There is no standard ('canonical') way to do this. Indeed, given one isomorphism $\pi_2(V, A) = Z \times Z$, the elements $(m, n)$ can be relabelled to $(m+k, n)$, $k$ being a fixed integer, without contradiction. Only if we prescribe the form of elements $(0, 1)$ and $(1, 1)$, as, for example, in fig. 22, the labelling scheme is unique.

In dipole-locked $^3$He-A the boundary conditions compel the vector $\hat{l} = \hat{e}_1 \times \hat{e}_2$ (§ 2.2.4) to stand perpendicular to the surface. The set $A = S^1 \times Z_2 = \mathrm{O}(2)$ contains the positions of the orthonormal pair $(\hat{e}_1, \hat{e}_2)$ in the plane, while $\hat{l}$ is fixed parallel or antiparallel to the normal. From $\pi_2(A) = 0$, $\pi_1(A) = Z$, $V = \mathrm{SO}(3)$, $\pi_2(V) = 0$ and $\pi_1(V) = Z_2$ it follows that $\mathrm{im}\,\sigma = 0$ and $\pi_2(V, A) = \ker \xi = 2Z = \{0, \pm 2, \pm 4, \ldots\}$. The surface point singularities are boojums (Mermin 1977 a, 1981), around which the pair $(\hat{e}_1, \hat{e}_2)$ rotates by an integer multiple of $4\pi$, and which can cause a decay of the supercurrent in $^3$He-A. Similarly $4\pi n$-vortices are expected on the surfaces of

Fig. 22




Nematic surface singularities (tangential boundary conditions) of indices (1, 1) and (0, 1), as viewed from the bulk.



cholesteric liquid crystals under tangential boundary conditions (Stein *et al.* 1978, Pisarski and Stein 1980). A thorough study of surface singularities was performed by Meyer (1972) on a nematic–isotropic interface.

Surface line defects are classified by the elements of the relative homotopy group $\pi_1(V, A)$, which is also deduced by use of the exact sequence. For dipole-locked $^3$He-A Volovik (1978) recovered the lines segregating areas of reversed $\hat{l}$.

### 4.4. *Defect transformations*

Exact sequences of homotopy groups also prove helpful in examining how defects transform, when the space of degeneracy is altered. This can happen either by a change of the length scale of the degeneracy parameter variations, or by a change of the symmetry group of the medium, for example in a phase transition.

#### 4.4.1. *Defect cores*

From §§ 2.2.3 and 2.2.4 we know that the space of degeneracy increases when certain terms in the free-energy vanish, or when the characteristic variation length $\lambda$ of the degeneracy parameter field becomes smaller than the corresponding coherence length. For a nematic liquid crystal the space of degeneracy is enlarged from $P^2$ to $S^4$, when the energy term proportional to $\operatorname{tr} Q^3$ is overcome, for $^3$He-A from SO(3) to $S^2 \times SO(3)/Z_2$, when the dipolar interaction becomes negligible compared to the elastic energy.

Assume a medium of space of degeneracy $V_2$, and a singularity surrounded by a Burgers circuit (or sphere) $F$ whose corresponding loop (or surface) $f$ in $V_2$ represents an element $\alpha_2 \in \pi_r(V_2, x_0)$, $r = 1$ or 2. In the vicinity of the singularity the field varies rapidly and takes values in an enlarged space $V_1 \supset V_2$. If $F$ is shrunk so that it passes through this region, its counterpart in $V_1$ is contained in a homotopy class $\alpha_1 \in \pi_r(V_1, x_0)$. Releasing a loop (or surface) from the subspace $V_2$ to the total space $V_1$ is described by the homomorphism

$$i_*^{(r)}: \pi_r(V_2, x_0) \to \pi_r(V_1, x_0)$$

of eqn. (3.9). It is part of the exact sequence of homotopy groups (eqn. (3.11)). Those defects in $V_2$, which have a non-singular core in $V_1$ are labelled by elements of the kernel of $i_*^{(r)}$ (Mermin *et al.* 1978).

Since the first and second homotopy groups of the space $V_1 = S^4$ vanish (§ 3.2), the cores of all defects in nematic liquid crystals are non-singular. How the singularity is avoided by an escape into biaxiality is demonstrated for a 180°-disclination in fig. 23 (according to Lyuksyutov 1978). The diameter of the biaxial core in the uniaxial phase is estimated to be about 200 Å.

For line singularities in $^3$He-A, where $\pi_1(\mathrm{SO}(3))=Z_2=\{1,-1\}$, and $\pi_1(S^2\times \mathrm{SO}(3)/Z_2)=Z_4=\{1,\alpha,\alpha^2,\alpha^3\}$ (§ 3.4), homomorphism $i_*^{(1)}$ associates the following elements: $1\to 1$, $-1\to\alpha^2$. Since element $-1$ is not in the kernel of $i_*^{(1)}$, the corresponding 360°-disclination in the tripod $(\hat{e}_1,\hat{e}_2,\hat{l})$ cannot be eliminated by dipole-unlocking.

In this homomorphism $\alpha$ and $\alpha^3$ have no counterimage. To see what happens with the corresponding singularities when $V_1$ is reduced to $V_2$, Mermin *et al.* (1978) applied the homomorphism $j_*^{(1)}$ following $i_*^{(1)}$ in the exact sequence:

$$\ldots\to\pi_1(V_2,x_0)\xrightarrow{i_*^{(1)}}\pi_1(V_1,x_0)\xrightarrow{j_*^{(1)}}\pi_1(V_1,V_2,x_0)\to\ldots$$

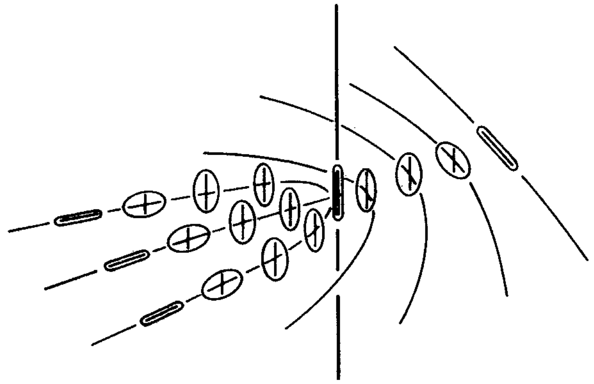
Since $\alpha$ and $\alpha^3$ are not in im $i_*^{(1)}=\ker j_*^{(1)}$, they are mapped into non-trivial elements of $\pi_1(V_1,V_2)$. This implies that on every Burgers circuit around the singular line a region must be traversed where values in $V_1$ are taken by the degeneracy parameter which do not belong to $V_2$. For energetic reasons this region will be as small as possible and form a wall terminating on the singular line. Around the singularity of type $\alpha$, for instance, the orthonormal pair of vectors $(\hat{e}_1,\hat{e}_2)$ rotates by 180° about $\hat{l}$, while simultaneously $\hat{d}$ turns into $-\hat{d}$ (fig. 24). This motion of $\hat{d}$ is also unavoidable in the dipole-locked phase. Within the singular wall $\hat{d}$ passes from the position parallel to $\hat{l}$ to one antiparallel, the degeneracy parameter thereby leaving the space $V_2=\mathrm{SO}(3)$.

Point singularities labelled by elements of $\pi_2(V_1)$, which are not in the image of homomorphism $i_*^{(2)}$ give rise to line singularities for $V_2$. Volovik and Mineev (1977 a) have analysed how a hedgehog in the vector field $\hat{d}$ breaks into lines when the dipole-free $^3$He-A phase is locked.

### 4.4.2. *Phase transitions*

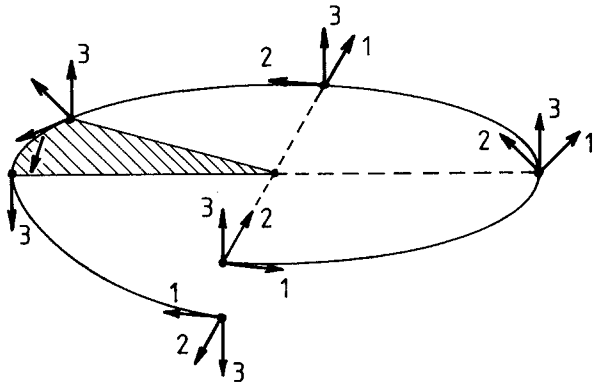
The behaviour of defects in the transition from the smectic-A to the smectic-C liquid crystalline phase was studied by Kléman and Michel (1977). Their work was generalized by Trebin (1981 a). Suppose that a uniform ordered medium, which is characterized by an order parameter $x_0$ of symmetry group $H_2\subset G$, is heated and

Fig. 23



Elimination of a 180°-disclination line of a uniaxial nematic liquid crystal by escape to biaxiality close to the singularity (according to Lyuksyutov 1978).

Fig. 24




Burgers circuit about a singular line of type $\alpha$ in dipole-free $^3$He-A. Along the circuit the pair of vectors $(\hat{e}_1, \hat{e}_2)$ (labelled 1, 2) rotates by 180°, whereas the vector $\hat{d}$ (labelled 3) turns into $-\hat{d}$. In the dipole-locked phase the region where $\hat{d}$ is rotated to $-\hat{d}$ forms a singular wall.

turns into a phase of order parameter $y_0$ and symmetry $H_1 \subset G$, where $H_2$ is a subgroup of $H_1$. If the lower symmetry phase is rotated by an element $g \in G$, its order parameter $gx_0$ turns into $gy_0$ in the higher symmetry phase. Thus we obtain a correspondence between the spaces of degeneracy $V_2 = G/H_2$ and $V_1 = G/H_1$, which in terms of homogeneous spaces is expressed by the mapping

$$\left.\begin{aligned} p\colon G/H_2 &\to G/H_1, \\ gH_2 &\mapsto gH_1. \end{aligned}\right\} \tag{4.3}$$

$gH_2$ is mapped into that coset of $H_1$ where it is contained.

Our conjecture postulates a transition so smooth that the phase remains uniform also above the critical temperature. Most probably this occurs in a second-order phase transition. For a weakly distorted phase 2, described by a field $\phi_2(\mathbf{r})$ valued in $V_2$, we assume that relation (4.3) is also valid locally, so that the field in phase 1 becomes $\phi_1(\mathbf{r}) = p(\phi_2(\mathbf{r}))$, up to continuous deformation. If the field values along a Burgers circuit $F$ form a loop $f(t)$ in $V_2$ before the transition, then afterwards they form a loop $p(f(t))$ in $V_1$. Associating the homotopy class of $f$ in $\pi_1(V_2, x_0)$ with that of $p\ f$ in $\pi_1(V_1, y_0)$ yields a homomorphism

$$p_*^{(r)}\colon \pi_r(V_2, x_0) \to \pi_r(V_1, y_0) \tag{4.4}$$

not only for $r = 1$ but for any integer $r \geqslant 1$. $p_*^{(r)}$ also maps the elements of an orbit of $\pi_r(V_2, x_0)$ (under the action of $\pi_1(V_2, x_0)$) into a unique orbit of $\pi_r(V_1, y_0)$ (under the action of $\pi_1(V_1, y_0)$). Equation (4.4) therefore constitutes the selection rule for defect transformations in a phase transition.

If $r = 1$ or 2, then by eqns. (3.13) and (3.14) $p_*^{(r)}$ is transferred to homomorphisms $H_2/H_2^0 \to H_1/H_1^0$ or $\pi_1(H_2^0) \to \pi_1(H_1^0)$, respectively (Trebin 1981 a). In the table these homomorphisms are presented for several phase transitions. In the reverse transition $1 \to 2$ those singularities whose corresponding elements in $\pi_r(V_1, y_0)$ have a counterimage, return to the respective defect in phase 2. The others break into singularities of higher dimension. This fact is elaborated for the transformation of point defects.

Transformation of defects in phase transitions†.

| Phase | $H$ | $\pi_1$ | $\pi_2$ |
|---|---|---|---|
| Uniaxial nematic | $T(3)\wedge D_{\infty h}$ | $Z_2$ | $Z$ |
| Biaxial nematic | $T(3)\wedge D_{2h}$ | $Q$ | 0 |
| Smectic-A | $(T(2)\times Z)\wedge D_{\infty h}$ | $Z\wedge Z_2$ | $Z$ |
| Smectic-C | $(T(2)\times Z)\wedge C_{2h}$ | $Z\wedge Z_4$ | 0 |

| Phase transition | $p_*^{(1)}$ | $p_*^{(2)}$ |
|---|---|---|
| Biaxial→uniaxial nematic | $\pm 1, \pm i\sigma_z \mapsto 0$<br>$\pm i\sigma_x, \pm i\sigma_y \mapsto 1$ | $0\mapsto 0$ |
| Smectic-C→smectic-A | $(n\|0), (n\|2)\mapsto(n\|0)$<br>$(n\|1), (n\|3)\mapsto(n\|1)$ | $0\mapsto 0$ |
| Smectic-A→nematic | $(n\|0)\mapsto 0$<br>$(n\|1)\mapsto 1$ | $n\mapsto n$ |
| Smectic-C→nematic | $(n\|0), (n\|2)\mapsto 0$<br>$(n\|1), (n\|3)\mapsto 1$ | $0\mapsto 0$ |

† In the first part the isotropy groups $H$ and the first and second homotopy groups are listed for several mesomorphic phases (of unbroken symmetry group $G=E(3)$). In the second part the homomorphisms $p_*^{(1)}$ and $p_*^{(2)}$ which constitute selection rules for the transformation of line and point singularities in the indicated phase transitions are presented. $\wedge$ denotes the semidirect product, $n$ is an integer and $Q$ is the quaternion group.

We apply an exact sequence slightly differing from that developed in § 3.3.2 (see, for example, Steenrod 1951, § 17.3):

$$\ldots\to\pi_2(G,H_2,e)\to\pi_2(G,H_1,e)\to\pi_1(H_1,H_2,e)\to\ldots \tag{4.5}$$

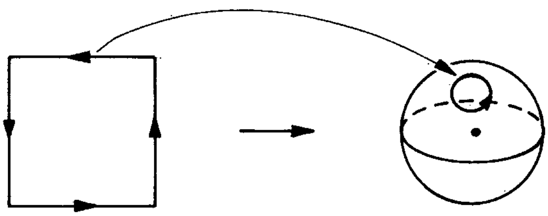
The second homotopy groups of the homogeneous spaces $G/H_k$ are identified with relative homotopy groups, whose elements are represented by mappings of the unit square into $G$, the boundary going into $H_k$ and the identity $e$. Imagine this square being deformed to a sphere with a hole (fig. 25) and in physical space being wrapped around the singular point. At the point on the sphere of coordinates $(t_1, t_2)$ the degeneracy parameter in phases 2 and 1 is $g(t_1,t_2)x_0$ and $g(t_1,t_2)y_0$, respectively. Information on defect types and transformation is already obtained from the restriction of the mapping to the boundary, i.e. to the loop $F$ encircling the hole. Since $\pi_1(G,H_k,e)=\pi_1(H_k^0,e)$ and $\pi_1(H_1,H_2,e)=\pi_1(H_1^0,H_1^0\cap H_2,e)$ (the loops can only reside in $H_1^0$), sequence (4.5) is equivalent to

$$\ldots\to\pi_1(H_2^0,e)\xrightarrow{\rho}\pi_1(H_1^0,e)\xrightarrow{\sigma}\pi_1(H_1^0,H_1^0\cap H_2,e)\to\ldots \tag{4.6}$$

Take a point singularity in phase 1 corresponding to an element $\alpha\in\pi_1(H_1^0)=\pi_2(G,H_1,e)$, which is not in im $\rho$. Because $\alpha$ is also not in ker $\sigma$, it is represented by a loop $h$ in $H_1^0$ which in its course must leave $H_2^0$ and $H_2$. Whereas before the phase transition 1→2 the degeneracy parameter along circuit $F$ is $h(t)y_0\equiv y_0$ and the hole can be closed, afterwards it is $h(t)x_0\neq$ const, so that $F$ encircles a line defect emerging from the singular point. This line singularity may split into several others, as illustrated in detail by Trebin (1981 a).

As an example we consider the hyperbolic point of smectic-A liquid crystals. It is a point singularity in the director, whose field lines—depicted in fig. 8—coincide

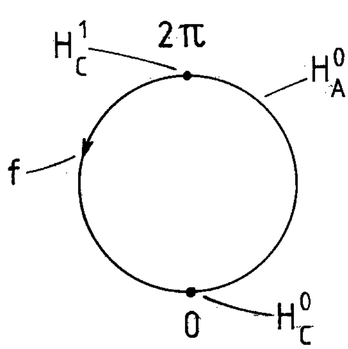
Fig. 25



Wrapping a square (the domain of a mapping into $G$) about a singular point whose behaviour is investigated in a phase transition.

with the layer normals. The second homotopy group for smectics of type A is $Z$, and the hyperbolic point carries the index $n=1$. In a phase transition to the smectic-C phase, which does not have stable point defects, we expect the hyperbolic point to break into line singularities. The respective symmetry groups, lifted into $\bar{E}_0(3)=T(3)\wedge SU(2)$ are $H_A=Z\wedge\bar{D}^z_\infty$, $H_C=Z\wedge\bar{C}^x_2$. $\bar{D}^z_\infty$ denotes the rotations by angles $\varphi(0\leqslant\varphi\leqslant4\pi)$ about the layer normal, and by integer multiples of $\pi$ (modulo $4\pi$) about all axes in the layer. $\bar{C}^x_2$ denotes the rotations, also by multiples of $\pi$(modulo $4\pi$), about that axis in the layer which is orthogonal to the projection of the tilted director. The discrete translational symmetry perpendicular to the layers, indicated by $Z$, is not involved in point defect processes. One obtains $H^0_A=\bar{C}^z_\infty$, $H^0_A\cap H_C=\{1,-1\}\subset SU(2)$. The loop $f$ for the hyperbolic point encircles $\bar{C}^z_\infty$ once (fig. 26), since the index is $n=1$. Therefore in the C-phase the circuit $F$ encloses a line singularity, around which the projection of the director to the smectic plane rotates by $4\pi$. It may break into two lines of vorticity $2\pi$. Perez *et al.* (1978) have observed a hyperbolic point in the smectic-A phase, terminating at a defect ring (fig. 27). Upon transition to the smectic-C phase two lines evolve inside the ring. For similar experiments and a detailed theoretical investigation referral is made to the work of Bourdon *et al.* (1982) and Bouligand and Kléman (1979). The lines do not extend beyond the ring, because there the field is uniform. The defect transformations examined by Cladis *et al.* (1979) in the transition from the smectic-A to the cholesteric phase cannot be discussed by our theory, since there is no subgroup relation of the symmetry groups.

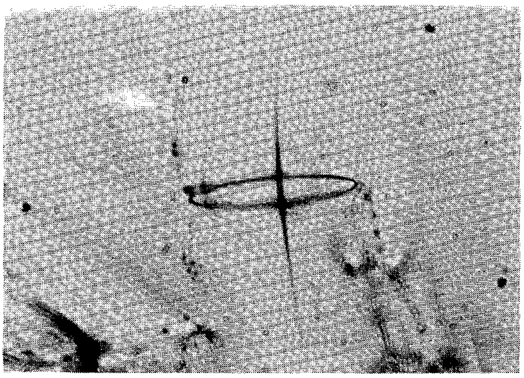
Fig. 26



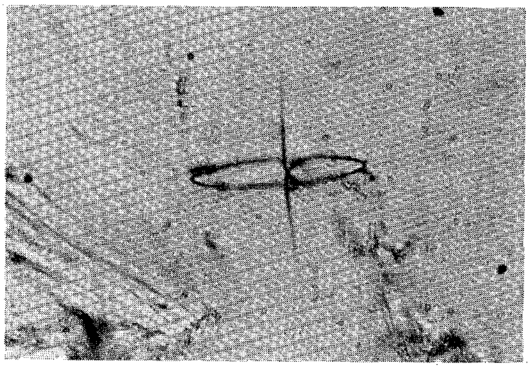

Loop $f$ in the component $H^0_A$ of the isotropy group of the smectic-A liquid crystalline phase, and components $H^0_C$, $H^1_C$ for the smectic-C phase.

Fig. 27

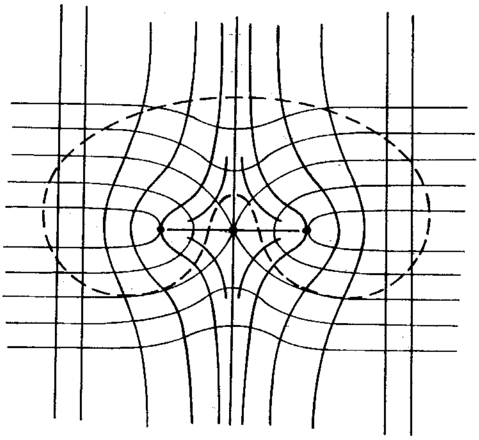
(*a*)



(*b*)



(*c*)



(*a*) Hyperbolic point in the smectic-A phase, terminating at a singular ring (an ellipse), from Perez *et al.* (1978). The hyperbola passing through the focus of of the ellipse is an unstable line defect. (*b*) After transition to the smectic-C phase, the singular point is broken into two singular lines joining hyperbola and ellipse. (*c*) Cross-section of the point defect in a case where the ellipse is degenerated to a circle and the hyperbola to a straight line. The full lines denote the layers and the normal field. Inside the ring, the normal field is hyperbolic, outside it, it is uniform, since the ring carries a topological charge opposite to that of the point. The dashed line marks a cross section of the Burgers sphere probing the charge of the ring.

The geometrical model of the defect transition should be correct in the far-field of a singularity, where the distortions are weak. The far-field, however, already determines the defect type. Transformations, which break the proposed selection rules, require a rearrangement of the far-field at the cost of energy.

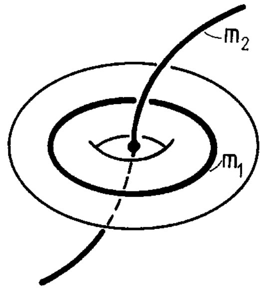
Defects in phase 2 which correspond to elements in $\ker p_*^{(r)}$ have a non-singular core of phase 1. They should be of lower energy than defects which are also singular in the higher symmetry phase. Thus $p_*^{(r)}$ introduces an energetical classification of the singularities, as requested by Bouligand *et al.* (1978).

Often defects are considered only in that part of the degeneracy parameter which is most easily manipulated, for instance, by boundary conditions. In a conjectured phase transition, where phase 1 is governed by the incomplete, phase 2 by the complete, degeneracy parameter, these defects can be related to the singularities of the actual space of degeneracy. Point singularities in the $\hat{l}$-vector of superfluid $^3$He-A, for instance, denoted 'vortons' by Blaha (1976), are line defects in the full dipole-locked degeneracy parameter, around which the pair $(\hat{e}_1, \hat{e}_2)$ rotates by an integer multiple of $4\pi$.

### 4.5. *Torus homotopy groups*

Homotopy classes are defined not only for mappings from $r$-spheres into the space of degeneracy but for continuous mappings between any two topological spaces, although these are rarely endowed with a group structure. Garel (1978) in particular examines mappings from $r$-dimensional tori into $V$. The two-dimensional torus $T^2$ is appropriate for the classification of closed defect lines. The homotopy classes of mappings from a tubular surface into $S^1$, for example, are labelled by two integers $(m_1, m_2)$ (fig. 28). While $m_1$ denotes the winding number of the enclosed singularity, $m_2$ is the index of the defect lines passing through the torus. For mappings $T^2 \to S^2$ the homotopy classes also carry integer numbers, which are the index sums of all point defects inside the torus. Three indices $(n, m_1, m_2)$ characterize a mapping $T^2 \to P^2$: $m_1$ and $m_2$ (both modulo 2) correspond to nematic disclination lines within the torus and traversing it, $n \in Z$ counts the enclosed topological point charge. Nematic defect loops can emit point defects, thereby lowering or raising the index $n$. Infinite lines may compensate the lost charge by retrieving it from infinity and thereby create singular points in any number (Dzyaloshinskii 1981). Only if $m_1$ or $m_2$ vanishes can the torus be closed to a sphere and the index $n$ be uniquely determined as usual. If $m_1 = m_2 = 1$, the line passing through the torus may extract

Fig. 28




Line singularities inside a torus and passing through it.

topological charge, so that it is impossible to define $n$ in a canonical way. The fact that a defect loop has properties of a point singularity allows the field of the hyperbolic point of fig. 27 to terminate on an oppositely charged defect ring.

## § 5. Topological solitons

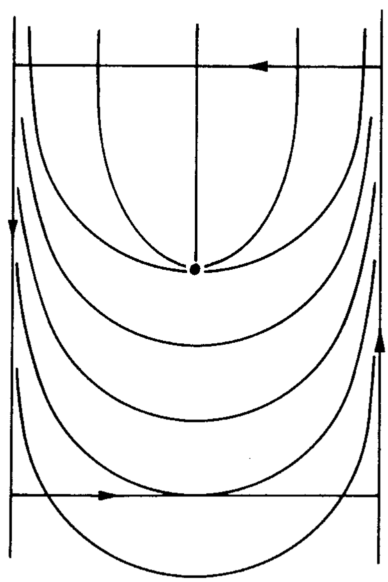
Thus far our interest has centred on non-uniform systems with a singularity in the degeneracy parameter field. If the singularity is topologically stable, it is not possible to smooth it out by local fluctuations. However, there are also non-singular fields, which, owing to boundary conditions, cannot be made uniform unless singularities are introduced. Such fields are named 'configurations'.

### 5.1. *Linear, planar and particle-like solitons*

Take, for instance, a uniaxial nematic liquid crystal subjected to the condition that far from the $y$–$z$-plane the director is parallel to the $z$-direction. The degeneracy parameter along any path connecting points with $x=-\infty$ and $x=+\infty$ forms a closed loop in $V$. If the loop is non-contractable, there is no way for the system to relax continuously to the uniform ground state. The distortion will prevail along a certain width $\Delta x$ minimizing the elastic energy, and gives rise to a domain wall (Mineyev and Volovik 1978, Mineev 1980), that is classified by a conjugation class of the fundamental group. The wall may terminate on a defect line parallel to the $y$–$z$-plane, which, if tested by the Burgers circuit of fig. 29, is seen to correspond to the same class as the wall. Because of their shape stability, domain walls are also named planar solitons.

In a more general sense planar solitons are fields in $V$ which take values in a subset $A \subset V$ far from a central plane. They are classified by use of the first relative

Fig. 29



Linear soliton in a nematic liquid crystal terminating on a stable line defect. The arrows mark the sense of a Burgers circuit testing the line singularity.

homotopy group $\pi_1(V, A)$. The set $A$ consists either of 'easy directions' (for example in an anisotropic ferromagnet), of 'vacuum states' (positions of lowest energy, for example in a magnetic field), or of directions admitted by the anchoring conditions on a surface. If $A$ has several disconnected components, and hence $\pi_1(V, A)$ is not a group, the domain walls cannot be bounded by a line singularity. These walls, like a 180° Bloch- or Néel wall, are termed 'classical' by Mineev (1980).

Linear solitons take values in $A$ far from a line. Accordingly they are described by elements of $\pi_2(V, A)$. They may terminate on point singularities labelled by the same homotopy class. Such point defects relieve a solitary field from strain. Pushing the singularity through the medium leaves the soliton in its wake.

Finally, there are the particle-like solitons, classified by $\pi_3(V, A)$, whose degeneracy parameter field is restricted everywhere at infinity to values of the set $A$. If $A$ is just one point, the boundary condition makes physical space equivalent to a three-sphere, since all points at infinity are considered identical. In this case particle-like solitons are not expected to exist for energetical reasons. Usually the elastic energy density of an ordered medium is a second-order polynomial in the gradient of the degeneracy parameter. If the diameter $L$ of the soliton is scaled down by a factor $\lambda < 1$ $(L \to \lambda L)$ the elastic energy density increases by $\lambda^{-2}$, but the volume decreases by $\lambda^3$, so that the total elastic energy is reduced by $\lambda$. The soliton will collapse to dimensions of the coherence length, where the order parameter can move out of the space of degeneracy, and will vanish away. Exceptions to this rule are assumed only for media with an internal length scale, like the pitch of cholesteric liquid crystals (Pisarski and Stein 1980). Stabilization of the soliton may also occur due to higher gradient terms, but only at a microscopic size (Shankar 1977). A dynamical stabilization of particle-like solitons was discussed (Mineyev and Volovik 1978), but is still in question (Mineev 1980).

The space of degeneracy $V$ is that subset of the order-parameter space $X$ whose elements are associated with the energetically degenerate states of minimum free-energy. Because $X$ is a vector space, any loop or surface in $X$ is contractable to a point, and the homotopy groups of $X$ are trivial. The exact sequence

$$\ldots \to \pi_{r+1}(X) \to \pi_{r+1}(X, V) \to \pi_r(V) \to \pi_r(X) \to \ldots \tag{5.1}$$

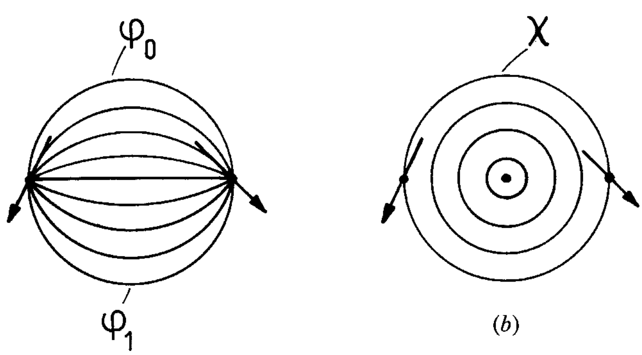
yields the isomorphisms $\pi_r(V) = \pi_{r+1}(X, V)$. Therefore in three-dimensional space point defects may be interpreted as particle-like solitons, line defects and singular walls as linear and planar solitons in the *order* parameter. Here the application of homotopy theory in condensed matter physics meet its use in field theory. The fields are mappings from space-time to a vector space $X$, the 'space of internal symmetries'. The values of those constant fields, which minimize a given lagrangian, form the vacuum set $V$. A field of finite energy must take values in $V$ at infinity. If the asymptotic field $\phi(\hat{r}, r \to \infty)$ represents a non-trivial element of $\pi_2(V) = \pi_3(X, V)$, the field has shape stability and is of non-zero energy, because there must be points in space, where values outside $V$ are assumed. Such fields describe particle-like states, the monopoles, which were discovered as solutions of field equations in the unified gauge field theories by t'Hooft (1974) and Polyakov (1974), and classified by the second homotopy group by Tyupkin *et al.* (1975) and Monastyrskii and Perelomov (1975) (see also, for example, Michel 1980, Appendix H). In field theory the application of homotopic methods was first proposed by Finkelstein (1966). He named the topologically stable states 'homotopons' and 'kinks'. The analogy of particle-like monopole states and defects in condensed matter physics bears resemblance to a theory by Burton (1892) who assumed matter to consist of structural defects in the ether.

## 5.2. *Fixed boundary conditions*

Homotopy groups also help to decide whether a non-singular degeneracy parameter field $\varphi_0$ can be continuously deformed into another field $\varphi_1$ at not necessarily uniform, but fixed, boundary conditions. The problem is illustrated by a two-dimensional ferromagnet in one spatial dimension along the presentation of Poénaru (1979). Given two fields $\varphi_0$ and $\varphi_1$, defined on the unit interval, with values in $V=S^1$, and with the same boundary conditions $\varphi_0(0)=\varphi_1(0)$, $\varphi_0(1)=\varphi_1(1)$: is it possible to deform $\varphi_0$ into $\varphi_1$ without changing the values on the boundary? For an answer the two intervals are glued together to form a mapping $\chi$ of a circle into $V=S^1$ (fig. 30). If $\varphi_0$ is deformable into $\varphi_1$ under the prescribed boundary conditions, the homotopy can be spread into the interior of the circle (fig. 30 (*a*)) and generates a continuous mapping of the entire disk into $V$. But this mapping provides a homotopy between $\chi$, which is a loop in $V$, and the constant loop (fig. 30 (*b*)). Therefore $\varphi_0$ is deformable to $\varphi_1$ under fixed boundary conditions if and only if $\chi$ represents the identity in $\pi_1(V)$. The same procedure, performed in three-dimensional space, leads to a composed mapping $\chi$ of the three-sphere into $V$. Unless $\chi$ represents the identity of $\pi_3(V)$, the deformation process is not possible.

For non-singular unit-vector fields in three-space the preceding observations guarantee the conservation of a topological quantity denoted linking number. Take two unit vectors $\hat{l}_1$, $\hat{l}_2 \in V=S^2$. The loci in space where the field takes the values $\hat{l}_1$ and $\hat{l}_2$ form loops $C_1$ and $C_2$, respectively, which might be entangled. The linking number counts how often $C_1$ passes through $C_2$. (In general there are several disjoint loops for $\hat{l}_1$ and also for $\hat{l}_2$. The exact way to determine the linking number, involving the orientation of the loops, is reported by Toulouse (1980 b), Appendix IV). In the case of constant uniform boundary conditions, the vector field is classified by an index $n \in \pi_3(S^2)=Z$. This index coincides with the linking number. If the boundary conditions are not uniform, but fixed, the loops cannot be disentangled, since glueing the original mapping on the boundary together with one of unlinked loops produces

Fig. 30




(*a*) (*b*)

(*a*) Homotopy between mappings $\varphi_0$ and $\varphi_1$ with fixed boundary conditions. (*b*) The homotopy between $\varphi_0$ and $\varphi_1$ provides a prescription of how to contract $\chi$ to a point.

a vector field on the three-sphere which does not represent the identity of $\pi_3(V)$. The linking number is also conserved in uniaxial nematic liquid crystals, because any non-singular director field represents a unique vector field.

In cholesteric liquid crystals Bouligand (1974) observed dark lines forming entangled double loops. He analysed that the lines marked 360°-disclinations of type $\lambda$ (§ 3.4) which were labelled by the element $-1\in\pi_1(V)=Q$, and were singular in the helix axis and binormal, but not in the director. The loops indicated positions in space of vertical director. When the degeneracy parameter field was lifted to a vector field, the arrows on one loop pointed upwards and on the other downwards. The loops simultaneously constituted cholesteric line singularities and nematic solitons of non-zero linking number. The second property prevented a disentanglement of the loops, although according to the cholesteric defect classification they were allowed to cross (the commutator being 1).



## § 6. Some differential geometry of defects

Whenever a homotopy group equals the additive group $Z$ of integer numbers, the corresponding singularities bear some analogy to electric charges. Actually we have already used the term 'topological charge'. Such defects are for instance vortices in superconductors, dislocations in crystals, point defects in isotropic ferromagnets or uniaxial nematic liquid crystals. Mathematically, the topological charge is the 'degree of a mapping' or a Hopf-index. The charges can be expressed as functionals of the degeneracy parameter field and therefore are denoted 'analytical topological invariants'. The analytic expressions, whose derivation is found in the textbooks on differential geometry (see, for example, Flanders, 1963)), were brought to the attention of physicists by Belavin *et al.* (1975), Blaha (1976), Volovik and Mineev (1977 a, b), de Vega (1978) and others, and are collected in § 6.1. In § 6.2 theorems of differential geometry are used to determine those defects whose presence can be enforced by boundary conditions. Finally, in § 6.3 some remarks are made on the description of many-defect systems.

### 6.1. *Analytical topological invariants*

The distorted two-dimensional ferromagnet is either described by a field $\hat{m}(\mathbf{r})=(m_1(\mathbf{r}), m_2(\mathbf{r}))$ of unit vectors, or by a complex field $\psi(\mathbf{r})=m_1(\mathbf{r})+im_2(\mathbf{r})$ of unit modulus. The angle, by which the vector moves on the unit circle when one proceeds a distance $d\mathbf{s}$ in physical space, is $d\varphi=\mathbf{a}\cdot d\mathbf{s}$, with

$$\mathbf{a}=-i\psi^*\nabla\psi=(m_1\nabla m_2-m_2\nabla m_1). \tag{6.1}$$

The expression $\mathbf{a}\cdot d\mathbf{s}$ is called the 'pullback' to real space of the volume form on the circle. In the presence of defects $\mathbf{a}\cdot d\mathbf{s}$ is not an exact differential form, since the index of the singularities enclosed by a Burgers circuit $C$ is an integral

$$n=\frac{1}{2\pi}\oint_C \mathbf{a}\cdot d\mathbf{s}, \tag{6.2}$$

that does not vanish in general. Applying Stokes' law we obtain an integral over the area $S$ enclosed by $C$ as

$$n=\int_S \mathbf{b}(\mathbf{r})\cdot d\mathbf{f}. \tag{6.3}$$

Here

$$b = \operatorname{curl} a \tag{6.4}$$

denotes an area density of point and line defects in two or three spatial dimensions, respectively.

Let us parametrize the points on a Burgers sphere $F$ as $\mathbf{r}(t_1, t_2)$. For a three-dimensional ferromagnet the corresponding surface in $V = S^2$ is then given by $\hat{m}(\mathbf{r}(t_1, t_2))$. The derivatives $\partial\hat{m}/\partial t_1$ and $\partial\hat{m}/\partial t_2$ are orthogonal to $\hat{m}$, and

$$d\Omega = \hat{m}\cdot\left(\frac{\partial\hat{m}}{\partial t_1} \times \frac{\partial\hat{m}}{\partial t_2}\right) dt_1 dt_2 \tag{6.5}$$

represents the area on the unit sphere swept by the magnetization vector, when in parameter space the rectangle of area $dt_1 dt_2$ is covered, or in physical space the area

$$d\mathbf{f} = \left(\frac{\partial\mathbf{r}}{\partial t_1} \times \frac{\partial\mathbf{r}}{\partial t_2}\right) dt_1 dt_2 \tag{6.6}$$

on the Burgers sphere. The index of the point singularities enclosed by the Burgers sphere equals the number of times which the unit sphere $V = S^2$ is swept by $\hat{m}$ as one moves once over $F$. From eqns. (6.5) and (6.6) this index follows as

$$n = \frac{1}{4\pi}\int_F d\Omega = \frac{1}{4\pi}\int_F d\mathbf{f}\cdot\mathbf{d}, \tag{6.7}$$

where

$$\mathbf{d} = \tfrac{1}{2}\varepsilon_{ijk} m_i (\nabla m_j \times \nabla m_k). \tag{6.8}$$

$\varepsilon_{ijk}$ is the completely antisymmetric third rank tensor. With Gauss' law, the index is formulated as integral over the volume $D$ bounded by $F$:

$$\left.\begin{aligned} n &= \int_D \rho(\mathbf{r}) d^3\mathbf{r}, \\ \rho(\mathbf{r}) &= \frac{1}{4\pi}\operatorname{div} d \end{aligned}\right\} \tag{6.9}$$

being a density of point singularities.

This index $n$ is identical to the degree of the mapping from the Burgers sphere to the space of degeneracy $V = S^2$ (Flanders 1963). The degree is quickly determined by the following procedure: look for the points on the Burgers sphere, where the field assumes a fixed regular value $\hat{m}_0 \in S^2$ (i.e. look for the inverse image of $\hat{m}_0$). These points, denoted by $P_l$, $l = 1, 2, \ldots$, form a finite set. To $P_l$ we assign the number $k_l = +1$ or $k_l = -1$ according to the sign of the jacobian of the mapping. To obtain this sign one chooses two non-collinear vectors $\mathbf{e}_1$, $\mathbf{e}_2$, that are tangential to the Burgers sphere and form a right-handed tripod $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ with the outer normal vector $\mathbf{e}_3$. Moving along $\mathbf{e}_1$ and $\mathbf{e}_2$, on the image sphere the corresponding vector $\hat{m}$ runs in the direction of two tangential vectors $\tilde{\mathbf{e}}_1$ and $\tilde{\mathbf{e}}_2$. Because $\hat{m}_0$ is a regular value, these are non-collinear and non-zero. The sign of the jacobian is positive if the tripod $(\tilde{\mathbf{e}}_1, \tilde{\mathbf{e}}_2, \hat{m}_0)$ is right-handed, otherwise it is negative. The index is $n = \sum_l k_l$.

Integer numbers also label non-singular textures ('configurations') of dipole-locked $^3$He-A with constant boundary conditions. The degeneracy parameter is the tripod $(\hat{e}_1, \hat{e}_2, \hat{l}=\hat{e}_3)$. $V=\mathrm{SO}(3)$ is the projective space $P^3$ (§§2.2.4 and 3.2). Since, due to the boundary conditions, physical space is equivalent to the three sphere $S^3$, the textures correspond to mappings $S^3 \to P^3$, which can be lifted to mappings $S^3 \to S^3$. The rotation describing the position of the tripod with respect to a fixed frame is either expressed by an orthogonal matrix of componetns $R_{ik}(\mathbf{r})$, or by a unit four-vector $\hat{m}(\mathbf{r})=(\omega_1 \sin\theta/2, \omega_2 \sin\theta/2, \omega_3 \sin\theta/2, \cos\theta/2)$, $\theta$ denoting the rotation angle, the unit vector $\hat{\omega}$ the rotation axis. The index $n \in \pi_3(S^3)=Z$ is the integral over the pullback of the volume form on $S^3$:

$$n=\frac{1}{(4\pi)^2}\int d^3\mathbf{r}\,\varepsilon_{\alpha\beta\gamma\delta}\varepsilon_{ijk}m_\alpha(\partial_i m_\beta)(\partial_j m_\gamma)(\partial_k m_\delta) \tag{6.10}$$

(Mineev 1980). The Greek indices run from 1 to 4. $\varepsilon_{\alpha\beta\gamma\delta}$ denotes the completely antisymmetric tensor of rank four. There is an alternative formulation by the contorsion tensor $K$ whose components are $K_{li}=\frac{1}{2}\varepsilon_{ijk}R_{jq}\partial_l R_{kq}$ (Nye 1953, Kröner 1960). The change $d\mathbf{b}$ of a vector $\mathbf{b}$, which moves with the tripod along a distance $d\mathbf{s}$, is $d\mathbf{b}=\mathbf{\Omega}\times\mathbf{b}$; the components of $\mathbf{\Omega}$ are $\Omega_i=ds_l K_{li}$. In terms of the contorsion tensor, the index is

$$n=\frac{1}{(4\pi)^2}\int d^3\mathbf{r}\,\det K \tag{6.11}$$

(Trebin 1981 b). Yet another expression is

$$n=\frac{1}{(4\pi)^2}\int d^3\mathbf{r}\,\mathbf{v}\cdot\mathrm{curl}\,\mathbf{v}. \tag{6.12}$$

The components of $\mathbf{v}$ are

$$v_i=\hat{e}_1\cdot\partial_i\hat{e}_2 \tag{6.13}$$

$\mathbf{v}$ and $\hat{l}$ are related by the equation

$$\mathrm{curl}\,\mathbf{v}=\tfrac{1}{2}\varepsilon_{ijk}l_i(\nabla l_j\times\nabla l_k) \tag{6.14}$$

(Kléman 1973, Mermin and Ho 1976).

Configurations of unit vector fields also carry an integer number, known as the Hopf-index, since $\pi_3(S^2)=Z$. Examples for such configurations are presented by Shankar (1977) and Michel (1980). The Hopf-index of a vector field $\hat{l}$ is given by eqns. (6.12) and (6.14), by the linking number (§5.2), or by the integral

$$n=\frac{1}{4\pi}\int_F d\mathbf{f}\cdot\mathrm{curl}\,\mathbf{v}=\frac{1}{4\pi}\int_C d\mathbf{s}\cdot\mathbf{v} \tag{6.15}$$

$C$ is the loop where the field values equal a fixed vector $\hat{l}_0 \in S^2$, $F$ a surface bounded by $C$.

### 6.2. *Boundary conditions enforcing defects*

In §4.3 those defects which possibly exist on a surface were classified. However, global properties of a surface often make the presence of singularities necessary. Surface defects of a unit vector (or director) field of tangential boundary conditions are labelled by an index (winding number, §4.3), if we do not care about their continuation to the bulk. For a compact, connected, two-sided surface the sum of the indices equals the Euler characteristic $\chi$, according to the Poincaré theorem. By covering the surface with a network of polygons and counting the number $V$ of vertices, $E$ of edges and $F$ of faces, the Euler characteristic is found to be $\chi = V - E + F$, independent of the particular network. $\chi$ is also determined by examination of the unit vector field $\hat{\mathbf{v}}(\mathbf{r})$ of the outer normals of the surface. The gaussian curvature (the product of the inverse main curvature radii) at a point on the surface is

$$k = \hat{v}\cdot\{\tfrac{1}{2}\varepsilon_{ijk}v_i(\nabla v_j \times \nabla v_k)\}. \tag{6.16}$$

According to the Gauss–Bonnet theorem, the total curvature is

$$\int df k = \int d\mathbf{f}\cdot\{\tfrac{1}{2}\varepsilon_{ijk}v_i(\nabla v_j \times \nabla v_k)\} = 2\pi\chi. \tag{6.17}$$

The compact surfaces are topologically equivalent to spheres with $s$ handles. $s$ is the genus of the surface, and $\chi = 2(1-s)$. A sphere has Euler characteristic $\chi = 2$, a torus $\chi = 0$

Tangential (or conical) boundary conditions are realized, for example, for nematic spherulites suspended in an isotropic liquid. On energetical grounds Dubois-Violette and Parodi (1969) argued that of the two quanta of vorticity one should rest on the north pole, the other on the south pole of the droplet, the nematic field lines running along the meridians. The texture, named 'onion skin', requires no further singularities in the bulk. It has been observed by Candau *et al.* (1973). The tangential field $(\hat{e}_1, \hat{e}_2)$ in $^3$He-A has been discussed by Mermin (1977 a, b: there Euler characteristic and Poincaré theorem are illustrated in detail) and by Anderson and Palmer (1977). On a spherical surface—the $\hat{l}$-vector standing parallel to the normal—the two quanta are supposed to be concentrated in one singular point of vorticity $4\pi$, which is the boojum mentioned in §4.3.

Non-singular degeneracy parameter fields on the boundary decide which defects must exist in the bulk. The boundary field on a sphere, representing an element of the second homotopy group, determines the total index of point singularities inside. In the case of homeotropic (i.e. perpendicular) boundary conditions for a ferromagnet, on a surface the normed magnetization vector is identical to the normal. Comparison of eqn. (6.7), (6.8) and (6.17) yields $n = \frac{1}{2}\chi$ for the sum of indices of point defects in the bulk (Stein 1979 b, Mineev 1980). Hedgehog point singularities in nematic droplets were actually seen by Meyer (1972) and others.

When $^3$He-A is enclosed in a spherical vessel, and $\hat{l}$ points radially outward, a point singularity in $\hat{l}$ of index 1 is expected in the volume, the vorton of Blaha (1976). As discussed in §4.4.2 it is the terminating point of a $4\pi$-vortex in the field $(\hat{e}_1, \hat{e}_2)$. Here, as in other cases, it is energetically favourable for the vorton to move to the surface and form a boojum connected to a non-singular bulk texture. A vorton-like structure appears in cholesteric droplets, the pitch axis corresponding to the $\hat{l}$-vector. Here the point singularity in the pitch stays in the centre of the spherulite and is attached to the surface by a $4\pi$-vortex in the director and binormal. The structure is known as 'Frank-Pryce texture' and was observed by Robinson *et al.* (1958) and Candau *et al.* (1973).

### 6.3. *Many-defect systems.*

We return to the description of the two-dimensional ferromagnet by a unimodular complex field $\psi(\mathbf{r})$ (§6.1), and perform a gauge transformation on $\psi$ by locally chaning the phase: $\psi(\mathbf{r})\to\psi(\mathbf{r})\exp i\chi(\mathbf{r})$. Then $\mathbf{a}$ turns into $\mathbf{a}+\nabla\chi$, but the vortex density $\mathbf{b}=\operatorname{curl}\mathbf{a}$ remains gauge-invariant. $\mathbf{b}$ is also subject to the conservation law $\operatorname{div}\mathbf{b}=0$, expressing the fact that the number of vortices moving into a finite volume is the same as that moving out, or, equivalently, that vortex lines cannot terminate in the volume. If $\psi$ is time-dependent, in addition to the 'vector-potential' $\mathbf{a}$ a 'scalar potential' $u=+i\psi^*\partial_t\psi$, and an 'electric' field $\mathbf{e}=-\partial_t\mathbf{a}-\nabla u$ is introduced. The fields $\mathbf{b}$ and $\mathbf{e}$ are invariant under the gauge transformation $\psi(\mathbf{r},t)\to\psi(\mathbf{r},t)\exp i\chi(\mathbf{r},t)$, implying the transitions $\mathbf{a}\to\mathbf{a}+\nabla\chi$, $u\to u-\partial_t\chi$. They satisfy the homogeneous Maxwell equations

$$\operatorname{div}\mathbf{b}=0,\qquad \partial_t\mathbf{b}+\operatorname{curl}\mathbf{e}=0, \tag{6.18}$$

which express that as much electromagnetic flux moves into a three-dimensional hypersurface of spacetime as moves out. The change of the phase of $\psi$ can be interpreted as local action of the 'gauge-group' U(1) on the degeneracy parameter.

Equations (6.7)–(6.9), too, lead to a conservation law. In addition to the vector field $\mathbf{d}$, which resembles a dielectric displacement, a field $\mathbf{h}$ of components $h_k=\hat{m}\cdot(\partial_t\hat{m}\times\partial_k\hat{m})$, $k=x,y,z$ can be defined, and in addition to the point defect density $\rho=\operatorname{div}\mathbf{d}/4\pi$ a current

$$\mathbf{j}=\frac{1}{4\pi}(\operatorname{curl}\mathbf{h}-\partial_t\mathbf{d}). \tag{6.19}$$

From these inhomogeneous Maxwell-type equations, which relate fields and currents, a continuity equation

$$\partial_t\rho+\operatorname{div}\mathbf{j}=0 \tag{6.20}$$

is derived. Although $\rho$ and $\mathbf{j}$ remain invariant under the transformations $\mathbf{d}\to\mathbf{d}+\operatorname{curl}\mathbf{v}$, $\mathbf{h}\to\mathbf{h}+\partial_t\mathbf{v}$, these are not caused by an action of a gauge group. Therefore $\rho$ and $\mathbf{j}$ are denoted 'gauge-like' variables (Julia and Toulouse 1979).

In both cases the analytical topological invariants gave rise to densities and currents of vortices and point defects, which obey conservation laws and thus represent reasonable physical quantities for the description of many-defect systems.

In the case of line defects in dipole-locked $^3$He-A (and also multisublattice ferromagnets like $UO_2$, see, for example, Dzyaloshinskii (1977)), there is no arithmetic addition law for singularities, since $\pi_1(SO(3))=Z_2$, hence also no prescription of how to express defect densities.

Dzyaloshinskii and Volovik (1978, 1980) referred to the property of the density $\mathbf{b}$ as gauge-invariant quantity and proposed the use of gauge fields for defect densities in those cases where analytical topological invariants are not available. The distortion $\mathbf{a}$ has components valued in the Lie-algebra of U(1), which is the set of real numbers. As distortion for tripod fields a vector field $\mathbf{A}$ is taken valued in the Lie-Algebra of SO(3). Its components are the antisymmetric matrices $A_i=-K_{ij}L_j$. Here $K$ denotes the contorsion tensor (§6.1), $L_j$ the matrices generating the Lie algebra of SO(3), of components $[L_j]_{mn}=-\varepsilon_{jmn}$. They coincide with the $l=1$ angular momentum operators in a cartesian basis. A gauge transformation performs a local rotation of the tripods by a field $g$ of orthonormal matrices: $\hat{e}_k(\mathbf{r})$

$\to g(\mathbf{r})\hat{e}_k(\mathbf{r})$. Then $\mathbf{A}$ turns into $g\mathbf{A}g^{-1} + g\nabla g^{-1}$. The gauge field corresponding to $\mathbf{b}$ is

$$\mathbf{B} = \text{curl}\,\mathbf{A} + \mathbf{A} \times \mathbf{A}. \tag{6.21}$$

In the gauge-transformation $\mathbf{B}$ is invariant up to local conjugation: $\mathbf{B} \to g\mathbf{B}g^{-1}$ (compare $\mathbf{b} \to (\exp + i\chi)\ \mathbf{b}\ (\exp - i\chi)$), which is of no influence, since the energy functionals containing $\mathbf{B}$ are local-invariant to rotations. $\mathbf{B}$ is applied as measure for disclination densities. Together with $\mathbf{A}$ a covariant derivative $\nabla_{\mathbf{A}} = \nabla + \mathbf{A}$ is defined, that makes the tripods appear parallel: $\nabla_{\mathbf{A}}\hat{e}_k = 0$. The components of the corresponding curvature tensor are $R_{ijkl} = \varepsilon_{ijm}[B_m]_{kl}$. So disclination densities may be interpreted as curvature. If we define a 'scalar potential' $U = -A_t = -K_{tj}L_j$, a disclination current is given by

$$\mathbf{E} = -\partial_t \mathbf{A} - \nabla U + [U, \mathbf{A}], \tag{6.22}$$

the bracket denoting the matrix commutator. $\mathbf{E}$ and $\mathbf{B}$ satisfy Young–Mills field equations or Bianchi-identities:

$$\left.\begin{aligned} \text{div}\,\mathbf{B} + \frac{1}{2}\sum_{i=1}^{3} [A_i, B_i] = 0, \\ \partial_t \mathbf{B} + \text{curl}\,\mathbf{E} - \tfrac{1}{2}[\mathrm{U}, \mathbf{B}] + \tfrac{1}{2}\{\mathbf{A} \times \mathbf{E} + \mathbf{E} \times \mathbf{A}\} = 0. \end{aligned}\right\} \tag{6.23}$$

Though there is no invariance under arbitrary continuous deformations, the choice of $\mathbf{B}$ as measure for disclination densities is justified by the gauge-invariance (up to local conjugation), but also by results of hydrodynamic theories on spin waves in the presence of disclination lines. If these lines are fixed (like an external field), the currents $\mathbf{E}$ vanish (Volovik and Dzyaloshinskii 1978, Dzyaloshinskii and Volovik 1980).

Note that for stable configurations of tripod fields, labelled by elements of $\pi_3(\mathrm{SO}(3)) = Z$, analytical topological invariants again do exist (eqn. (6.11)), from which densities and currents are derived (Dzyaloshinskii 1981).

Media, whose degeneracy parameter is acted on by SO(3), in general are also characterized by a non-trivial symmetry group $H$. For uniaxial nematic liquid crystals Dzyaloshinskii (1981) has taken care of this fact by declaring the gauge potentials involved in rotations about the director axes inefficient in the free-energy and in hydrodynamic equations. The symmetry group already bears information on certain phenomena appearing in two-defect interactions, like the topological obstruction for crossing of defects. There are still no hints how these two-body effects can be incorporated into a many-defect picture (Julia and Toulouse 1979), so that the expected topological rigidity finds expression in equations of motion.

When line singularities are brought into a system of point singularities of a uniaxial nematic liquid crystal, the conservation of the topological charge is broken (§4.1.1). The classifying second homotopy group $\pi_2(P^2) = Z$ must then be replaced by the orbit group $\pi_2(P^2)/D_2 = Z_2$ (§4.1.2), which does not provide analytical topological invariants any more.

Gauge concepts were also recently applied to the study of many-defect systems in crystals (Kadić and Edelen 1982), a subject of long and successful history (Kröner 1960, Anthony 1970). By use of $\mathrm{E}_0(3) = \mathrm{T}(3) \wedge \mathrm{SO}(3)$ as gauge group, the gauge fields arising from the action of SO(3) were recognized as coupled disclination and dislocation densities, those from the action of T(3) as pure dislocation densities.

## § 7. Defects in systems of broken translational symmetry

For the investigation of defects in crystals modern methods of mathematical physics have been employed, like non-riemannian differential geometry (Bilby *et al.* 1955, Kröner 1960), quantum field theory (Wadati *et al.* 1978) and gauge theory (Kadić and Edelen 1982, Edelen 1982). Crystals are also the first condensed matter systems to which homotopy theory was applied, but this application has been controversial ever since. Finkelstein (1966) described a deformed crystal as a field of local distortion tensors. These are $3\times 3$-matrices of positive determinant forming the group $\mathrm{GL}_+(3,R)$. Since $\pi_3(\mathrm{GL}_+(3,R))=Z$, Finkelstein assumed topologically stable configurations to exist in crystals, but cautiously mentioned that the distortion tensors must satisfy compatibility conditions. These indeed prevent the existence of kinks (§ 7.2). Rogula (1976) was the first to classify point and line singularities in ferromagnets and crystals by homotopic methods. As an unbroken symmetry group, he used the group Aff(3) of affine transformations of three-space. But Aff(3) is not the invariance group of the bulk free-energy. Its elements even transform one Bravais lattice into any other. Consequently Rogula discovered, in addition to dislocations and disclinations, also 'shear-type' defect lines. Classifying crystal defects by the homotopy groups of a 'space of Bravais lattices' instead of a space of degeneracy violates the assumptions of the London limit as reported in § 2.1. Therefore Rogula's theory was opposed by Michel (1978, 1980), and replaced by a version (Kléman *et al.* 1977) that is based on the euclidean group as an unbroken symmetry group (§ 7.1). This theory, in turn, was criticized by Mermin (1979), who claimed that fields in the degeneracy parameter involving translational elements are not only required to be continuous, but, rather, that values at a point be related to those in the neighbourhood by non-locality conditions yet to be specified. In § 7.2 Mermin's objections are materialized and some suggestions are provided on how to incorporate the additional requirements into homotopy theory.

### 7.1. *Defects in crystals*

#### 7.1.1. *Dislocations only*

First, we restrict ourselves to translational displacements within a crystal, the orientations of the crystal axes remaining fixed. In three spatial dimensions the unbroken symmetry group is the group T(3) of pure translations. As isotropy group serves the group of discrete translations, isomorphic to $Z^3$. As already indicated in § 2.2.5, the space of degeneracy, $V=\mathrm{T}(3)/Z^3$, is the three-dimensional torus $T^3=S^1\times S^1\times S^1$, of fundamental group $\pi_1(T^3)=Z^3$. Each element $(l,m,n)\in\pi_1(T^3)$ corresponds to a vector $\mathbf{b}=l\mathbf{a}_1+m\mathbf{a}_2+n\mathbf{a}_3$ of the Bravais lattice, where $(\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3)$ denotes the set of primitive lattice vectors. Vector $\mathbf{b}$ is the familiar Burgers vector describing the closure failure of the path accompanying a Burgers circuit in an undistorted Bravais lattice. No referral is made to the orientation of $\mathbf{b}$ with respect to the direction $\hat{d}$ of the dislocation line. Hence edge ($\mathbf{b}\perp\hat{d}$) and screw ($\mathbf{b}\|\hat{d}$) dislocations of the same Burgers vector are topologically equivalent, and indeed, one can be deformed continuously into the other (Mermin 1979). Since $\pi_2(T^3)=\pi_3(T^3)=0$, stable point singularities and configurations are not predicted for this special case.

#### 7.1.2. *All defect types*

If the orientation of the crystal axes is allowed to vary in space, in $d$ dimensions the full euclidean group $\mathrm{E}(d)$ has to be taken as an unbroken symmetry group.

According to the discussion of § 2.2.5, the space of degeneracy is $V=\mathrm{E}(d)/H$, $H$ denoting the discrete space group of the crystal under consideration.

Here for the first time we meet wall defects in three-space. Denote by $H'=H\cap E_0$ the set of elements of $H$ not containing reflections. If $H=H'$, the crystal differs from its mirror image, and $\pi_0(\mathrm{E}(3)/H)=Z_2$. Stable planar singularities exist, forming twin boundaries.

Since $H$ is discrete, there are no topologically stable point singularities (§ 3.3.3). The fundamental group $\pi_1(V)$ is equal to the lift $\bar{H}'=\varphi^{-1}(H')$ of $H'$ into the universal covering group $\bar{\mathrm{E}}_0(d)$ of $\mathrm{E}_0(d)$. In two and three dimensions we obtain: $\bar{\mathrm{E}}_0(2)=\mathrm{T}(2)\wedge\mathrm{T}(1)$, $\bar{\mathrm{E}}_0(3)=\mathrm{T}(3)\wedge\mathrm{SU}(2)$.

Hence in three-space, the line singularities are labelled by the conjugation classes of $\bar{H}'$. This group is generated by translations, rotations and screw displacements. After encircling the defect line, the accompanying reference crystal is either translated by a lattice (Burgers) vector, or rotated by a discrete angle $\theta$, $0\leqslant\theta<4\pi$, or rotated in combination with a translation along a non-primitive lattice vector. The corresponding singularities are the dislocations, disclinations and dispirations (Harris 1970).

Let us investigate the triangular plane lattice of sixfold rotational symmetry. The group $\bar{H}'$ is isomorphic to $(Z\times Z)\wedge Z$. An element $(n,m)\in Z\times Z$ marks a translation by the vector $t=n+\omega m$, $\omega=\exp(i\pi/3)$, if we describe two-dimensional vectors by points in the complex plane. An element $r\in Z$ labels a rotation by $r\cdot 60°$, of fractional winding number $r/6$. The multiplication law is given by $\{t_1|r_1\}\{t_2|r_2\}=\{t_1+\omega^{r_1}t_2|r_1+r_2\}$, and the conjugate of an element by

$$\{t_2|r_2\}\{t_1|r_1\}\{t_2|r_2\}^{-1}=\{(1-\omega^{r_1})t_2+\omega^{r_2}t_1|r_1\}. \qquad (7.1)$$

The conjugation class of $\{t|r\}$ has the form $\{T|r\}:=\{\{t'|r\}|t'\in T\}$, where $T$ denotes a subset of the Bravais lattice points. A pure dislocation is labelled by the conjugation class $\{T|0\}$ of an element $\{t|0\}$. Here $T$ is the star $\{\omega^r t|0\leqslant r\leqslant 5\}$ of the Burgers vector $t$, since, on guiding the dislocation about a disclination, the Burgers vector changes direction by a crystallographic rotation. A pure disclination corresponds to the conjugation class $\{T|r\}$ of an element $\{0|r\}$. For $r=1$ and 5, $T$ is the entire Bravais lattice, for $r=2$ and 4 one-third of it (spanned by $1+\omega$ and $1-\omega$), for $r=3$ the quarter lattice spanned by 2 and $2\omega$. The elements $t\in T$, in the case of pure disclinations, have the form $(1-\omega^r)t'$, where lattice vector $t'$ is the position of the disclination core with respect to the origin, about which the rotations of the reference crystal are performed. Two disclinations of indices $r$ and $-r$, and separated by the vector $t'$, are equivalent to a single dislocation of Burgers vector in the star of $t$. Such a dislocation can decay into two disclinations. This decay is of importance in the theory of defect-mediated two-dimensional melting (Halperin and Nelson 1978). The transition from the hexatic phase, which contains many free disclocations and possesses bond-orientational order only, to the isotropic phase is due to the liberation of bound disclination pairs.

For the triangular lattice the commutator subgroup is the translational subgroup $Z\times Z$, and the homology group is isomorphic to the point group of the lattice. Disclinations in the hexagonal lattice of vortex lines of a type II superconductor have been observed by Träuble and Essmann (1968).

As seen by the example, the fundamental group is non-abelian even for very simple crystal structures, and characteristic features are expected to occur in defect processes. Some, such as the rotation of the Burgers vector of a dislocation moved about a disclination line, or the ambiguities in defect combinations, have been pointed out prior to the discovery of the homotopic defect classification. Others, like locks of partial dislocations and disclinations, which remind of the topological obstructions for the crossing of line singularities, still wait for an explanation or refutation by the homotopy scheme. Illustrative presentations on the subject of disclinations and related phenomena are provided by Harris (1977), Kröner and Anthony (1975), de Wit (1973) and Nabarro (1967, chapter 3.1).

For all crystallographic groups H the third homotopy group $\pi_3(\mathrm{E}(3)/H)$ equals the set of integers (Bott 1954). Just as Finkelstein (1966), who started from $\mathrm{GL}_+(3, R)$ as the space of degeneracy, we expect non-trivial configurations to exist in crystals.

The description of the non-uniform crystal as a field valued in $\mathrm{GL}_+(3, R)$ or $\mathrm{E}(3)/H$, however, contains redundant information. These spaces are of dimension nine and six, respectively, whereas a crystal is well characterized by a three-dimensional displacement field in simply connected regions outside the singularities. Hence, to remove the redundance, the fields must be subjected to certain restrictions, which may necessitate severe modifications of the classification scheme as developed above.

### 7.2. *Restricted homotopies*

Mermin's criticism (1979) of the generalization of the homotopic defect classification to systems of broken translational symmetry essentially contains three points. First it is questioned that a uniform system can be adjusted uniquely to the distorted structure. Second, the incorporation of restrictive conditions for the degeneracy parameter fields is assumed to prevent the realization of entire defect classes predicted by homotopy theory. And third, even if such classes are realizable, it is doubted whether all defects within the class can be deformed into one another by interpolating fields that satisfy the conditions: defect classes are supposed to split.

#### 7.2.1. *The adjustment process*

Even a weak deformation of a crystal affects the unit cell. So in adjusting the uniform crystal to the local structure of the distorted crystal a rigid body operation will hardly be sufficient. Rather, shear and compression must also be applied. But then the operations along the Burgers circuit about the singular line do not form a loop in the homogeneous space $\mathrm{E}(d)/H$ but in $\mathrm{Aff}(d)/H$, where $\mathrm{Aff}(d)$ is the group of affine transformations of the euclidean space. An element of $\mathrm{Aff}(d)$ consists of a translation and a distortion expressed by a $d \times d$-matrix of non-zero determinant. Any loop in $\mathrm{Aff}(d)/H$ can be represented as a path in $\mathrm{Aff}(d)$, which, after suitable multiplication from the right by an element $a \in \mathrm{Aff}(d)$, starts at an element of $H$ and terminates at the identity. In Appendix 2 it is demonstrated, how, fixing starting and terminating point, such a path is continuously deformed into one resting in $\mathrm{E}(d)$. Simultaneously the loop in $\mathrm{Aff}(d)/H$ is continuously deformed into a loop in $\mathrm{E}(d)/H$. Hence $\pi_1(\mathrm{Aff}(d)/H) = \pi_1(\mathrm{E}(d)/H)$, and the use of $V = \mathrm{E}(d)/H$ as space of degeneracy is justified. Note that in contrast to Rogula's procedure (1976), $H$ is still the isotropy group of the uniform crystal in $\mathrm{E}(d)$, and not in $\mathrm{Aff}(d)$. As mentioned by Kléman *et al.* (1977), a theorem of Stewart (1960) allows the proof that even $\pi_1(\mathrm{Diff}(d)/H) = \pi_1(\mathrm{E}(d)/H)$, where $\mathrm{Diff}(d)$ is the group of differentiable deformations of euclidean $d$-space.

7.2.2. *Existence of singular fields*

Let $\mathbf{r}$ be the radius vector of a point $P$ in the distorted crystal, and $g(\mathbf{r}) = \{\mathbf{t}(\mathbf{r})|R(\mathbf{r})\} \in E(d)$ the operation adjusting the uniform reference crystal to the local structure of $\mathbf{r}$. Then the point in the uniform crystal corresponding to $P$ has the radius vector $\mathbf{v} = g^{-1}(\mathbf{r})\mathbf{r} = R^{-1}(\mathbf{r})\cdot(\mathbf{r}-\mathbf{t})$. The jacobian of the vector function $\mathbf{v}(\mathbf{r})$ must be equal to the rotational part $R^{-1}$ of the rigid motion $g^{-1}$, up to a dilatation:

$$(\partial_1\mathbf{v}, \partial_2\mathbf{v}, \partial_3\mathbf{v}) = \Lambda R^{-1}, \tag{7.2}$$

where $\Lambda$ is a positive definite diagonal matrix. From this requirement follows an interdependence of rotational and translational field:

$$\partial_i\mathbf{t} = (R\partial_i R^{-1})\cdot(\mathbf{r}-\mathbf{t}) - R(\Lambda - 1)R^{-1}\cdot\hat{e}_i \tag{7.3}$$

(Kutka and Trebin 1982). The consequences of the non-locality condition (7.3) have not yet been fully explored, and we shall make no use of it. Instead, a model description for layers and crystals is introduced which contains some of the properties of fields valued in $E(d)/H$, and points out possible restrictions and their impact on the homotopic classification. Thereby we shall concentrate on disclinations and configurations.

A layered system (of codimension 1) is described by a smooth scalar function $f$ defined everywhere in space. A layer consists of the points where $f(\mathbf{r})$ is constant. Disclinations are defects in the normal field $\nabla f/\|\nabla f\|$ of the layers, and occupy the sites where $\nabla f$ vanishes (the 'singularities' of $f$). Hence the study of disclinations of layered systems is replaced by the investigation of zeros of vector fields that are gradients and as such irrotational.

The number of layers traversed by a closed loop $C$,

$$\oint_C \nabla f\cdot d\mathbf{s} = \oint_C df, \tag{7.4}$$

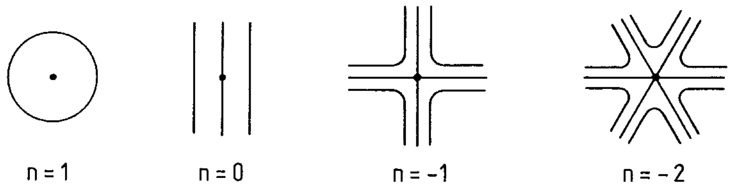
vanishes, which guarantees that no extra layers terminate in the volume. Thus the integrability condition for absence of dislocations is satisfied. Moreover, the model contains a regularity condition assuring that close to the singularity the layer separation, proportional to $1/\|\nabla f\|$, does not become arbitrarily small.

As for unit vector fields, in two spatial dimensions the homotopic defect classification predicts disclinations for any winding number, since $\pi_1(S^1) = Z$. In three dimensions, point singularities and configurations are expected to exist for any integer index, since $\pi_2(S^2) = \pi_3(S^2) = Z$.

For layered systems in two dimensions (the striped plane) it was suspected by Mermin (1979) and proved rigorously by Poénaru (1981), that—within the present model—disclinations of winding number larger than 1 do not exist. This statement becomes intelligible by the following consideration: let us move the (isolated) singularity of $f$ to the origin and adjust $f$ by a constant such that $f(\mathbf{0}) = 0$. In a small neighbourhood of the origin the layer $f(\mathbf{r}) = 0$ then either forms a single point, or an even number $q(\geqslant 0)$ of rays emanating from the origin (fig. 31). As is quickly checked, the winding number of the gradient field is $n = 1 - q/2 \leqslant 1$. Note that in the excluded case of $n = 2$ (fig. 6, p. 208, the field lines can be seen as layers), the stripes touch each other at the origin.

We describe two-dimensional crystals by two layer systems in the plane. The corresponding two scalar functions, $f_1$ and $f_2$, if viewed as components of a vector function $\mathbf{f}$, define a mapping from the plane to the plane. Disclinations are those

Fig. 31




Possible layer structures near a singular point in the striped plane, illustrating Poénaru's theorem.



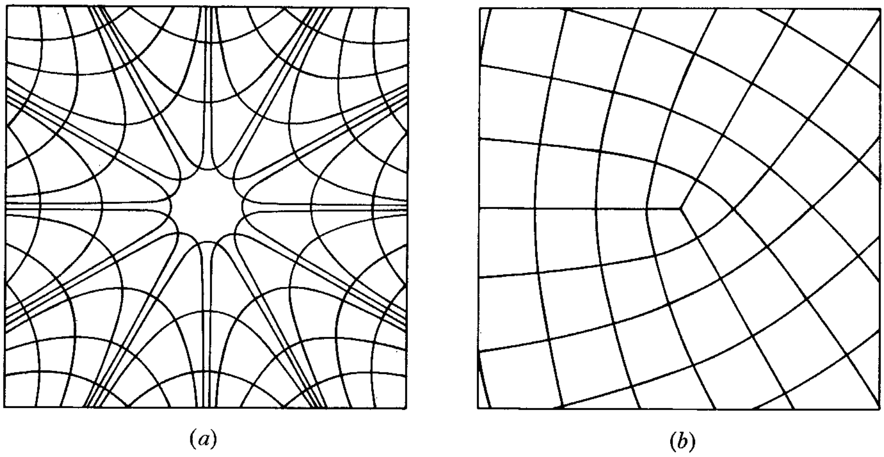
isolated points where the jacobian of $\mathbf{f}$ is zero. Therefore outside the singularities $\nabla f_1$ and $\nabla f_2$ do not vanish, and the layers always intersect at a finite angle ($\nabla f_1$ is not collinear to $\nabla f_2$). The two vectors reciprocal to $(\nabla f_1, \nabla f_2)$ comprise the distorted lattice vectors. The disclinations are labelled by the winding number of the field of lattice vectors or layer normals. Owing to Poénaru's theorem, this number is less or equal to 1. However, $n=1$ also is not allowed due to the following observation: for $n=1$ the layers of one system, say $f_1$, form concentric circles close to the singularity. But the projection of $\nabla f_2$ onto these circles ought to form closed field lines, which is not possible for a gradient field.

Placing the crystal into the complex plane $C$, we can express the mapping $\mathbf{f}$ by a complex function of a complex variable. For example polynomials $w=z^k$, $z \in C$, with integer $k>0$ describe distorted quadratic crystals. The layers are the lines of constant real and imaginary part of $w$. The winding number is equal to $n=1-k<1$ (see fig. 32 (*a*) for the case $k=3$).

Until now we have considered only well-oriented layers and crystals, with disclinations of integer winding numbers. But, for the system of stripes and for two-dimensional crystals of $q$-fold rotational symmetry, indices occur, that are multiples of $\frac{1}{2}$ or $1/q$, respectively. An example of a 'Moebius-crystal' of winding number $n=\frac{1}{4}$, described by the function $w=z^{3/4}$, is depicted in fig. 32 (*b*). One layer system goes over into the other. We obtain an oriented system if we lift the crystal to the riemannian surface of the multivalued function $z^{1/4}$. The winding number $m$ on this surface is the same as that of a crystal obtained if we squeeze the Moebius crystal into a section of $360°/q$ of the complex plane, and fill the rest of the plane with identical sections (this crystal is described in our example by $w=z^3$, fig. 32 (*a*)). The relation between the winding number $n$ of the Moebius crystal and $m$ of the lifted crystal is (compare the exponents of $z$ in our example) $1-m=q(1-n)$, or $n=(m-1)/q+1$. For stripes, where $m \leqslant 1$, $q=2$, we find $n \leqslant 1$, for crystals, where $m<1$ and $q>0$, the indices are restricted to $n<1-1/q<1$. This result holds true also for crystals on simply connected surfaces. Note that the sign of the winding number here is different from the convention of Nabarro (1967).

Three-dimensional distorted crystals are described by three scalar functions $(f_1, f_2, f_3)$, mapping three-space on itself. For configurations this mapping is regular (of non-zero jacobian) everywhere, and is the identity mapping outside a solid three-dimensional ball. It was pointed out by Gunn and Ma (1980) that the compatibility conditions for the absence of dislocations require Finkelstein's distortion tensor field to be derived from such a mapping: the tensor at $\mathbf{r}$ transforms a triple of undistorted primitive lattice vectors into a distorted one which is the triple reciprocal to $(\nabla f_1, \nabla f_2, \nabla f_3)$. Now from several mathematical theorems, cited in Appendix 3, it is

Fig. 32



Distorted square crystal, whose lattice planes are described by Re $w$ = const and Im $w$ = const of a complex function $w = z^k$: (*a*) $k = 3$, winding number $m = 1 - k = -2$; (*b*) $k = \frac{3}{4}$, winding number $n = 1 - k = \frac{1}{4}$.

derived that a continuous family of differentiable vector-functions $\mathbf{f}_t$, $0 \leqslant t \leqslant 1$, exists, each member having the same properties as $\mathbf{f}$, such that $\mathbf{f}_0 = \mathbf{f}$, and $\mathbf{f}_1$ is equal to the identity mapping. Thus any configuration of a crystal can be deformed continuously to the uniform state and is therefore unstable. Also in Appendix 3 it is proved that stable configurations of layer systems in three-space do not exist.

These examples confirm Mermin's conjecture that non-locality and compatibility conditions prohibit the existence of singularities which homotopy theory predicts. This is, however, not true for all types of singularities. In three-space point disclinations of single layer systems exist for any index. To construct the corresponding scalar function one starts from a system of stripes in two dimensions, described by a function $f(x, y)$ with an isolated singularity at the origin of index $n$. The function is extended to three dimensions by forming $F_{\pm} = f(x, y) \pm \frac{1}{2} z^2$. Inspection of the normal field $\nabla F_{\pm} / \| \nabla F_{\pm} \|$ according to the rules of § 6.1 reveals that the singularity of $\nabla F_+$ is of index $n$, that of $\nabla F_-$ of index $-n$. Since $n$ can be any integer not larger than 1, point disclinations for all integer indices are realized in three-space. Examples are provided by the two-dimensional sink and source, characterized by scalar functions $f_1(x, y) = -\frac{1}{2}(x^2 + y^2)$ and $f_2(x, y) = \frac{1}{2}(x^2 + y^2)$, both of winding number $n = 1$. Upon extension to three dimensions these describe the vector fields $\nabla F_1$ of the hyperbolic point and $\nabla F_2$ of the hedgehog (fig. 8, p. 209), where $F_1(x, y, z) = \frac{1}{2}(z^2 - x^2 - y^2)$ and $F_2(x, y, z) = \frac{1}{2}(z^2 + x^2 + y^2)$. Without restrictions, these singularities are equivalent (see fig. 8 for the homotopy). But, as shown in the next section, under the integrability conditions they are topologically distinct.

### 7.2.3. *Equivalence of defects*

According to our original definition, two singularities are equivalent if the loops (surfaces) in the space of degeneracy, which correspond to the Burgers circuits (spheres) in physical space, are freely homotopic. When degeneracy parameter fields are restricted, it is required, in addition, that the homotopy can be spread out in space (the core of one defect being replaced by the core of the other) such that outside the singularity the non-locality condition is satisfied. That no gradient field exists interpolating between hyperbolic and radial point, has already be seen in fig. 8: the vector field has a closed field line. For a general proof of this statement assume that the field of the hyperbolic point prevails inside a sphere of radius $R_0$ about the origin, that of the radial point outside a sphere of radius $R_1$. Now enclose the field in a ball of radius $R_2 > R_1$ and wrap this ball about the three-sphere $S^3$ (just as a two-dimensional disk is wrapped about the two-sphere) so that the origin touches the south pole, and all the points on the surface meet at the north pole. Since there is a maximum at the north pole, there must be a minimum at the south pole, in contradiction to our assumption that there is already a hyperbolic (saddle) point. Hence the two singularities, although of the same homotopy index, are not equivalent. The example displays that for gradient fields there must be a second topological quantum number distinguishing the singularities of index $n=1$. This additional label is the Morse-index. It counts the minus signs of the polynomials $F_1$ and $F_2$ and is 2 for $F_1$, 0 for $F_2$.

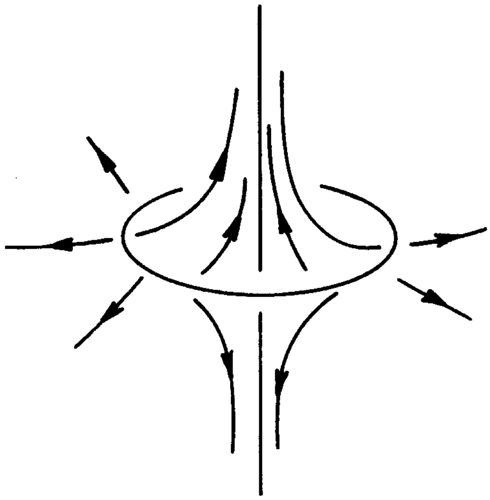
Morse-singularities are the zeros of a scalar function, that, in a suitable coordinate system in the neighbourhood of the singularity, can be written as polynomial $k_1x^2+k_2y^2+k_3z^3$, $k_1, k_2, k_3 \in \{\pm 1\}$. If it is possible to place several Morse-singularities on a compact manifold, as in the above example, the sum of their homotopy indices equals the Euler characteristic, according to the Poincaré theorem (§ 6.2). But the Morse-inequalities must also be satisfied: these relate the numbers $C_m$ of singularities of Morse-index $m$ to the Euler characteristic $\chi$ and the Betti numbers $R_m$ of the $d$-dimensional manifold (Milnor 1963):

$$\left.\begin{array}{l} C_0 - C_1 + C_2 - \ldots \pm C_d = \chi, \\ \left.\begin{array}{l} C_m \geqslant R_m, \\ C_m - C_{m-1} + \ldots \pm C_0 \geqslant R_m - R_{m-1} + \ldots \pm R_0 \end{array}\right\} \quad m=0,1,\ldots,d \end{array}\right\} \tag{7.5}$$

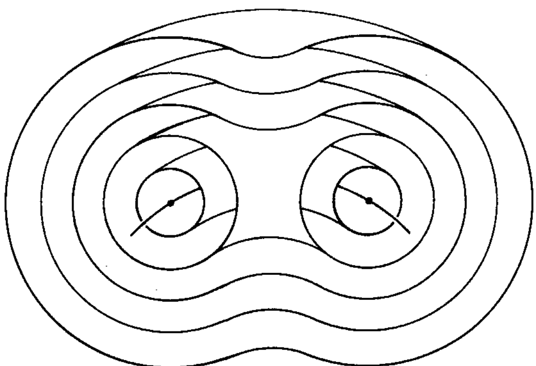
For $S^3$ we have: $\chi=0$, $R_0=R_3=1$, $R_1=R_2=0$. From these equations it follows that the above maximum and saddle point can exist on the three-sphere in the presence of either an additional maximum and minimum, or an additional minimum and saddle point of type $\frac{1}{2}(x^2+y^2-z^2)$. These extra defects of opposite charge can also be smeared out into a ring of vanishing charge from which the field lines emanate perpendicularly (fig. 33). If by a slight deformation the corresponding layers are made equidistant, an unstable defect line arises along the $z$-axis (fig. 34). The resulting structure is a special case of a focal conic texture (Bouligand 1972), where the ellipse is degenerated to a circle, and the hyperbola to a straight line. Thus focal conic textures, which for a long time could not be incorporated into the homotopic defect classification, are recognized as a transition field of two $n=1$ smectic-A point singularities, where the integrability conditions enforce the presence of a defect ring. Apparently this field is favoured energetically over the pure hyperbolic or pure radial point defects (Trebin and Kutka 1981, Kutka 1981).

The branch of mathematics dealing with the decomposition of a manifold into layers or 'leaves', is the theory of foliations. A complete classification of defects in systems of broken translational symmetry certainly must take advantage of the concepts developed there. An introduction to the theory is presented by Lawson (1974). Another concept to describe systems of broken translational symmetry, viz. by the notion of 'semilocal structures', and remarks on defect structures thereof are reported by Thom (1981).

Fig. 33



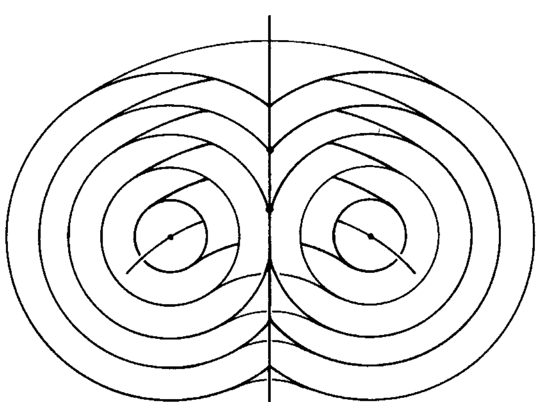
(*a*)



(*b*)

Transition between hyperbolic and radial point of a smectic layer system: (*a*) normal field; (*b*) corresponding layers.

Fig. 34



Layers of a focal conic texture.

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## APPENDIX 1

### *Factorization of spaces*

The representation of the space of degeneracy $V$ as coset space $G/H$ is an example of a frequent practice in topology to reduce a complicated space, like $V$, to one whose properties are well-known (here the Lie-group $G$), and which is subdivided into equivalence classes. In the case of the coset space, two elements $g_1, g_2 \in G$ are equivalent (notation $g_1 \sim g_2$), if $g_1^{-1} g_2 \in H$. The relation $\sim$ is an equivalence relation, since it is reflective ($g_1 \sim g_2$), symmetric (if $g_1 \sim g_2$, then $g_2 \sim g_1$) and transitive (if $g_1 \sim g_2$ and $g_2 \sim g_3$, then $g_1 \sim g_3$), and allows $G$ to be arranged into disjoint sets of mutually equivalent elements, denoted by $[g]$. These are, in the present example, the left cosets $gH$ of $H$ in $G$. Most frequently (and also for coset spaces) the equivalence relation is induced by a group action: if $X$ is a space, for example the order parameter space $X = R^3$ of a three-dimensional ferromagnet, and $F$ a group acting on $X$, here $F = \mathrm{SO}(3)$, then two elements $x_1$, $x_2 \in X$ are equivalent, if there is an element $f \in F$ transforming $x_2$ into $x_1$: $x_1 = fx_2$. Evidently the equivalence class $[x]$ is the orbit $Fx$. The set of equivalence classes is denoted $X/F$. In our example, an orbit is a two-sphere of radius $m$, and $X/F$ is the ray $[0, \infty)$ of non-negative real numbers. The bulk free-energy is a function on $X/F$.

The little group $F_x$ of a point $x$ in $X$ consists of those elements $f$ of $F$, for which $fx = x$. The action is called free, if $F_x = 0$ for all $x \in X$. In this case the exact sequence (3.12) is valid also for factorized spaces, where $X$ takes the part of $G$, and $F$ that of $H$:

$$\dots \to \pi_r(F) \to \pi_r(X) \to \pi_r(X/F) \to \pi_{r-1}(F) \to \dots$$

For a base point $x_0 \in F$ the isomorphism $\pi_r(X, Fx_0, x_0) = \pi_r(X/F, Fx_0)$ holds.

## APPENDIX 2.

### *Continuous deformation of paths in* Aff($d$) *into paths in* E($d$)

Denote by $g(t) = \{\tau(t)|A(t)\}$, $0 \leqslant t \leqslant 1$, the points on a path in Aff($d$) starting at $h \in H \subset \mathrm{E}(d)$ and terminating at the identity. $A$ is a real $d \times d$-matrix of non-zero determinant. Define the matrices

$$M(t) = [A(t)A^{\mathrm{T}}(t)]^{1/2},$$

$$R(t) = M^{-1}(t)A(t),$$

$$C(t) = \ln M(t).$$

$M(t)$ is real and symmetric, $R(t)$ is orthogonal. $M$, $R$ and $C$ are well defined and depend continuously on $t$. $A(t)$ can be written as $A(t) = [\exp C(t)]R(t)$. By the family of paths

$$g(t, s) = \{\tau(t)|[\exp sC(t)]R(t)\},$$

$0 \leqslant s,\ t \leqslant 1$, the original path in Aff($d$) is continuously deformed into one in E($d$), starting and terminating points being held fixed.

## APPENDIX 3

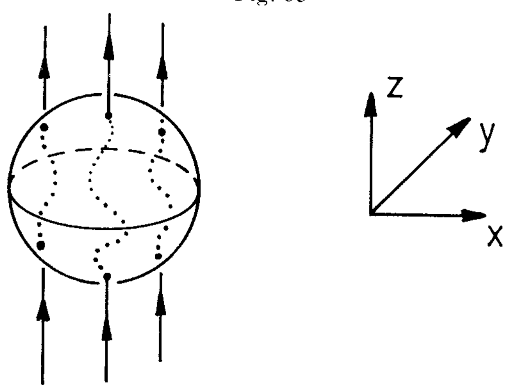
### *No configurations in crystals and layer systems*

Configurations in crystals and layer systems are unstable. The proof of this statement is sketched here. Several steps of this proof were pointed out to me by Th. Bröcker, K. Jänich and Ch. Meier. The details of the proof will be presented in a forthcoming publication.

A configuration of a crystal is described by a differentiable, orientation preserving mapping $\varphi: R^3 \to R^3$, which is regular everywhere, and is the identity mapping outside a three-ball. By stereographic projection of three-space on the three-sphere $\varphi$ is transformed into a mapping $\tilde{\varphi}: S^3 \to S^3$, that is the identity in a neighbourhood of the north pole. A regular differentiable mapping between compact manifolds is a local diffeomorphism and a covering, that is universal, since its domain is simply connected (similarly as SU(2) with the projection $\varphi$: SU(2)→SO(3) is a universal covering of SO(3)). The number of points of $\tilde{\varphi}^{-1}(x)$, $x \in S^3$, equals the number of leaves of the covering and is identical to the order of the fundamental group of the image set (Massey 1967, chapter 5). Since $\pi_1(S^3)=0$, there is only one leaf: $\tilde{\varphi}$ is therefore a diffeomorphism. According to a theorem of Cerf (1968), the group Diff $S^3$ of orientation preserving diffeomorphisms of $S^3$ is connected, so that a continuous path leads from any element to the identity. If the initial diffeomorphism is the identity in a neighbourhood of the north pole, a path can be chosen along which this property is preserved. By reversal of the stereographic projection, $\varphi$ is transformed into the identity mapping on $R^3$, and the initial configuration into the uniform crystal, without ever introducing disclinations (points of vanishing jacobian).

Configurations of layer systems are characterized by differentiable mappings $f$: $\mathrm{R}^3 \to \mathrm{R}$, of non-vanishing gradient, and with $f(\mathbf{r})=z$ (the three-coordinate) outside a three-ball. The layers are inverse images $f^{-1}(u)$, $u \in R$. Associated with the gradient field is a family of flow lines $\alpha_\rho(t)$, $\rho$ denoting the family index, such that $(d/dt)$ $\alpha_\rho(t)=\nabla f$ at point $\alpha_\rho(t)$. The flow lines traverse the three-ball and run parallel to the

Fig. 35




Flow lines of the gradient field $\nabla f$ corresponding to a configuration of a layer system in three-space.

$z$-axis outside it (fig. 35). A line, entering the ball from below, must leave it in an upward direction, since it follows the gradient. It is possible to deform the function $f$ continuously such that the $x$ and $y$ coordinates of the exit point of every line are the same as of the entrance point. So we can use these coordinates for the label $\rho$. Outside the ball the line parameter $t$ is chosen to coincide with $z$. Then the mapping $\chi: R^3 \to R^3$, $(x, y, z) \to \alpha_{xy}(z) = (f_1(\mathbf{r}), f_2(\mathbf{r}), f_3(\mathbf{r}))$ is differentiable, everywhere regular and the identity mapping outside the ball. Via a continuous family of vector functions of components $(f_{1s}, f_{2s}, f_{3s})$, $0 \leqslant s \leqslant 1$, it can be deformed to the identity mapping of $R^3$. The family $\{f_{3s}\}$ of scalar functions describes the smoothing down of the configuration that is recognized as unstable.



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