IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Relations between defects in the bulk and on the surface of an ordered medium: a topological investigation

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1995 J. Phys. A: Math. Gen. 28 2005

(http://iopscience.iop.org/0305-4470/28/7/020)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.70
The article was downloaded on 02/06/2010 at 03:50

Please note that terms and conditions apply.

J. Phys. A: Math. Gen. 28 (1995) 2005–2014. Printed in the UK

Relations between defects in the bulk and on the surface of an ordered medium: a topological investigation

Hans-Rainer Trebin† and Robert Kutka‡

† Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany
and Isaac Newton Institute for Mathematical Sciences, Cambridge, UK
‡ Siemens AG, Zentralabteilung Forschung und Entwicklung, Otto-Hahn-Ring 6, D-81739 München, Germany

Received 24 November 1994

Abstract. Starting from a proposal of Volovik we investigate surface point, line, and wall defects with the aid of relative homotopy groups. The exact sequence of homotopy groups is used in interpreting the relations between surface and bulk singularities. In particular, we consider the possibilities for surface singularities to move into the bulk, for bulk singularities to leave the medium through the surface, and for singular loops to be broken apart by the surface. The theory is extended to the case where the surface induces a thermodynamic phase differing from that in the bulk. An example is given of a biaxial nematic surface with the Klein bottle as the order-parameter space. Due to the fundamental theorem for homotopy groups of fibre bundles, the classification scheme of surface defects is identical for all pairs of bulk and surface order-parameter spaces which are related by an inverse-bundle projection.

1. Introduction

Ordered media, such as nematic liquid crystals, s-type superconductors, superfluid ^{3}He or quantum matter fields in cosmological theories, are described as continuous mappings from real space to a reduced order-parameter space (ROPS) [1]. For nematic liquid crystals, which are anisotropic fluids due to a spontaneous alignment of the molecular long axes, the reduced order parameter is the local optical axis [2, 3], and the ROPS is the set of rays through the origin, the projective sphere P^2. For s-type superconductors the ROPS is the set of phase factors, forming the circle S^1. For the superfluid phases of ^{3}He many ROPS exist, depending on the energy scale, the simplest being the orthogonal group $SO(3)$. For cosmological quantum fields it is the set of degenerate vacuum states, whose shape depends on the grand unification model used and in the simplest cases is either a circle or an n-sphere [4].

At a surface or an interface, ordered media can display an enormous wealth of phenomena, and these have been addressed in many papers during the last decade (for a review see [5]). Far from transition temperatures as a rule the ROPS are restricted at the surface to a *subspace*. On nematic surfaces only a subset of orientations of the optical axes (the 'directors') is admitted, as, for example, a tangential, conical or orthogonal ('homeotropic') orientation. The ROPS is thus reduced from the projective plane P^2 to the projective line P^1, the circle S^1 or a point, respectively. The physical origin of this 'anchoring' along selective directions is a subject of intensive investigation.

Denote the ROPS by V, its restriction to the surface by $A \subset V$. Bulk defects were classified at the end of the seventies by the homotopy groups of V and $\pi_n(V)$ [1, 6–10].

For the classification of surface defects, the homotopy groups of A and $\pi_n(A)$ have been applied [11].

But bulk and surface defects are not mutually isolated. An essential step to connect the singular order-parameter fields on the surface with their neighbouring volume was made by Volovik [12]. He proposed to surround a surface point defect by a hemisphere $D^n, n = 2$, whose boundary ∂D^n lies in the surface, and to consider the mappings $(D^n, \partial D^n) \to (V, A)$ from this hemisphere into V, and from its boundary into A. Hence surface point defects are classified by the relative homotopy groups $\pi_n(V, A),\ n = 2$.

The three types of homotopy groups are related by an exact sequence of homomorphisms, which has been exploited by Volovik to calculate $\pi_2(V, A)$. But the exact sequence allows much more interpretation. For the classification of surface defects of dimension $r = 2 - n, n = 2, 1, 0$, in section 2 we use it to answer questions such as which surface defects can be restricted entirely to the surface, which must continue into the bulk, which can leave the surface and move into the bulk? Which bulk defects can terminate at the surface, which can leave the volume through the surface, which cannot approach the boundary? We also discuss the question under what circumstances a surface is able to break up defect loops.

Close to a phase transition temperature, the surface may be covered by another thermodynamic state of the medium, for example, on a free nematic surface, smectic layers may be forming [5], hence new types of order can emerge, requiring an *extension* of the order-parameter space. Defects arising in a sequence of two phase transitions, when the unbroken symmetry group G is broken into a subgroup $H_1 < G$ and from there further to a subgroup $H_2 < H_1$, have been extensively dealt with by the present authors [16, 10, 14] under the heading 'semidefects' and, in cosmological field-theoretic models under the name 'hybrid defects' by [15, 16]. In section 3 we make an attempt to classify singularities on phase transforming surfaces by combining the concept of semidefects and Volovik's classification concept by relative homotopy groups. Parts of this concept are realized in a classification scheme of Misirpashaev [17] for defects at a phase interface.

2. Surfaces restricting the reduced order-parameter space

We assume now as above, that on the surface considered the ROPS V is restricted to a subspace A. To be precise, in the following we denote the defects described by $\pi_n(A)$ as 'boundary defects', and those characterized by $\pi_n(V, A)$ and taking regard of the nearby bulk structure as 'surface defects'.

The three types of homotopy groups are related by the exact sequence of homomorphisms [18]:

$$\cdots \xrightarrow{i_n} \pi_n(V) \xrightarrow{j_n} \pi_n(V, A) \xrightarrow{\partial_n} \pi_{n-1}(A) \xrightarrow{i_{n-1}} \pi_{n-1}(V) \xrightarrow{j_{n-1}} \cdots \qquad (1)$$

where i_n and j_n are inclusion homomorphisms and ∂_n is the boundary homomorphism.

The sequence has been used by Volovik to calculate the relative homotopy group $\pi_2(V, A)$ by applying the isomorphism theorem $\pi_2(V, A)/\ker(\partial_2) = \mathrm{Im}(\partial_2)$ together with the exactness properties of the sequence $\ker(\partial_2) = \mathrm{Im}(j_2)$ and $\mathrm{Im}(\partial_2) = \ker(i_1)$ to show that

$$\pi_2(V, A)/\mathrm{Im}(j_2) = \ker(i_1)\,. \qquad (2)$$

$\pi_2(V, A)$ now results as a group extension Ext(Im (j$_2$), ker (i$_1$)) [1], its elements being pairs (α, β). $\alpha \in \mathrm{Im}(j_2)$ labels the image under j_2 of a bulk point singularity transferred to

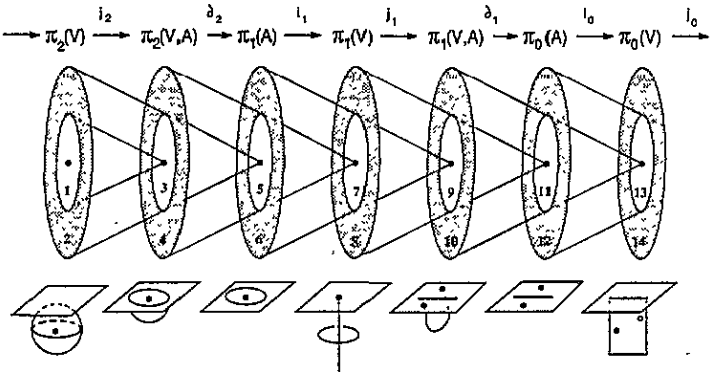

Figure 1. Exact sequence of homotopy groups. For the interpretation see the text.

the surface, and $\beta \in \ker(i_1)$ labels the enclosed boundary point singularity. In many cases this group extension is a direct product [12] (see also the discussion in [19, p 204].

But the exact sequence contains much more information, which we illuminate and depict in figure 1. The outer circles symbolize the full group, the inner circles the image of the preceding mapping, which due to the exactness property equals the kernel of the following, and the point the unit element.

In general, the sequence terminates at $\pi_1(V)$, as the subsequent sets must not have a group structure. There are many instances, where a group structure can be imposed (see the discussion in [10, p 215]), and in the following we assume this to be the case.

The different parts of the circles can now be interpreted in the following way:

(1) Elements of $\ker(j_2)$ correspond to bulk defects, which may penetrate through the surface and leave the volume, as, after being surrounded by the hemisphere, they belong to the trivial element of $\pi_2(V, A)$.
(2) Elements outside $\ker(j_2)$ cannot escape .
(3) The homotopy group $\pi_2(V, A)$ classifies fields, which are contained in the hemisphere, i.e. surface point defects with a bulk structure and bulk point defects, but not boundaries of bulk line singularities. Only those surface defects, whose group elements are in $\mathrm{Im}(j_2)$ can move from the surface into the bulk, as their inverse images correspond to bulk defects. Due to the the exactness property $\mathrm{Im}(j_2) = \ker(\partial_2)$ they are mapped to the trivial element of $\pi_1(A)$. Hence they are unstable as pure boundary point singularities, in contrast to:
(4) elements of $\pi_2(V, A)\backslash\mathrm{Im}(j_2)$, which do not have a correspondence among the bulk point singularities, hence cannot move into the bulk and are stable as boundary point singularities.
(5) Boundary point singularities are tested by a Burgers circuit. Those belonging to $\ker(i_1)$ are unstable if extended into the bulk.
(6) But there are also those taken into account, which are continued along a line into the volume. They correspond to elements outside of $\mathrm{Im}(\partial_2)$, as these lines cannot be confined to the hemisphere. Due to $\mathrm{Im}(\partial_2) = \ker(i_1)$ they are mapped to the classes for stable bulk line singularities.
(7) Among the bulk line defects the exact sequence determines those which can terminate on the surface, $\mathrm{Im}(i_1)$, as they have a correspondence with boundary point singularities, $\pi_1(A)$. Surprisingly, these can escape through the surface, because they also belong to $\ker(j_1)$ and are mapped to the trivial element of $\pi_1(V, A)$, which describes surface

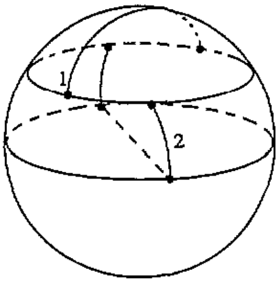

Figure 2. Tubular surface surrounding a line singularity which is connected with both ends to the boundary.

wall defects.

There are, however, circumstances possible, which nevertheless prevent the escape. A closed line singularity can also carry a point charge [10]. If such a loop touches the surface, and if its line characteristics belongs to $\mathrm{Im}\,(i_1)$, it can break and be connected with the boundary at two points. A tubular surface testing can be extended to a hemisphere (figure 2). When the corresponding element of $\pi_2(V, A)$ is outside $\ker(j_2)$ the loop is not able to leave the volume through the boundary.

(8) The elements of $\pi_1(V)$ outside $\mathrm{Im}\,(i_1)$ cannot terminate on the surface. They either form closed loops, or they contribute to the volume structure of surface wall singularities, since their image under j_1 is not trivial.

(9) The line surface singularities of $\mathrm{Im}\,(j_1)$ can leave the surface to form bulk line singularities, according to their inverse image, but they also are unstable if considered as boundary line defects under the mapping ∂_1.

(10) Elements of $\pi_1(V, A)\backslash\mathrm{Im}\,(j_1)$ must stick to the boundary, cannot move into the bulk, and contribute to stable boundary lines.

(11) Elements of $\ker(i_0)$ are pure boundary line singularities and do not bound walls in the bulk, whereas:

(12) elements of $\pi_0(A)\backslash\ker(i_0)$ are mapped to stable bulk walls, which they bound.

(13) Elements of $\ker(j_0)$ describe walls in the volume, which terminate at surface line singularities and can escape through the boundary.

(14) Finally, the elements of $\pi_0(V)\backslash\ker(j_0)$ label walls separating the boundary and the bulk, as their image, of $\pi_0(V, A)$, takes values in the bulk and on the boundary, which belong to different connected components of the ROPS V.

Let us apply these interpretations to the standard example of a nematic liquid crystal. If tangential boundary conditions prevail, $V = P^2$ and $A = P^1$. The relative sequence is now†

$$\begin{array}{ccccccccccccccc}
\cdots & \xrightarrow{i_2} & \pi_2(P^2) & \xrightarrow{j_2} & \pi_2(P^2, P^1) & \xrightarrow{\partial_2} & \pi_1(P^1) & \xrightarrow{i_1} & \pi_1(P^2) & \xrightarrow{j_1} & \pi_1(P^2, P^1) & \xrightarrow{\partial_1} & \pi_0(P^1) & \xrightarrow{i_0} & \cdots \\
 & & 2Z & \to & 2Z \times Z & \to & \frac{1}{2}Z & \to & Z_2 & \to & 0 & \to & 0 & & \\
 & & z & \mapsto & (z, 0) & & v & \mapsto & (2v) \bmod 2 & & & & & & \\
 & & & & (z, u) & \mapsto & u & & w & \mapsto & 0. & & & &
\end{array} \qquad (3)$$

No stable bulk point singularity can leave the volume through the boundary ($\ker(j_2) = 0$). Only surface defects of type $(z, 0)$, forming $\ker(\partial_2)$, can move into the bulk. Boundary point defects of half-integer winding number extend as line singularities into the bulk, those of integer winding number are without bulk structure, as $\mathrm{Im}\,(\partial_2) = \ker(i_1) = Z$.

† The integers denote a winding number, which we define as multiples of 2π. Winding numbers of spheres, which are multiples of the full solid angle 4π, hence are considered as even integers, and $\pi_2(P^2)$ is denoted by $2Z$, $\pi_2(P^2, P^1)$ is denoted by $2Z \times Z$.

All bulk line singularities can terminate on the surface, because $\mathrm{Im}\,(i_1) = Z_2 = \pi_1(P^2)$, all can leave the volume through the boundary ($\mathrm{Im}\,(i_1) = \ker(j_1) = \pi_1(P^2)$). There are no surface line singularities, because $\mathrm{Im}\,(j_1) = \ker(\partial_1) = 0$, and ∂_1 is injective, thus $\pi_1(P^2, P^1) = 0$.

Loop defects can break up when they touch the boundary. Considered as surface point defects, they are labelled by an element $(z, 0) \in 2Z \times Z$. If the first entry z of the pair is non-zero, they cannot leave the volume. This may be one reason why disclination lines, which are characteristic for the nematics, do not escape through the boundary. There may further be terms in the Frank–Oseen energy [3] preventing it, but also small deviations from the tangential boundary conditions.

The situation changes considerably with conical boundary conditions, A turning into S^l. The case has intensively been investigated in hybrid alignment films by Lavrentovich and Rozhkov [20]. The sequence becomes

$$\begin{array}{ccccccccccccccc} \cdots & \xrightarrow{i_2} & \pi_2(P^2) & \xrightarrow{j_2} & \pi_2(P^2, S^l) & \xrightarrow{\partial_2} & \pi_1(S^l) & \xrightarrow{i_1} & \pi_1(P^2) & \xrightarrow{j_1} & \pi_1(P^2, S^l) & \xrightarrow{\partial_1} & \pi_0(S^l) & \xrightarrow{i_0} & \cdots \\ & & 2Z & \rightarrow & 2Z \times Z & \rightarrow & Z & \rightarrow & Z_2 & \rightarrow & Z_2 & \rightarrow & 0 & & \\ & & z & \mapsto & (z, 0) & & v & \mapsto & 0 & & & & & & \\ & & & & (z, u) & \mapsto & u & & w & \mapsto & w & \mapsto & 0. & & \end{array} \tag{4}$$

As in the case of tangential boundary conditions, bulk point singularities cannot leave the volume through the boundary, and of the surface point singularities only the type $(z, 0)$ can move into the bulk. However, none of the boundary point singularities now extends along a singular line into the bulk ($\ker(i_1) = \pi_1(S^1)$). This is quite obvious, as bulk line defects of integer winding number can vanish by escape to the third dimension. Bulk line singularities cannot terminate on the surface ($\mathrm{Im}\,(i_1) = 0$) and cannot escape through the boundary any more ($\ker(j_1) = 0$). They either form closed loops, or they contribute to the one stable surface line singularity existing. It forms a 180° Bloch wall. Representatives of the two classes of paths in $\pi_1(P^2, S^1)$ are shown in figure 3.

The situation is still changing for homeotropic, i.e. orthogonal anchoring, $A = 1$ consisting of one point:

$$\begin{array}{ccccccccccccccc} \cdots & \xrightarrow{i_2} & \pi_2(P^2) & \xrightarrow{j_2} & \pi_2(P^2, 1) & \xrightarrow{\partial_2} & \pi_1(1) & \xrightarrow{i_1} & \pi_1(P^2) & \xrightarrow{j_1} & \pi_1(P^2, 1) & \xrightarrow{\partial_1} & \pi_0(1) & \xrightarrow{i_0} & \cdots \\ & & 2Z & \rightarrow & 2Z & \rightarrow & 0 & \rightarrow & Z_2 & \rightarrow & Z_2 & \rightarrow & 0 & & \\ & & z & \mapsto & z & \mapsto & 0 & \mapsto & 0 & & & & & & \\ & & & & & & & & w & \mapsto & w & \mapsto & 0. & & \end{array} \tag{5}$$

No bulk point singularities can leave the fluid through the boundary, because $\ker(j_2) = 0$. All surface singularities can move from the surface into the bulk, since $\mathrm{Im}\,(j_2) = \pi_2(P^2, 1)$. There are no stable boundary point singularities ($\pi_1(1) = 0$), and no bulk line defects can terminate on the surface ($\mathrm{Im}\,(i_1) = 0$) or escape through the surface. They merely contribute to surface line singularities ($\mathrm{Im}\,(j_1) = \pi_1(P^2, 1)$). All surface line defects can move accordingly into the bulk.

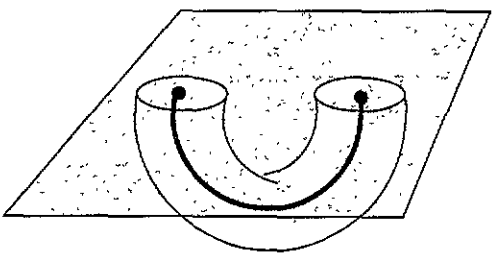

Figure 3. ROPS $V = P^2$, subspace $A = S^l$ and representative loops of the two types of homotopy classes of $\pi_1(P^2, S^l)$.

Finally let us consider the surface defects of dipole-locked superfluid ^{3}He-A (see also [12]). The reduced order parameter is a right-handed orthonormal tripod (e_1, e_2, l), where l denotes the angular momentum vector of the Cooper pair. Thus $V = SO(3)$. The boundary conditions are such that l stands either parallel or antiparallel to the surface, which implies $A = D_\infty \subset SO(3)$. The relative homotopy groups are known from the defect structure of uniaxial nematic liquid crystals, because $\pi_n(SO(3), D_\infty) = \pi_n(P^2)$, and we obtain the sequence:

$$\begin{array}{ccccccccccc} \pi_2(SO(3)) & \xrightarrow{j_2} & \pi_2(SO(3), D_\infty) & \xrightarrow{\partial_2} & \pi_1(D_\infty) & \xrightarrow{i_1} & \pi_1(SO(3)) & \xrightarrow{j_1} & \pi_1(SO(3), D_\infty) & \xrightarrow{\partial_1} & \pi_0(D_\infty) \\ 0 & \rightarrow & 2Z & \rightarrow & Z & \rightarrow & Z_2 & \rightarrow & Z_2 & \rightarrow & Z_2 \\ & & z & \mapsto & z & & w & \mapsto & 0 & & \\ & & & & u & \mapsto & (2u) \bmod 2 & & v & \mapsto & v\,. \end{array} \tag{6}$$

The surface point singularities are the well known boojums [21]. They are bound to the surface and cannot move into the bulk ($\mathrm{Im}\,(j_2) = \ker(\partial_2) = 0$). Boundary point singularities of odd winding number bound bulk disclination lines ($\ker(i_1) = 2Z \subset Z$). The bulk line singularities, 360° disclination lines in the tripod, can terminate on the surface and are also allowed to leave the bulk through the boundary. Finally, there are surface line singularities which separate domains of oppositely pointing vectors l. They cannot move into the bulk (as $\ker(\partial_1) = 0$), and are identical with the boundary line defects (∂_1 is bijective).

3. Surfaces inducing a phase transition

As a surface breaks the isotropy of space, it frequently induces a different thermodynamical phase, and phase transitions as a rule set in from the surface.

If there are different phase structures in the bulk and on the boundary, it is favourable to describe the reduced order-parameter spaces as coset spaces G/H_i, $i = 1, 2$, where G is the unbroken symmetry group, $H_1 < G$ the broken symmetry group in the bulk, and H_2 the broken symmetry group on the boundary. For simplicity here we deal with the case that H_2 is a subgroup of H_1. A standard example—easy to visualize—is the transition of an isotropic nematic liquid with $G = SO(3)$ to a uniaxial nematic phase, where $H = D_\infty$ is the cylindrical symmetry group of the director, and from there to a biaxial nematic phase with H_2 being the dihedral symmetry group D_2 of a cross. Such a transition is predicted in theories of surface wetting [22].

Defects in the bulk that develop in two successive phase transitions with symmetry breaking steps $G \rightarrow H_1 \rightarrow H_2$ have been treated in [14–16]. There, one has investigated the connectivity properties of the space G/H_2, which forms a fibre bundle with base space G/H_1, fibre H_1/H_2, and projection

$$\begin{array}{rccc} p: & G/H_2 & \rightarrow & G/H_1 \\ & gH_2 & \mapsto & gH_1\,. \end{array} \tag{7}$$

The homotopy groups of the three spaces are related by an exact sequence similar to that of (1) [18]:

$$\cdots \xrightarrow{i_n} \pi_n(G/H_2) \xrightarrow{p_n} \pi_n(G/H_1) \xrightarrow{\Delta_n} \pi_{n-1}(H_1/H_2) \xrightarrow{i_{n-1}} \pi_{n-1}(G/H_2) \xrightarrow{p_{n-1}} \cdots\,. \tag{8}$$

Here $\pi_n(G/H_2)$ describes defects in the fully broken phase, $\pi_n(G/H_1)$ defects in the partially broken phase, and $\pi_n(H_1/H_2)$ defects which arise from a uniform or singularity free partially broken phase, denoted as semidefects. The latter vanish in the symmetry restoring phase transition $2 \rightarrow 1$, which is described by the projection mapping of (7). If the partially broken phase 1 contains singularities, these may break in the second step into semidefects of one dimension more according to the homomorphism Δ_n of (8).

In the case of surfaces inducing a phase transition the ROPS in the bulk is undoubtedly G/H_1, whereas there is a variety of possibilities for the boundary. In the most general case the ROPS on the boundary is the entire bundle space G/H_2, but anchoring conditions might reduce it to a subset $U \subset G/H_2$. For a uniaxial nematic liquid crystal with a biaxial surface this subset could come from tangential anchoring conditions of the major director, the second axis pointing orthogonal to the surface, and U being P^1, which seems natural from the point of symmetry breaking. U can also stem from orthogonal boundary conditions of the major director with free rotation of the side axes, and then equals H_1/H_2.

Whereas in all cases the bulk singularities are classified by homotopy groups $\pi_n(G/H_1)$, and the boundary singularities by $\pi_n(U \subset G/H_2)$, the classification of surface point singularities is done by the homotopy classes of mappings of the hemisphere D^2 into the following spaces:

$$\begin{array}{rccc} f: & D^2 & \longrightarrow & G/H_1 \\ g: & \partial D^2 = S^1 & \longrightarrow & U \subset G/H_2 \\ & f|\partial D^2 & = & p|U \circ g\,. \end{array} \tag{9}$$

Misirpashaev [17] has listed these equations for a special set U.

We denote the set of classes of these mappings, under the assumption that they are based, sloppily by $\pi_2(G/H_1, U)$. If one is taking exact sequences as for the surface defects in (1) separately for phase 1 and phase 2, these sets are in between, leading to the following commuting diagram of mappings:

$$\begin{array}{ccccccccccccc} \cdots & \rightarrow & \pi_2(G/H_2) & \rightarrow & \pi_2(G/H_2,U) & & \rightarrow & & \pi_1(U) & \rightarrow & \pi_1(G/H_2) & \rightarrow & \cdots \\ & & & & & \searrow & & \nearrow & & & & & \\ & & \downarrow & \nearrow & \downarrow & & \pi_2(G/H_1,U) & & \downarrow & & \downarrow & \nearrow & \\ & & & & & \swarrow & & \searrow & & & & & \\ \cdots & \rightarrow & \pi_2(G/H_1) & \rightarrow & \pi_2(G/H_1,pU) & & \rightarrow & & \pi_1(pU) & \rightarrow & \pi_1(G/H_1) & \rightarrow & \cdots . \end{array} \tag{10}$$

The diagram has to be evaluated on a case to case basis. Here we do it for the following wide class of transitions:

Denote by $A \subset G/H_1$ the surface order-parameter space of phase 1. If $U = p^{-1}A$, the fundamental theorem for homotopy groups of fibre bundles [18, p 90] states, that

$$\pi_n(G/H_2, U) = \pi_n(G/H_1, A)\,. \tag{11}$$

According to the diagram of (10), $\pi_n(G/H_1, U)$ is equal to these two groups. It follows from this very general result, that *the classification of surface singularities remains invariant in a phase transition, if the boundary order-parameter space is being lifted in the same way as the bulk ROPS to the bundle space describing the new phase.* The statement is valid whether the transition happens only at the surface or proceeds into the bulk. A construction of the classifying group according to (9) is not necessary. For the interpretation of the surface processes the two parallel exact sequences have to be analysed:

$$\begin{array}{ccccccccccccc} \rightarrow & \pi_2(G/H_2) & \rightarrow & \pi_2(G/H_2,U) & \rightarrow & \pi_1(U) & \rightarrow & \pi_1(G/H_2) & \rightarrow & \pi_1(G/H_2,U) & \rightarrow & \pi_0(U) & \rightarrow \\ & \downarrow & & \| & & \downarrow & & \downarrow & & \| & & & \\ \rightarrow & \pi_2(G/H_1) & \rightarrow & \pi_2(G/H_1,A) & \rightarrow & \pi_1(A) & \rightarrow & \pi_1(G/H_1) & \rightarrow & \pi_1(G/H_1,A) & \rightarrow & \pi_0(A) & \rightarrow . \end{array} \tag{12}$$

If $U = G/H_2$ then $A = G/H_1$, and there are no surface singularities.

If $A = H_1$, i.e. a single order-parameter value is allowed on the boundary of phase 1, then $U = H_1/H_2$. Along a certain chain of the diagram (12) we recover the exact sequence of (8) for semidefects. The surface point singularities in the generalized sense of

Volovik [12] turn out to be the bulk point singularities in phase 1 with those semidefects of $\pi_n(U = H_1/H_2)$ attached to the boundary, into which they would break in a phase transition $1 \to 2$.

Among the boundary point singularities in $\pi_1(H_1/H_2)$ those are of special interest, which are outside $\mathrm{Im}\,(\Delta_2)$: when upon cooling the phase transition proceeds from the surface into the bulk, they develop into stable bulk line singularities according to the homomorphism i_1. Such boundary point singularities place the seed for line singularities in the bulk.

As a particular example let us consider a uniaxial nematic liquid crystal ($V_u = SO(3)/D_\infty$) with a biaxial surface ($V_b = SO(3)/D_2$) and tangential boundary conditions $A = P^1$. The lift of this set into $SO(3)/D_2$ yields an order-parameter space, where the major axis of the biaxial cross stays tangential to the surface, and the side axis rotates freely about it. The boundary order-parameter space U is determined in the following way: place an orthonormal tripod $\{e_1, e_2, e_3\}$ to the surface, with e_1 and e_2 in the boundary plane, and e_3 orthogonal to it. Orient the main director along e_2, the side axis along e_3. All the points of U are obtained by rotating the tripod with rotation operators $R(\alpha, \beta, \gamma = 0)$, α, β, γ being Eulerian angles, $0 \leqslant \alpha, \beta \leqslant \pi$. α is the rotation angle about e_3, turning e_2 into e_2', β the rotation angle about e_2'. Due to the identification of points $(\alpha, \beta = 0)$ with $(\alpha, \beta = \pi)$ and of points $(\alpha = 0, \beta)$ with $(\alpha = \pi, \pi - \beta)$ (figure 4), the manifold U is the Klein bottle. These boundary conditions are interesting, as the fundamental group of the Klein bottle is non-abelian: $\pi_1(U) = \frac{1}{2}Z \wedge \frac{1}{2}Z = \{(v, u)\}$, v denoting the winding number for the angle α (i.e. of the major director), u for the angle β (i.e. of the side axis). The semidirect product is defined by

$$(v_1, u_1)(v_2, u_2) = (v_1 + v_2, u_1 + (-1)^{2v_1} u_2)\,. \tag{13}$$

The Klein bottle is also the ROPS of the striped plane (which could serve as the boundary order-parameter space of smectic A liquid crystals in the bookshelf configuration). Due to its non-abelian fundamental group a singularity can change its homotopy label when guided about another one, as discussed by Poénaru and Toulouse [23] (see also the extensive discussion of the case in [19, p 199]. The biaxial nematic surface displays the same features, but has the advantage that the restrictions of the topological defect classification for systems of broken translational symmetry [9, p 638] do not apply.

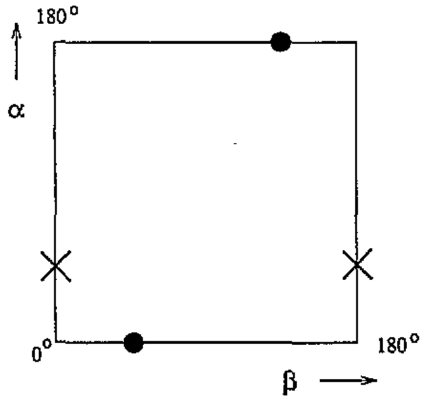

Figure 4. A Klein bottle as a boundary order-parameter space for a biaxial nematic surface. Points to be identified are marked.

The two connected exact sequences of (12) have following form:

$$\begin{array}{cccccccccccccc} \cdots & \to & 0 & \to & 0 & \to & F & \to & \frac{1}{2}Z \wedge \frac{1}{2}Z & \overset{i_1^\flat}{\to} & Q & \to & 0 & \to \cdots \\ & & \downarrow & & \downarrow & & \| & & \downarrow & & \downarrow & & \| & \\ \cdots & \to & 0 & \to & 2Z & \to & F & \to & \frac{1}{2}Z & \overset{i_1^\natural}{\to} & Z_2 & \to & 0 & \to \cdots \end{array} \tag{14}$$

where $Q = \{\pm 1, \pm \mathrm{i}\sigma_1, \pm \mathrm{i}\sigma_2, \pm \mathrm{i}\sigma_3\}$ denotes the quaternion group, σ_i a Pauli matrix.

The central part of the diagram is executed in terms of the group elements as

$$\begin{array}{ccc} (v, u) & \overset{i_1^\natural}{\mapsto} & (\mathrm{i}\sigma_2)^{-2u}(\mathrm{i}\sigma_3)^{-2v} \\ \bar{\downarrow} & & \bar{\downarrow} \\ v & \overset{i_1^\natural}{\mapsto} & (2v) \bmod 2\,. \end{array} \tag{15}$$

Due to the exactness property of the upper row the group F is kernel of homomorphism $i_1^\flat$, which is the abelian subgroup of $\frac{1}{2}Z \wedge \frac{1}{2}Z$ generated by the elements $(2, 0)$, $(1, 1)$ and $(0, 2)$, i.e. by the 4π-rotations of the biaxial cross. From the fundamental theorem we know, that $F = \pi_2(P^2, P^1)$, which in the exact sequence of (3) has been identified as $2Z \times Z$. The second factor denotes the winding number of the major axis (corresponding to e_2) in multiples of 2π and therefore is to be interpreted as the winding number v, the first one as the sum of v and u. The isomorphism connecting the two forms of F hence is

$$\begin{array}{ccccccc} \langle(2,0),(1,1),(0,2)\rangle & \to & 2Z \times Z & ; & 2Z \times Z & \to & \langle(2,0),(1,1),(0,2)\rangle \\ (v, u) & \mapsto & (v+u, v) & ; & (s, t) & \mapsto & (t, s-t)\,. \end{array} \tag{16}$$

It is to be noted, that with an odd winding number of e_2 there is always connected an odd winding number of e_3 (the side axis), hidden in the uniaxial case.

Due to the fundamental theorem the homotopy groups $\pi_n(V, A)$ are identical for all pairs of sets, which are related by an inverse bundle projection. Thus (P^2, P^1) shares these identities not only with $(SO(3)/D_2, U = \text{Klein bottle})$, but also with (i) (S^2, S^1) for a three-dimensional ferromagnet, (ii) $(SO(3), T^2)$ for a tripod field, and (iii) $(SU(2), \overline{T}^2)$. Here, $\overline{T}^2$ is the lift of the torus T^2 into $SU(2)$ under the canonical projection, and is the central torus in the foliation of $SU(2)$.

The respective three exact sequences according to (12) are

$$\begin{array}{lcccccccccccccc} \text{(i)} & \ldots & \to & 2Z & \to & 2Z \times Z & \to & Z & \to & 0 & \to & 0 & \to & 0 & \to \cdots \\ \text{(ii)} & \cdots & \to & 0 & \to & 2Z \times Z & \to & Z \times Z & \to & Z_2 & \to & 0 & \to & 0 & \to \ldots \\ \text{(iii)} & \cdots & \to & 0 & \to & 2Z \times Z & \to & 2Z \times Z & \to & 0 & \to & 0 & \to & 0 & \to \cdots \end{array} \tag{17}$$

although in cases (ii) and (iii) the symmetrical representation of F is more adequate.

Thus a deeper understanding is obtained of the surface classification for uniaxial nematic liquid crystals with tangential boundary conditions.

Acknowledgments

This research has been funded by the Deutsche Forschungsgemeinschaft under project number Tr 154/12-1. The work has been completed during the workshop 'Topological Defects' of the Isaac Newton Institute, Cambridge, UK, and one of the authors (HRT) is most thankful to the Institute for its hospitality and financial support.

References

[1] Michel L 1980 *Rev. Mod. Phys.* **51** 617

[2] Chandrasekhar S 1992 *Liquid Crystals* (Cambridge: Cambridge University Press)

[3] De Gennes P G and Prost J 1993 *The Physics of Liquid Crystals* (Oxford: Clarendon)

[4] Vilenkin A and Shellard E P S 1994 *Topological Defects in Cosmology* (Cambridge: Cambridge University Press)

[5] Jérôme B 1991 *Rep. Prog. Phys.* **54** 391

[6] Toulouse G and Kléman M 1976 *J. Physique Lett.* **37** L 149

[7] Volovik G E and Mineev V P 1976 *Pis. Zh. Eksp. Teor. Fiz.* **24** 605 (1976 *JETP Lett.* **24** 561)

[8] Rogula D 1976 *Trends in Applications of Pure Mathematics to Mechanics* ed G Fichera (New York: Pitman) p 311

[9] Mermin N D 1979 *Rev. Mod. Phys.* **51** 591

[10] Trebin H-R 1982 *Adv. Phys.* **31** 195

[11] Stein D L, Pisarski R D and Anderson P W 1978 *Phys. Rev. Lett.* **40** 1269

[12] Volovik G E 1978 *Pis. Zh. Eksp. Teor. Fiz.* **28** 65 (1978 *Sov. Phys. JETP Lett.* **28** 59)

[13] Trebin H-R 1981 *MATCH* **10** 211

[14] Kutka R, Trebin H-R and Kiemes M 1989 *J. Physique* **50** 861

[15] Kibble T W B, Lazarides G and Shafi Q 1982 *Phys. Lett.* **113B** 237

[16] Bais F 1981 *Phys. Lett.* **98B** 437

[17] Misirpashaev T Sh 1991 *Zh. Eksp. Teor. Fiz.* **99** 1741 (1991 *Sov. Phys.–JETP* **72** 973)

[18] Steenrod N 1951 *The Topology of Fibre Bundles* (Princeton, NJ: Princeton University Press)

[19] Kurik M V and Lavrentovich OD 1988 *Usp. Fiz. Nauk* **154** 381 (1988 *Sov. Phys. Usp.* **31** 196)

[20] Lavrentovich O D and Rozhkov S S 1988 *Pis. Zh. Eksp. Teor. Fiz.* **47** 210 (1988 *JETP Lett.* **47** 254)

[21] Mermin N D 1977 *Quantum Fluids and Solids* ed S B Trickey, E Adams and J Duffy (New York: Plenum) p 3

[22] Sluckin T J and Ponierwierski A 1985 *Phys. Rev. Lett.* **55** 2907

[23] Poénaru V and Toulouse G 1977 *J. Physique* **8** 887