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BOUNDARY CONDITIONS FOR TEXTURES AND DEFECTS

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Résumé. — Nous étudions l'influence des conditions aux limites sur l'existence et la coexistence des distorsions (textures, défauts) dans les milieux ordonnés. La classification topologique habituelle est fondée sur les applications de sphères dans la variété des états internes (qui caractérise l'ordre). Avec des conditions aux limites périodiques, ou partiellement périodiques, les sphères sont remplacées par des tores, ou quasitores. Les modifications induites dans la classification des distorsions, et dans leurs propriétés d'association, sont illustrées par quelques cas physiques pertinents.

Abstract. — We study the influence of boundary conditions on the existence and coexistence of distortions (textures, defects) in ordered media. The standard topological classification is based on mappings from spheres into the manifold of internal states (characterizing the order). For periodic, or partly periodic boundary conditions, the spheres have to be replaced by tori, or quasitori. The modifications which occur in the classification of distortions, and in their association properties, are illustrated in some physically relevant cases.

1. Introduction. — Ordered media are seldom perfectly ordered and many properties are sensitive to the distortions from perfect regularity. A general classification of these distortions is useful and has been developed in the past; it is based on a criterion of topological stability. Two kinds of distortions have been considered:

(i) Non-singular configurations or textures [1]; their classification is given by \( \pi_d(V) \), the homotopy group of order \( d \) (\( d \) is the space dimensionality) of a manifold \( V \) (this manifold, called the manifold of internal states, characterizes the order).

(ii) Singular configurations or defects [2]; their classification is given by the lower homotopy groups, \( \pi_r(V) \), with \( r < d \); the defects of dimensionality \( d' \) are classified by \( \pi_r \) with \( r = d - d' - 1 \).

The elements of a homotopy group \( \pi_r(M) \) are homotopy classes of mappings from a sphere \( S^r \) into a manifold \( M \). The question is frequently asked: why consider mappings from spheres?

In the case of non-singular configurations, this means that one considers configurations with a particular boundary condition (identical value of the order parameter everywhere at infinity; this effectively endows the space with the topology of a sphere). This is an interesting choice of a boundary condition; in a perfectly ordered medium, one can imagine the thought experiment of making a cavity, keeping the order parameter frozen outside it; then filling the cavity with a distorted non-singular configuration, and requiring the preceding boundary condition, in order to ensure continuity at the cavity surface. This operation can then be repeated elsewhere in space and one can eventually fill a sample in this way with topologically stable lumps [3]. Interesting as this may be, it is quite natural to wonder what sort of classification is obtained if one chooses a different boundary condition, such as, for instance, the popular (in condensed matter physics) periodic boundary condition (which endows the space with the topology of a torus); or the boundary condition (partly periodic) which would be appropriate if the cavity above were the space between two coaxial tori.

In the case of singular configurations (defects), the consideration of mappings from spheres means that one surrounds the defect with a spherical subspace. For instance, in dimension \( d = 3 \), one surrounds a wall with two points, a line with a loop, a point with a sphere. Again, it is quite natural to ask what would be predicted if a different surrounding subspace was chosen.

The aim of this paper is to show what sort of changes occur if one considers mappings from, say, tori rather than spheres. Is the number of homotopy classes changed or unchanged? Do the homotopy classes still possess a natural group structure? What is the physical significance of the possible changes?

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This paper is written in a very mathematically naive way, and apologies are due to the mathematicians; in fact, it is hoped that this may help them in understanding what the physicists see and need. In section 2, we give some general mathematical considerations. In section 3, we summarize some known results on mappings between spheres and tori. Some physical consequences and illustrations are presented in section 4.

2. Some mathematical considerations on homotopy classes of mappings. — The set of homotopy classes of pointed mappings from an n-dimensional manifold \( X^n \) into an m-dimensional manifold \( Y^m \) is denoted \((X^n, Y^m)\). Pointed mappings mean that we assume that some arbitrarily chosen point of \( X^n \) is always mapped into the same arbitrarily chosen point of \( Y^m \).

If \( X^n = S^n \), it is well known that the set of homotopy classes has a natural group structure; it is called the \( n \)th homotopy group of \( Y^m \) and it is denoted \( \pi_n(Y^m) \). For \( n \geq 2 \), \( \pi_n \) is necessarily abelian; \( \pi_1 \) may be non-abelian (the physical consequences of non-commutativity have been discussed [4]).

A set \( \{X, Y\} \) is said to have a natural group structure (n.g.s.) if there is a natural composition law, which describes, in physical terms, the addition of two defects [5]. In the case of spheres, \( X^n = S^n \), the restriction to pointed mapping is enough to have a n.g.s., for \( n > 1 \). But \((S^0, Y)\) does not in general have a n.g.s., and \( \pi_0(Y) \) is the set of connected components of \( Y \). These considerations lead to the following two questions:

What are the conditions on \( Y \) for \((X, Y)\) to have a n.g.s., whatever \( X \)?

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The answer to the first question is that \( Y \) must be an H-space [6, 7] (H stands for Hopf); the answer to the second question is that \( X \) must be an H'-space [6, 7] (also called H-cogroup).

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\( Y \) is an H-space if a mapping \( Y \times Y \to Y \) is defined, which satisfies the group axioms, up to homotopy. It is therefore a generalization of the notion of topological group. A topological group is an H-space; but for instance, the seven-dimensional sphere \( S^7 \), though not a topological group, is an H-space [8]. The formal definition of an H-space would require a little more explanation; it is sufficient to show here that the spheres \( S^n \) (\( n \geq 1 \)) are H'-spaces but that the tori \( T^n \) (\( n \geq 2 \)) are not. This can be understood easily, by the following argument.

Let \( X \) be the unit n-cube; a point \( x \in X \) is defined by \((x_1, x_2, \ldots, x_n)\) with \( 0 \leq x_i \leq 1 \). Consider mappings \( X \to Y \) with periodic boundary conditions:

\[
f(x_1, x_2, \ldots, x_n) = f(x_1, x_2, \ldots, x_i = 1, \ldots, x_n).
\]

In general, one does not see how to define a product \( f \cdot g \). However with the additional condition

\[
f(x_1 = 0, x_2, \ldots, x_n) = y^*, \quad y^* \in Y
\]

one can define a product \( h = f \cdot g \) by

\[
h(x_1, x_2, \ldots, x_n) = f(2x_1, x_2, \ldots, x_n)
\]

for

\[
0 \leq x_1 \leq \frac{1}{2}
\]

\[
h(x_1, x_2, \ldots, x_n) = g(2x_1 - 1, x_2, \ldots, x_n)
\]

for

\[
\frac{1}{2} \leq x_1 \leq 1
\]

In this way one obtains the torus homotopy groups \( \tau_n \) of R. H. Fox [9]. The usual homotopy groups \( \pi_n \) are obtained when one requires spherical boundary conditions in all directions (not just one):

\[
f(x_1, x_2, \ldots, x_n, x_{n+1}) = y^*
\]

if

\[
x_i = 0 \quad \text{for some} \quad i = 1, 2, \ldots, n
\]

So the n-cube with the mixed Fox boundary conditions (periodic in \((n - 1)\) directions, spherical in one direction) is an H'-space.

Note however that there is an interesting difference between the \( \tau_n \) and the \( \pi_n \); although the latter are abelian for \( n \geq 2 \), the former are not necessarily so. For instance \( \tau_3(S^2) \) is not abelian.

3. Results for spheres and tori. — In order to give a specific illustration, we shall discuss the cases when the manifolds \( X \) and \( Y \) are spheres \( S \) or tori \( T \). That is, we shall consider the four different situations:

\((S^n, S^m) \), \((S^n, T^m) \), \((T^n, S^m) \), \((T^n, T^m) \).

3.1 MAPPINGS FROM SPHERES TO SPHERES. — \( S \) is an H'-space and \((S^n, S^m) \) is a group: \( n \)th homotopy group of \( S^m \). For \( n < m \), \( \pi_n(S^m) = 0 \); for \( n = m \), \( \pi_n(S^m) = Z \), the additive group of integers; for \( n > m \), there is the rich structure of higher homotopy groups [10].

3.2 MAPPINGS FROM SPHERES TO TORI. — Again \( S^* \) is an H'-space. In addition, \( T^m \) is an H-space. Therefore, there are \( a \) priori two ways of defining a group structure for \( (S^n, T^m) \), but one can show that the two definitions agree and moreover, that the group structure is abelian. The group \((S^n, T^m) \) is \( \pi_n(T^m) \), the \( n \)th homotopy group of \( T^m \). By definition, \( T^m \) is a direct product of \( S^1 \), taken \( m \) times. As a consequence,

\[
\pi_n(T^m) = (\pi_n(S^1))^m.
\]

Therefore, for \( n = 1 \), \( \pi_1(T^m) = Z^m \); for \( n > 1 \), \( \pi_n(T^m) = 0 \). These two cases 3.1 and 3.2 belong to
the well-known theory of homotopy groups. We consider the last two more unusual cases [11] \((T^n, T^m)\) and \((T^n, S^m)\).

### 3.3 Mappings from Torus to Tori.

- \(T\) is an H-space, because it is a topological group; it is a topological group because it is a direct product of topological groups \(S^1 (S^1 = \text{SO}(2))\). Therefore the set \((T^n, T^m)\) has a natural group structure. Actually it can be shown that

\[
(T^n, T^m) = Z^n. 
\]

Note that this formula is consistent with the fact \(T^1 = S^1\).

### 3.4 Mappings from Tori to Spheres.

This case deserves a lengthier discussion. We consider \((T^n, S^m)\):

1. For \(n = 1, m\) arbitrary, this is \(\pi_1(S^m)\);
2. For \(n\) arbitrary, \(m = 1, 3, 7\) this is also a group because \(S^1, S^3, S^7\) are H-spaces \((S^1 = \text{SO}(2)\) and \(S^3 = \text{SU}(2)\) are even topological groups);
3. For \(n\) and \(m\) such that \(n \leq 2m - 2\), a composition law can be generally defined, which gives to the set \((T^n, S^m)\) a group structure [10, 12] called the \(m\)th cohomotopy group of \(T^n\), and denoted \(\pi^m(T^n)\). The cohomotopy groups are always abelian. In particular:

\[
\pi^n(T^m) = Z, \quad \pi^n(T^n) = 0 \quad \text{for} \quad n < m. 
\]

A simple conclusion which can be drawn from these results is that it makes a difference whether one considers mappings from spheres or from tori (that is, to assume spherical boundary conditions or periodic boundary conditions). \((S^n, S^m)\) is always a group, whereas \((T^n, S^m)\) is not always one. Even when \((T^n, S^m)\) is a group, it is not necessarily the same as \((S^n, S^m)\). As a simple example, compare

\[
(S^n, S^1) = \pi_n(S^1) = 0 \quad \text{for} \quad n > 1, 
\]

and

\[
(T^n, S^1) = Z^n. 
\]

Another remark may be introduced here. When \(X\) and \(Y\) are manifolds of equal dimensionality, it is possible to define the degree of a mapping \(X \rightarrow Y\). This degree is a topological invariant: all homotopic mappings have the same degree. If \(X\) and \(Y\) are orientable, the degree is an integer; if either \(X\) or \(Y\) is non-orientable, the degree is an integer modulo 2. From the preceding results, it can be seen that

\[
(T^n, T^m) = Z^{m}. 
\]

This proves that the degree of a mapping is not sufficient in general to characterize a homotopy class. Another example is \(\pi_2(P^2) = Z\), where \(P^2\) is the projective plane (non-orientable). This may have some physical consequences (difficulty of assigning unambiguously a topological number to a given texture or defect).

### 4. Physical Consequences and Illustrations.

In this section, we wish to consider various types of ordered media. The order defines a particular manifold of internal states. The mappings from spheres or tori into this manifold may lead to different classifications and we wish to interpret the similarities and differences in physical terms.

#### 4.1 The Order Parameter is a Two-Dimensional Vector.

This type of order parameter describes superfluids (like He₄), superconductors, planar spin magnets (the so-called \(XY\) model), etc... In this case, the manifold of internal states is a circle,

\[
V = S^1. 
\]

Both types of mappings \((S^n, S^1)\) and \((T^n, T^1)\) have a natural group structure. The results for \(n = 1, 2, 3\) are summarized in the following table

<table>
<thead>
<tr>
<th>(n)</th>
<th>((S^n, S^1))</th>
<th>((T^n, T^1))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(n = 1)</td>
<td>(Z)</td>
<td>(Z)</td>
</tr>
<tr>
<td>(n = 2)</td>
<td>(0)</td>
<td>(Z^2)</td>
</tr>
<tr>
<td>(n = 3)</td>
<td>(0)</td>
<td>(Z^3)</td>
</tr>
</tbody>
</table>

In a sample of space dimensionality \(d = 2\), the mappings \((n = 1)\) describe singular points and the mappings \((n = 2)\) describe non-singular textures. We see that mappings from spheres or tori lead obviously to the same prediction for point vortices, classified by an integral index (the circulation). However we see also that, while there are no non-trivial textures with spherical boundary conditions, there is a doubly-indexed infinity with periodic boundary conditions. These non-trivial textures can be seen as frozen spin waves, extended over the sample (Fig. 1).

![Fig. 1. Example of texture for the two-dimensional planar spin (XY) model with periodic boundary conditions.](image-url)
In a sample of space dimensionality \( d = 3 \), and in the case of spheres, the mappings \((n = 1)\) describe singular lines, the mappings \((n = 2)\) describe singular points, and the mappings \((n = 3)\) describe non-singular textures. \((S^2, S^1) = 0\) says that there are no singular points, while \((T^2, S^1) = Z^2\) describes vortex rings, which are localized defects. A vortex ring is naturally to be surrounded by a tubular subspace and that is precisely what \( T^2 \) is. The double index corresponds to the integral circulation of the vortex and to the total flux of other vortices passing through the vortex ring. So, the consideration of mappings from tori, in this most simple case, draws our attention to the possibility of a vortex closing on itself to form a localized defect, a vortex ring; and to the possibility of vortices being entangled. Here two vortex rings can disentangle at no topological cost because \( \pi_1 \) is commutative [4]. Finally, as far as the textures are concerned, the discussion for \( d = 2 \) can be repeated.

4.2 The order parameter is a three-dimensional vector. — This would describe an isotropic magnet (the so-called Heisenberg model). The manifold of internal states is a sphere, \( V = S^2 \).

The results for mappings \((S^n, S^2)\) and \((T^n, S^2)\), \(n = 1, 2, 3\) are given below

<table>
<thead>
<tr>
<th>( n )</th>
<th>( S^n, S^2 )</th>
<th>( T^n, S^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>( Z )</td>
<td>( Z )</td>
</tr>
<tr>
<td>3</td>
<td>( Z )</td>
<td>no natural group structure</td>
</tr>
</tbody>
</table>

In a space of dimensionality \( d = 3 \), \((S^2, S^2)\) describes singular points (in a sphere), while \((T^2, S^2)\) describes singular points (in a torus); the classification is the same. With \((T^3, S^2)\) we meet our first example of a set of homotopy classes which has no natural group structure; a complete physical understanding of the consequences has not yet been achieved. Note however, as a possible hint, that the corresponding Fox homotopy groups (Section II) \( \pi_3(S^2) \) is non-abelian; and the Whitehead product \([13, 14]\) of \( \pi_3(S^2) \) and \( \pi_4(S^2) \) is non-trivial.

Remark. — We can summarize the previous results in a more simple way by saying that the mapping \((T^n, S^n)\) contains the information relative to the mappings \((S^n, S^n)\) with \( n' \leq n \). For instance, we saw that \((T^2, S^1)\) describes textures in the case \( d = 2 \), but does not describe singular points in the case \( d = 3 \), since \((S^2, S^1) = 0\) then implies the non-existence of such points. In the same way, for \( d = 3 \), \((T^2, S^2)\) contains the information relevant to both singular points \((\pi_3(S^2) = Z)\) and to textures \((\pi_3(S^2) = Z)\).

These remarks also apply to the cases treated below.

4.3 The order parameter is a three-dimensional director. — This is the case for the liquid crystals of nematic type (ordinary nematics, i.e. uniaxial). The manifold of internal states is \( P^2 \), the projective plane, \( V = P^2 \).

The results for mappings \((S^n, P^2)\) and \((T^n, P^2)\), \(n = 1, 2, 3\) are in the table below:

<table>
<thead>
<tr>
<th>( n )</th>
<th>( S^n, P^2 )</th>
<th>( T^n, P^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( Z_2 )</td>
<td>( Z_2 )</td>
</tr>
<tr>
<td>2</td>
<td>( Z )</td>
<td>no natural group structure</td>
</tr>
<tr>
<td>3</td>
<td>( Z )</td>
<td>no natural group structure</td>
</tr>
</tbody>
</table>

In a space of dimensionality \( d = 3 \), nematics present one type of singular line, which is its own anti-defect \((Z_2\) is the additive group of integers modulo 2). There is a family of additively charged singular points, classified by \((S^2, P^2) = \pi_3(P^2) = Z \). The set \((T^2, P^2)\) can be classified as \( Z \times Z_2 \times Z_2 \), the first factor corresponding to points, the second to rings, the third to entangled rings, but there is no natural unit in this set and no natural group structure. Note that the Whitehead product of \( \pi_2(P^2) \) and \( \pi_3(P^2) \) is non-trivial, or equivalently that \( \pi_3(P^2) \) acts non-trivially on \( \pi_2(P^2) \).

4.4 The manifold of internal states is a torus or a Klein bottle. — These cases are of interest for two-dimensional crystal lattices and charge (or matter) density waves. The manifolds considered here are then \( V = T^2 \) or \( V = K \).

The results for the mappings \((S^n, T^2)\), \((T^n, T^2)\), \((S^n, K)\), \((T^n, K)\), \(n = 1, 2\) are given in the table below

<table>
<thead>
<tr>
<th>( n )</th>
<th>( S^n, T^2 )</th>
<th>( T^n, T^2 )</th>
<th>( S^n, K )</th>
<th>( T^n, K )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( Z^2 )</td>
<td>( Z^2 )</td>
<td>( Z \times Z )</td>
<td>( Z \times Z )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>( Z^4 )</td>
<td>0</td>
<td>no natural group structure</td>
</tr>
</tbody>
</table>

We see that periodic boundary conditions allow a wealth of non-singular textures \((T^2, T^2) = Z^2 \) which do not survive with spherical boundary conditions. \((S^2, T^2) = 0\); one of these textures is shown in figure 2. In the Klein bottle case, we remember that \( \pi_1(K) \) is non-commutative [4] (cross product of \( Z \) by \( Z \)) and we observe that \((T^2, K)\) has no natural group structure.

5. Discussion. — The classification of textures and singularities in terms of homotopy groups involves consideration of mappings from spheres (spherical boundary conditions or spherical surrounding subspaces). It is natural physically to consider mappings...
Fig. 2. — Example of texture for a two-dimensional polarized charge density wave with periodic boundary conditions.

from manifolds other than spheres and, in particular, from tori. This corresponds to periodic boundary conditions for textures and to tubular surrounding subspaces for defects (this allows the recognition, among localized defects, of closed rings, besides points). The existence or non-existence of a natural group structure for such a set of homotopy classes of mappings gives us information on the laws of coexistence for the corresponding textures and defects. This information is apparently contained also in the Whitehead product of homotopy groups or in the commutativity properties of the Fox homotopy groups. We believe that these various viewpoints are all useful to understand and predict the subtle chemistry of textures and defects in ordered media, and this paper has been written to stimulate further steps in this direction.

Acknowledgments. — It is a pleasure for the author to thank G. Toulouse and V. Poénaru for illuminating advice and discussions, and critical reading of the manuscript.

References

[5] We do not demonstrate stricte sensu that, for a general set \( \{ X, Y \} \), the natural composition law corresponds to the addition of defects. Nevertheless, this can be checked on some examples of section IV.
[11] In particular, the results of section IV rely heavily on these cases which are not to be confused with Fox’ torus homotopy groups.