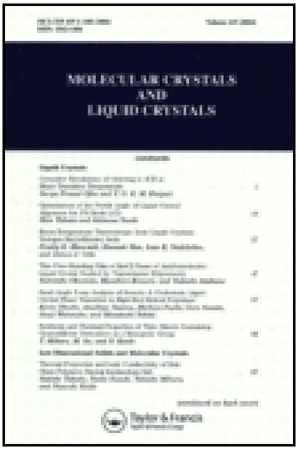

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Frustration and Related Topology of Blue Phases

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Frustration and Related Topology of Blue Phases

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CONTENTS

1. INTRODUCTION

Blue Phases remained up to very recent years quite mysterious. First observations were done at the end of the last century by Reinitzer in 1888 and by Lehmann in 1906.[1] The precise nature of these phases was a puzzling problem. At present it is firmly established that they are real phases and not textures of other phases. These Blue Phases are observed in a very narrow range of temperature in between the isotropic and the cholesteric phases.[2,3] Up to now, three different Blue Phases have been discovered. They appear in the following order by increasing the temperature:

Cholesteric	BP1 Blue Phase 1	BP2 Blue Phase 2	Blue Fog	Isotropic

→ T

Most of the time they occur in binary mixtures of nematic and cholesteric liquid crystal.[2] Their existence and the range ΔT of temperature where they do appear depend strongly on the pitch $p = 2\pi/q$ of the cholesteric. The influence of the twist is preponderant; these phases mainly exist for very small pitch i.e. strong twist (high q).

Thermodynamical studies reveal first order phase transitions.[2,3] The striking features of these Blue Phases is that, despite their high optical activity (as in cholesteric), they are optically isotropic.[3] Moreover, the BP1 and BP2 phases grow as crystals[4] and reflect selectively visible light. One observes Bragg reflection in the blue for instance, as suggested by their historical denomination. Blue fog is, at the moment, still in the mist and we let its description open for the future. We shall further on focus our attention only on the BP1 and BP2 crystalline phases.

The analysis of Bragg reflections specifies a cubic structure for both of them. Saupe[5] was the first to propose a model where both a twist and a cubic structure were associated. With the benefit of hindsight it appears that, in his geometrical model, a double twist was already present.

Unlike the cholesteric phases where a twist does exist in one direction of the space (one dimensional helix), the Blue Phases, as sketched by the Saupe model, present twist in several directions of the space. In this model the axes of the molecules are assumed to be directed along the edges of a cube. This geometrical constraint induces the presence of defects. One can qualitatively expect these phases to be stabilized near the isotropic transition where the cost of energy due to the defects is lower. In order to prove it, one should do an exact but difficult calculation of the free energy.

A first theoretical prediction of a crystalline phase was given by Brazowskii and Dimitriev[6] with use of a Landau expansion[21] of the free energy in terms of a tensorial order parameter Q_{ij}. They reported the existence of an hexagonal phase close to the isotropic one. This theory has been developed by Hornreich and Shtrikman who computed with approximations the minima of the free energy and found several crystalline phases with cubic symmetry.[7] Minimization of the energy is obtained by a balance of two terms.[8,9] A bulk term F_{bulk} (expansion in Q) favors, at lowest order in Q, a uniaxial order parameter Q. The other term F_{grad} (expansion in ∇Q) favors a biaxial order parameter Q and twist. In the following we shall focus our attention on the limit case of a uniaxial order parameter which raises a topological question of great interest. The minimization of $F_{\rm bulk}$ is then satisfied and one is left with the problem of searching structures lowering the remaining term $F_{\rm grad}$. In order to solve the problem one must build a director field $\mathbf{n}(r)$ (uniaxial order parameter) satisfying the local minimum of the free energy $F_{\rm grad}$. This will reveal, as we shall see in more detail in section 2, to be the *double twist condition*. This local condition leads to frustration in $\mathbf{R}^3$ *i.e.* it cannot be fulfilled over large distances. A first type of models (section 3) proposes a structure of Blue Phases as a lattice of disclinations where the double twist is only achieved in small regions of the space. An alternative approach (section 4) consists in satisfying the double twist condition everywhere but in a curved space.[8,11]

2. DOUBLE TWIST AND FRUSTRATION

If one imposes uniaxiality to the Landau tensor Q_{ij} one can express it in terms of the director $\mathbf{n}$ (mean orientation of the molecules):

$$Q_{ij} = S_0\left(n_i n_j - \frac{1}{3}\delta_{ij}\right) \tag{1}$$

where S_0 is the directional order parameter, $\mathbf{n}$ a unit vector with the condition that $+\mathbf{n}$ and $-\mathbf{n}$ are equivalent. The free energy $F_{\rm grad}$ can be expanded in terms of $\mathbf{n}$[11] as:

$$F_{\rm grad} = \int \mathcal{F}\ \mathrm{vol} \tag{2}$$

with

$$2\mathcal{F} = K_{11}(\mathrm{div}\ \mathbf{n})^2 + K_{22}(\mathbf{n}.\mathbf{curl}\ \mathbf{n} + q)^2 + K_{33}(\mathbf{n}\wedge\mathbf{curl}\ \mathbf{n})^2$$
$$- (K_{22} + K_{24})\ \mathrm{div}\ (\mathbf{n}.\mathbf{curl}\ (\mathbf{n}) + \mathbf{n}\ \mathrm{div}\ \mathbf{n}) \tag{3}$$

where q is the pitch of the cholesteric.

Expansion of the elastic constants in powers of S gives at second order in S[13]:

$$\begin{aligned} K_{11} &= K_{33} \\ K_{24} &= 0 \end{aligned} \tag{4}$$

The last term is a surface term often disregarded. It is of importance in the case of the Blue Phase since it leads to contributions when disclinations are present.

Expression (3) can be simplified in the one elastic constant approximation: $K_{11} = K_{22} = K$:

$$\mathcal{F} = K \sum_{k,j} (\partial_k n^j + q\epsilon_{kji} n^i)^2 - q^2 \tag{5}$$

An absolute minimum of the free energy would be reached if the condition:

$$\partial_k n^j + q\epsilon_{kji} n^i = 0 \tag{6}$$

could be satisfied everywhere. Let us point out that (6) is the double twist condition.

If one assumes an initial orientation $n_o^z = 1$ along the z direction, condition (6) only induces components $\delta n^y(r)$ and $\delta n^z(r)$ such that:

$$\begin{aligned} \frac{\delta n^y}{\delta x} &= q\epsilon_{zyx} n_0^z = -q \\ \frac{\delta n^x}{\delta y} &= q\epsilon_{yzx} n_0^z = +q \end{aligned} \tag{7}$$

Notice that $\delta n^z \equiv 0$.

Twist is then achieved in the two directions Ox and Oy perpendicular to the initial orientation n_0^z as indicated in Figure 1. But the main question is: what happens at large distances if one prescribes the orientation of **n** step by step by the local condition (6)? In other words, knowing the orientation of the director $\mathbf{n}_A$ at point A, does the rule (6) allow to define the orientation $\mathbf{n}_B$ at point B? The answer is given in Figure 2. The orientation of **n** at point B deduced by the rule (6) depends on the path used to go from point A to point B. There is frustration since the orientation is not well defined at point B. The mathematical traduction of this frustration is that a director

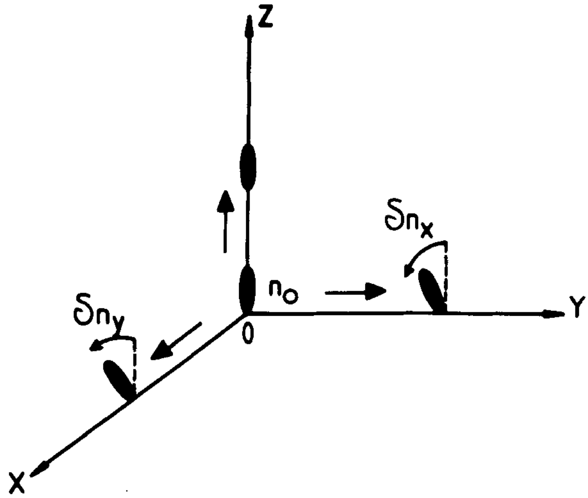

FIGURE 1 Geometrical interpretation of the double twist condition. Small displacements in the x and y directions induce a rotation of the molecules.

field does not exist satisfying the double twist condition. The physical implication is that double twist cannot be achieved everywhere in $\mathbf{R}^3$ but only locally. This important point was first noticed by Sethna[14] who proposed to release this frustration by changing the curvature of the space.

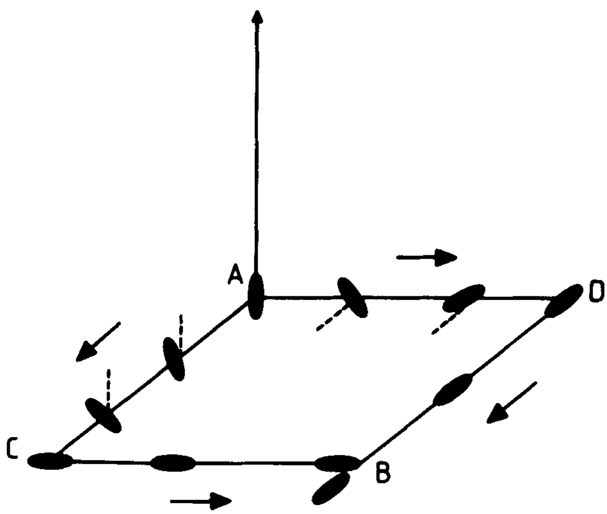

FIGURE 2 Following the rule given in Figure 1, one prescribes the molecular orientation along two different paths ACB and ADB. The resulting orientation at point B depends on the path. Frustration occurs since the orientation is not defined at point B.

3. GEOMETRICAL MODELS

Assuming that the order parameter is a director **n**, nice geometrical interpretations of the different crystalline structures have been exhibited. Saupe[5] was the first to propose a cubic configuration incorporating double twist of the director and singularities. In his model, the director is constrained to lie along the edges of a cube. In the same vein, all the geometrical models can be built by imposing the orientation of the director along some particular axes of a cubic cell. It is then possible to extend the director field in the vicinity of the axes by applying the double twist rule. Around the z axis for instance one can consider a director of the form:

$$\mathbf{n} = \sin(qr)\,\mathbf{e}_\theta + \cos(qr)\,\mathbf{e}_z \tag{8}$$

where (r, θ, z) are the usual polar coordinates around the z axis. This configuration gets a zero elastic free energy in the vicinity of the line ($r \rightarrow 0$). The elastic energy is $Kq^2/2$ for a cholesteric configuration. The director field defined by Equation 8 is visualized in Figure 3. The director is aligned along the tube axis but twists away from this direction when moving radially outward (increasing r).

Crystalline structures can be built by stacking finite or infinite tubes filled with the director field given by Equation 8. The problem is then to obtain cubic arrangements with a given symmetry such as O^2 = P 4_232, O^5 = F 432, O^8 = I 4_132. The radius of a tube is determined by the value of the tilt angle μ at the surface of this tube (Figure 3). This angle is adjusted to fit tubes together.

Models with adjacent tubes

The condition of double twist being more or less satisfied inside each tube, frustration strongly appears in between neighbouring cylinders. Let us consider three non-intersecting tangent tubes parallel to the three axes of a cube. As shown in Figures 4 and 5, such an arrangement produces either an $S = -\frac{1}{2}$ (Figure 4) or an $S = +1$ disclination line (Figure 5). Only the $S = -\frac{1}{2}$ disclination leads to a discontinuity in the director field and is a real defect. By setting such arrangements of cylinders in a cubic network, one gets geometrical configurations with different symmetry groups as shown in Figures 6 and 7. A network of $S = -\frac{1}{2}$ disclination lines is associated to each stacking of infinite cylinders. Along these lines it is assumed that there is no orientational order as in the isotropic phase. In the simple cubic

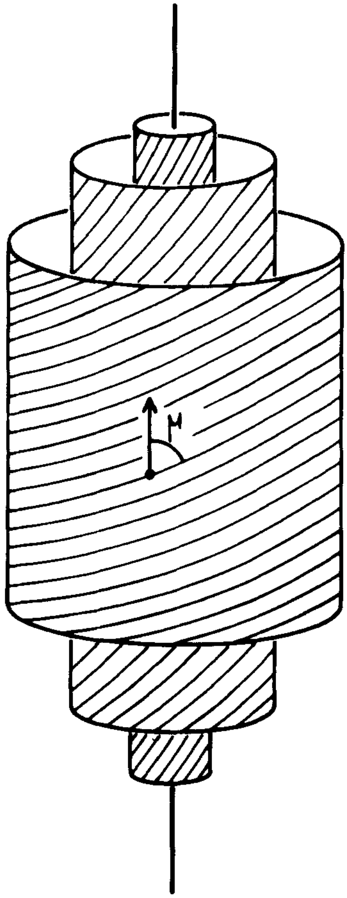

FIGURE 3 Director field lines inside a cylinder. The director is more and more tilted when moving away from the axis.

structure (Figure 6) proposed by Meiboom *et al.*,[15] sets of cylinders are arranged parallel to the cube axes producing intersecting $S = -\frac{1}{2}$ disclinations along the [111] directions of the cube. In the O^8 model sketched by Hornreich and Shtrikman,[7] the cylinders are still parallel to the cube axes and the disclinations, still in the [111] directions, are not intersecting. Notice that the O^8 model can be obtained from the O^2 model by taking away half of the cylinders.

Models with intersecting tubes

Another way to generate $S = -\frac{1}{2}$ disclination lines is to consider intersecting double twist tubes instead of tangent infinite double twist

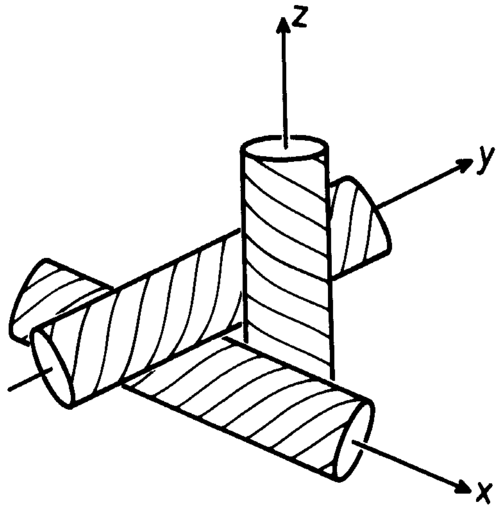

FIGURE 4a First way to stack three non-intersecting perpendicular cylinders tangent per wise.

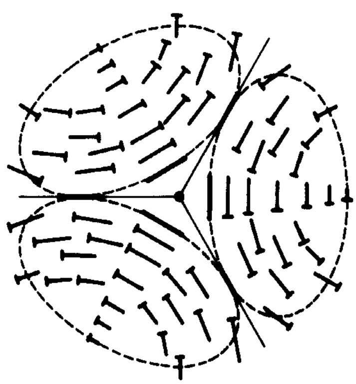

FIGURE 4b Section by the plane containing the three tangencies. The director field is represented in the elliptic sections of the cylinders with the usual projective convention.

cylinders as shown in Figures 8 to 10. In these configurations, the pieces of tubes are always situated along symmetry axes: A_4 in Figure 8a, A_2 in Figure 9, A_3 in Figure 10.

The simplest model shown in Figure 8 corresponds to the Saupe model.[5] It does not lead to defect points as expected by Saupe but to defect lines. The network of $S = -\frac{1}{2}$ disclination lines is indicated in Figure 8b.

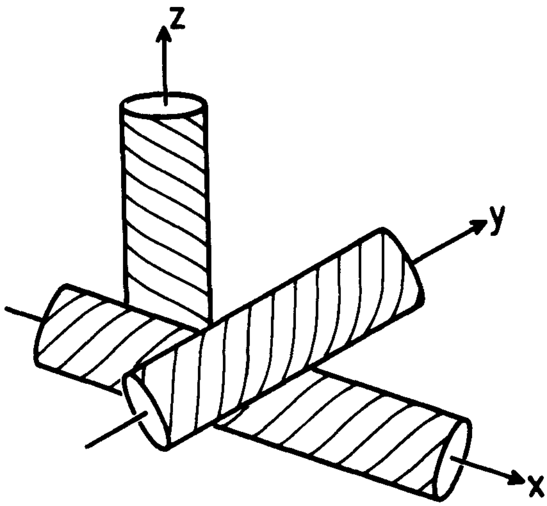

FIGURE 5a Second way to stack three non-intersecting perpendicular cylinders tangent per wise.

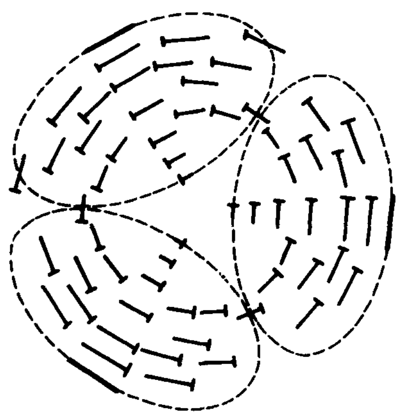

FIGURE 5b Section by the plane containing the three tangencies. This configuration leads to a $S = +1$ disclination line. There is no singularity since the director field can "escape" in the third dimension.

The other structures we exhibit in this paper (Figures 9 and 10) are reminiscent of the models proposed by Luzzati[16] for cubic lyotropic phases. In these phases, the amphiphilic molecules aggregate in small cylinders joined together (the rods of the figures). They build two infinite lattices which are unconnected, mutually interwoven and separated by one infinite aqueous medium.[17] The analogy between these systems and the Blue Phase is certainly very deep. Indeed one

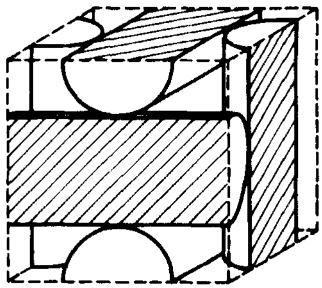

FIGURE 6a One of the simplest cubic arrangements of infinite double twist cylinders. Its symmetry is $O^2 = P4_232$.

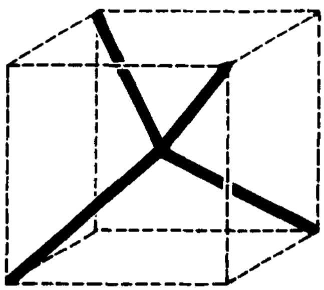

FIGURE 6b The corresponding network of $S = -\frac{1}{2}$ disclination lines.

can recover the symmetry groups observed in Blue Phases by removing the mirror operations (incompatible with the chirality) from the different symmetry groups of the cubic lyotropic phases. In the same spirit, Finn and Cladis[18] suggested that Blue Phases may be two phase regions of cholesteric and isotropic liquid similar to a current model for microemulsions.

Link between the different models

The problem is then to find the possible link between two stackings of tubes with the same symmetry in the Blue Phase and in the lyotropic models as for instance in Figures 6 and 10. In the model of Figure 6, cylinders parallel to the cube are tangent per wise. Such an array produces either $S = -\frac{1}{2}$ or $S = +1$ disclination lines (Figures 4 and 5) along the body diagonals of the cubic cell. The two types of configuration are in equal number. Half of a body diagonal is therefore a defect line ($S = -\frac{1}{2}$) as represented in Figure 6b. The other half is an $S = +1$ disclination line. The "escape" of the director field along this line forms in fact a double twist tube. This leads to the

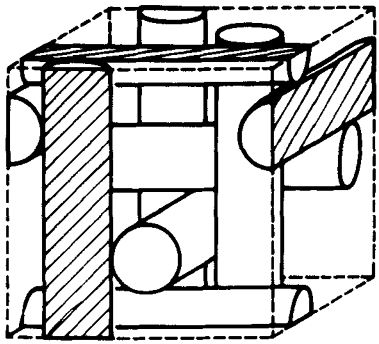

FIGURE 7a Another arrangement of infinite double twist cylinders leading to the symmetry group $O^8 = I4_132$.

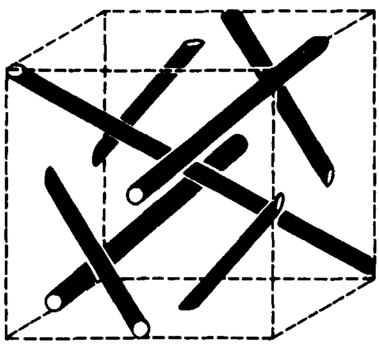

FIGURE 7b The corresponding network of $S = -\frac{1}{2}$ disclination lines.

configuration of Figure 10 where the tubes lie along the half of the body diagonals.

This comparison between the two models prove that several arrays of cylinders can lead to an equivalent distribution of directors. Nevertheless the existence of different representations is very useful to understand the topology of this distribution and fill the "holes" between the tubes.

Let us now compare the models of Figures 7a and 9 which have the same symmetry $O^8 = I4_132$. In that case the answer is given in Figure 11. In between some cylinders of Figure 9, represented by the black rods, one can insert a double twist tube of Figure 7a that lies along the helicoidal axis 4_1. That means that, in that case, the two stackings lead to the same distribution of directors and that the double twist condition is perfectly fulfilled along the 4_1 axes as well as along the A_2 axes. The question is now to understand what happens in

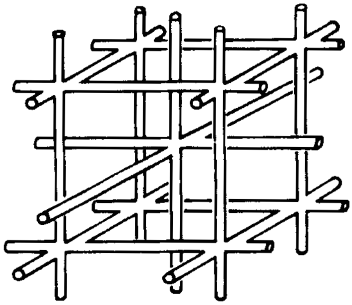

FIGURE 8a Stacking of pieces of double twist cylinders. They lie along the four-fold axes of a cube and intersect at the nodes of the centered cubic cell. The symmetry group is $O^5 = I432$.

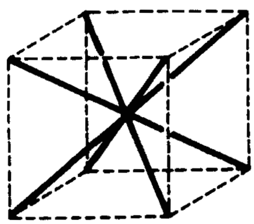

FIGURE 8b The corresponding network of $S = -\frac{1}{2}$ disclination lines.

between the cylinders represented by the white rods in Figure 9, i.e. along the 4_3 axis. Figure 12 shows the variation of the director on the 4_3 axis. It is interesting to look at the field around the axis. We suggest the following approximation of the director field:

$$\begin{aligned} n_z &= \sin qu \\ n_x &= \cos qz \cos qu \\ n_y &= \sin qz \cos qu \end{aligned} \tag{9}$$

with

$$u = -x \sin qz + y \cos qz \tag{9a}$$

where z is the coordinate along the axis. It is easy to verify that such a configuration satisfies the double twist condition when $u \rightarrow 0$, i.e. on the 4_3 axis. It is drawn in Figure 12b in a plane perpendicular to the axis in order to show the twist in the u direction. The twist in the

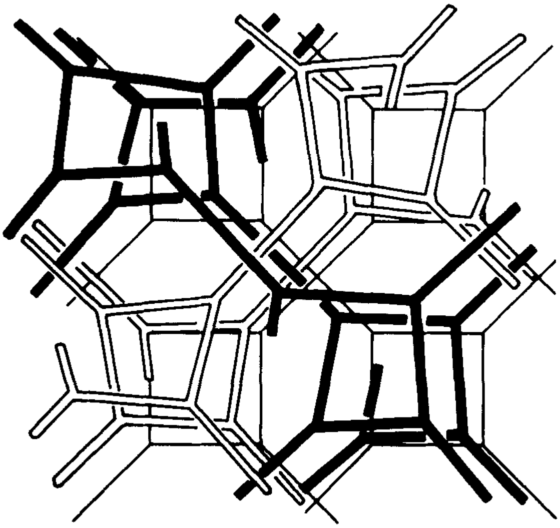

FIGURE 9 The symmetry group of this arrangement is $O^8 = I4_132$ as in Figure 7. Caution: the rods represent the core of the double twist cylinders. The black rods and the white rods are equivalent but their distinction makes easier the visualization of the structure. They lie along the two-fold axes of the symmetry group. The network of disclination lines is identical to the one of Figure 7b. It is also given by the three-fold axes.

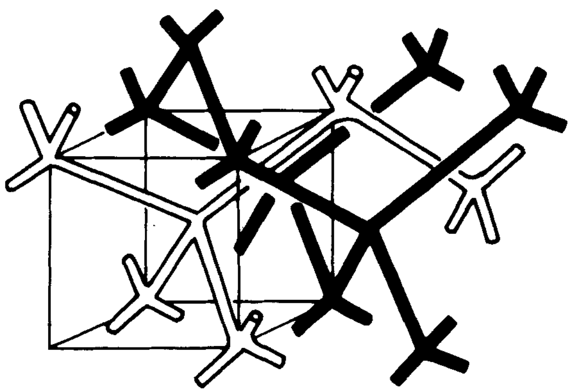

FIGURE 10 As in Figure 9, the rods represent the core of the double twist cylinders. Black rods and white rods are still equivalent. The symmetry group is $P4_232 = O^2$.

This arrangement can be compared to the one of Figure 4a of the same symmetry. Between the rods of Figure 8, one can glide infinite double twist cylinders (along the 4_2 axis) and thus recover the stacking of Figure 4a.

These two models lead to the same distribution of directors with the same network of disclination lines. The double twist condition is perfectly realized on the axes 4_2, and parts of the A_3 axes.

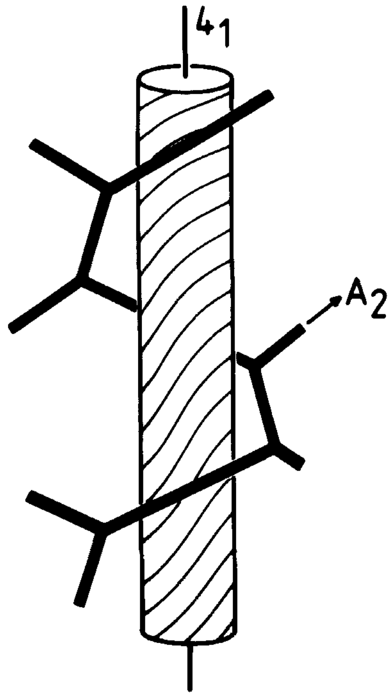

FIGURE 11 The link between the configuration of Figure 9 and the one of Figure 7 (with the same symmetry group O^8) is shown in this Figure. Indeed, in the O^8 group, the two-fold axes A_2 (cylinders of Figure 7a) form a kind of helix around the four-fold axes 4_1. An infinite double twist cylinder can then be set along this axis as in Figure 5a.

z direction sketched in Figure 12a is associated to the rotation of this plane around the *z* axis when moving along this axis.

Geometrical models and free energy

Referring to the models previously described, some points need to be emphasized:

—Several arrays of cylinders can lead to equivalent distributions of directors.
—The director field is perfectly twisting only along symmetry axes. Nevertheless, its approximation is too rough in between the axes to enable fine computation of the energy in order to establish a phase diagram. Therefore, a computer calculation is necessary to compare energetically the different structures.[10]

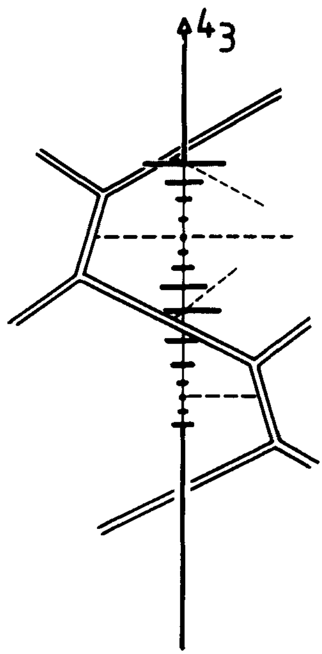

FIGURE 12a Director field along the 4_3 axis in between the white rods of Figure 7.

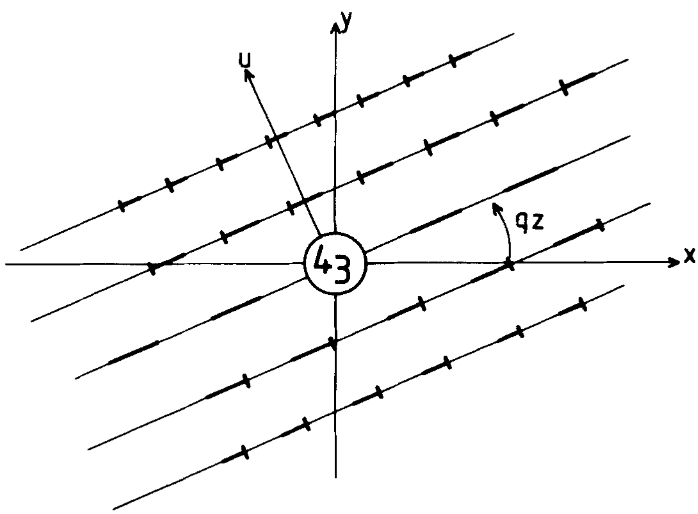

FIGURE 12b Approximated director field around the 4_3 axis taken as the z axis. It is represented in a plane perpendicular to the axis in order to show the twist in the u direction. The twist in the z direction sketched in Figure 10a is obtained by rotating this plane around the z axis when moving along it.

4. THE DOUBLE TWIST SEEN AS A RULE OF TRANSPORT

Let us now introduce some concepts of differential geometry which will reveal of main importance to describe a perfect Blue Phase without defects. Our purpose is to show that the double twist condition is in terms of mathematics a *linear connection*. As long as one is concerned with manifolds different from $\mathbf{R}^n$ the notion of connection is fundamental. It allows to compare what happens at two different points of the manifold.

We now want to introduce this notion in a very crude way, extracting from mathematics a simple presentation. At each point of a manifold one can define tangent vectors as vectors tangent to curves on the manifold. A linear connection is a rule of transport for a tangent vector. On a given manifold one can define different connections with different properties. We shall focus our attention on the notion of the curvature of a connection. Let us now give an example of connection, the Levi-Cività connection (which is linked to the metric of the manifold) on two different manifolds.

For a Levi-Cività connection the rule of transport is the following: along geodesics (shortest line between two points) a vector is transported with a constant angle with the geodesics.

a) Let us first consider this connection in $\mathbf{R}^2$ (plane) and emphasize some properties. Consider a vector $\mathbf{V}_A$ at point A. The parallel transport of the vector $\mathbf{V}_A$ by the Levi-Cività connection is indicated in Figure 13 along two different paths from point A to point B. First, along the geodesic (straight line) AB, $\mathbf{V}_A \rightarrow \mathbf{V}_E \rightarrow \mathbf{V}_B$ and then along the two geodesics AC and CB, $\mathbf{V}_A \rightarrow \mathbf{W}_F \rightarrow \mathbf{W}_C \rightarrow \mathbf{W}_B$. At point B, $\mathbf{V}_B \equiv \mathbf{W}_B$ *i.e.* the vector which has been parallel transported by the connection along AB is the same as the one obtained by transport along the line ACB. Then the *vector, parallel transported by the connection, defines in that case a vector field.*

b) We now want to give the example of the Levi-Cività connection on the manifold S^2 (sphere). We start again from a point A (Figure 14) and build the vector parallel transported from A to B along two different paths. First one moves directly from A to B along the geodesic which is, in that case, a great circle. One obtains a vector $\mathbf{V}_B$ at point B. Then one moves along ACB. One first travels along the great circle passing through points AC. The vector $\mathbf{V}$ is transported in $\mathbf{W}_D \rightarrow \mathbf{W}_C$, vectors doing a constant angle $\pi/2$ with the great circle passing through A, C. Then one moves from C to B along a meridian, one arrives with a vector $\mathbf{W}_B$ in B which is different from the vector $\mathbf{V}_B$ previously transported along the other path. In that case, *the vector, parallel transported, does not define a vector field.*

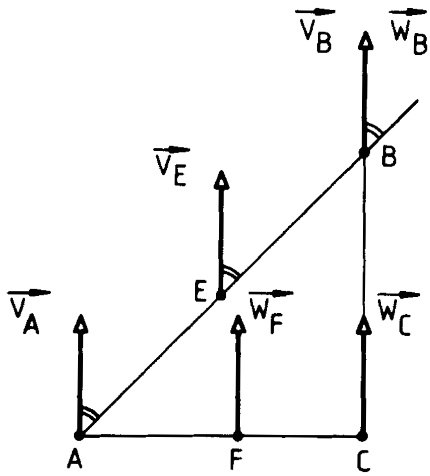

FIGURE 13 Parallel transport by the Levi-Cività connection in $\mathbf{R}^2$. The rule of transport defines a vector field: $\mathbf{V}_B \equiv \mathbf{W}_B$.

Looking at the two preceding examples, we see that the rule of transport given by the connection allows to find a vector field which is parallel transported by this connection in case a but not in case b. This is the characteristic property of a connection without curvature (case a) and with curvature (case b).

Care should be taken not to confuse between the curvature of an arbitrary connection and the intrinsic curvature of the manifold. We

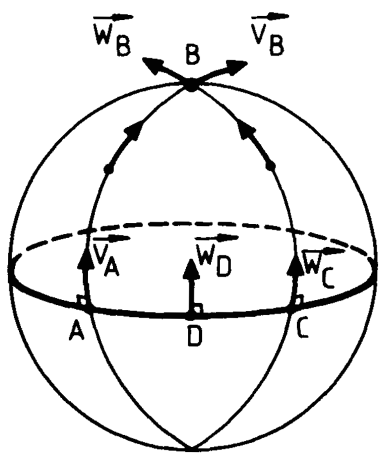

FIGURE 14 Parallel transport by the Levi-Cività connection in S^2. The rule of transport does not define a vector field: $\mathbf{V}_B \neq \mathbf{W}_B$.

emphasize that the curvature of a connection on a given manifold (curved space or flat space) reflects the obstruction to find a vector field which is parallel transported by the connection. A quantitative measure of this obstruction is given by the curvature tensor R^i_{jkl} (where indices are related to local coordinates). The variation δV of a vector parallel transported by the connection along a small circuit as indicated in Figure 15 is:

$$V^i = V^i_o + \delta V^i \tag{10}$$

The circuit is characterized by the element $dx^k \wedge dx^l$ and R^i_{jkl} is the infinitesimal rotational matrix:

$$\delta V^i = R^i_{jkl} V^j_o dx^k \wedge dx^l \tag{11}$$

One recovers that if $R^i_{jkl} = 0$ on the whole manifold then $\mathbf{V}_o = \mathbf{V}$ and there exists a vector field parallel transported by the connection.

Let us say as a conclusion we have seen that on a given manifold a linear connection defines a rule of transport for tangent vectors. Connections with or without curvature do exist on a given manifold, itself with or without intrinsic curvature. On a flat space (manifold without intrinsic curvature), there exist connections with curvature.

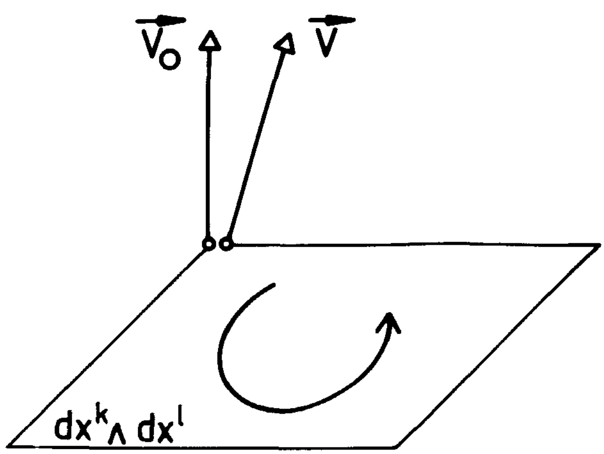

FIGURE 15 The vector $\mathbf{V}_0$ is parallel transported by the connection along a circuit defined by $dx^k \wedge dx^l$. After transport the new vector $\mathbf{V}$ is defined by:

$$V^i = V^i_0 + R^i_{jkl} V^j_o \, dx^k \wedge dx^l.$$

A good example is the double twist rule of transport (6) which is a connection in $\mathbf{R}^3$. We have seen that this rule leads to frustration i.e. one cannot find any vector field satisfying this rule of transport. The double twist condition (6) defines a linear connection with curvature in $\mathbf{R}^3$. Conversely on a curved space there may exist connections without curvature. It will be the case of the double twist connection built in S^3.

At this stage, one would like to be a little more precise about the notion of intrinsic curvature of a manifold. We are used to some intuitive notion of curvature as in the case of a soap bubble (2d surface). In that case, we see the soap bubble in our physical space $\mathbf{R}^3$. We look to the manifold "soap bubble" as embedded in $\mathbf{R}^3$. The vague notion of curvature of the soap bubble may be precised by considering at any point the tangent space and the normal to the soap bubble. The notion of normal indicates that, in that case, we look at the soap bubble as embedded in $\mathbf{R}^3$. The physical notion of principal curvatures reveals this embedding.

But if one wants to define an intrinsic property of a manifold one must consider this manifold without any embedding. This is the situation for example of an ant moving on an oak leaf. What could be the test for that ant in order to know whether it moves on the leaf or on a waterdrop fallen on that leaf? (see Figure 16). If the ant goes for a walk without observing the surrounding landscape the test will be related to the distance covered. If the ant just walks a distance L

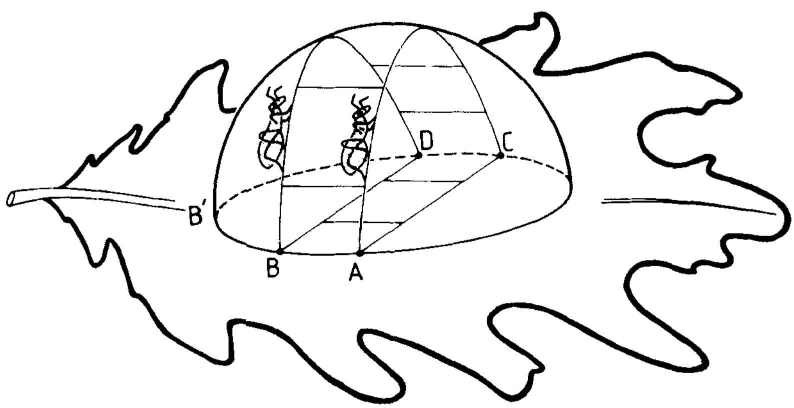

FIGURE 16 Test to know about curvature of the space: The distances covered by two ants walking at constant distance:

—are the same on the oak leaf (flat space)

—differ on the waterdrop (curved space).

it will be unable to know whether it travels directly on the leaf or on the water drop (see Figure 16). A little more is known if the ant wants to walk along the shortest path from one point to the another one. Then the ant will travel along the geodesic (shortest distance); straight lines on the leaf or great circles on the water drop. But the knowledge of the curvature of the space implies comparison and for that conversation will help as we shall see. Assume the ant just meets another ant and wants to chatter with it; the second ant will stay within earshot i.e. walk at a constant distance from the first one. What about the distances they have been walking after chattering for a while? The answer depends on what they are walking on. As a result, after chattering on the oak leaf, the two ants have covered the same distance, two parallel straight lines (see Figure 16). But the situation is different on the water drop. Let us assume that the first ant walks on a geodesic (great circle) from point A to C. This implies that the second one moves on a parallel circle (not a great circle) from B to D (see Figure 16). In that case the distance covered by the second ant differs from that covered by the first one. This reveals the curvature of the space. At first sight one could be surprised that the ant walking on a geodesic has walked a longer distance. The point is that the first one has covered the shortest distance to go from point A to C. The second ant is not going from A to C but from B to D. If this ant did not care for a conversation and just wanted to go alone by the shortest way from point B to D, it should have gone along the geodesic BB′D (great circle) as shown in Figure 16. These remarks suggest a relation between the metric (distances) and an intrinsic property (scalar curvature) of the manifold. As we have seen previously, among all connections which do exist on a manifold, there exists a unique one (without torsion) linked to the metric. This is the Levi-Cività connection. The notion of geodesic (related to distances) takes the metric into account. The curvature of the Levi-Cività connection allows to define an intrinsic property of the manifold. This is the scalar curvature R of the manifold. This scalar curvature is defined from the curvature tensor R^i_{jkl} of the Levi-Cività connection.

$$R = R^i_i \tag{12}$$

with the summation convention on equal indices

$$R^i_i = \sum_k R^k_k \tag{13}$$

$$R^j_h = g^{kj} R_{kh}$$
$$R_{kh} = R^j_{khj} \tag{14}$$

This quantity R is well defined whatever the dimension of the manifold is. If one computes for example the scalar curvature R in the case of the Levi-Civitá connection on a 2d-sphere of radius R_o one finds that R is constant over all the sphere and is related to R_o:

$$R = 2/R_o^2. \tag{15}$$

In the same spirit, the Levi-Civitá connection on the hypersphere S^3 of radius R_1 leads to an intrinsic curvature $R = 6/R_1^2$.

We are now able to give the chain of reasoning leading to the construction of an unfrustrated Blue Phase. Here again our purpose is to avoid mathematical details already given in (10) and only sketch main ideas. As we claimed several times the double twist condition can be seen from a mathematical standpoint as the rule of parallel transport characteristic of a connection hereafter referred to as double twist connection. This connection in $\mathbf{R}^3$ can be expressed in terms of some connection of reference. More precisely the double twist connection in $\mathbf{R}^3$ is the sum of two terms: the first one is the Levi-Civitá connection and the second one a corrective term. Remember that the Levi-Civitá connection of $\mathbf{R}^3$ is a connection without curvature in $\mathbf{R}^3$. Then the fact that it does not exist any vector field satisfying the double twist rule results from the corrective term. Due to that term the double twist connection gets curvature. But now we can still express this connection on S^3 with use of the Levi-Civitá connection and with a corrective term. The main point is that the Levi-Civitá connection on S^3 has curvature. The corrective term of the double twist connection characterizes the physical twist, the strength of which is measured by q. As we have seen before, the curvature of the Levi-Civitá connection on the sphere S^3 is scaled by the inverse R_1^{-1} of the radius of the sphere. Then if one chooses the radius of the sphere R_1 equal to the pitch of the cholesteric q^{-1}, the part of the Levi-Civitá connection which leads to curvature is cancelled by the corrective term. Then for $R_1 = q^{-1}$ the resulting double twist connection is without curvature. This implies that there exists a vector field parallel transported for that connection. It *means that on* S^3 *one can find a vector field or director field which satisfies everywhere the double twist condition.* Such a field describes a texture of perfect blue phase.

5. WHAT IS A TRANSLATION IN S^3?

In this section, we exhibit a simple analytical method to move in S^3 and in its tangent space. In the same way as a circle S^1 can be described with use of unit complex numbers, the S^3 sphere is isomorphic to the group of *unit* quaternions. The operations associated to this group are probably the best tools for transporting points and vectors. Moreover this presentation will reveal the analogy between the Blue Phase in S^3 and the Nematic Phase in $\mathbf{R}^3$.

What is a quaternion?

The circle S^1, embedded in $\mathbf{R}^2$, is often described with the complex notation

$$z = x_1\mathbf{1} + x_2 i \qquad x_1, x_2 \in \mathbf{R}$$

$$\text{with } \|z\|^2 = x_1^2 + x_2^2 = 1 \tag{16}$$

$$\text{and } i^2 = -\mathbf{1},\ \mathbf{1}i = i\mathbf{1} = i$$

In the same spirit, the sphere S^3, embedded in $\mathbf{R}^4$, can be described with use of unit quaternions:

$$q = x_1\mathbf{1} + x_2 i + x_3 j + x_4 k \tag{17}$$

where x_1, x_2, x_3, x_4 are four coordinates of $\mathbf{R}^4$ such that:

$$\|q\|^2 = x_1^2 + x_2^2 + x_3^2 + x_4^2 = \mathbf{L}. \tag{18}$$

Product of the basic quaternions $\mathbf{1}$, i, j, k, follows the rules:

$$\begin{cases} i^2 = j^2 = k^2 = -\mathbf{1} \\ ij = -ji = k \\ jk = -kj = i \\ ki = -ik = j \end{cases} \tag{19}$$

Notice that the product of quaternions is not commutative. To each quaternion q is associated a conjugate quaternion $\bar{q}$:

$$\bar{q} = x_1\mathbf{1} - x_2 i - x_3 j - x_4 k \tag{20}$$

x_1 is called the real part of q, $x_2 i + x_3 j + x_4 k$ is the imaginary part of q.

The scalar product of two quaternions is defined by

$$\langle q_1 | q_2 \rangle = Re\ (\bar{q}_1 q_2) \tag{21}$$

where Re = real part.
The norm of a quaternion is

$$\|q\|^2 = \langle q | q \rangle = x_1^2 + x_2^2 + x_3^2 + x_4^2 \tag{22}$$

The S^3 sphere is therefore isomorphic to the set of unit quaternions. It is a group since each element q has an inverse: $q^{-1} = \bar{q}$.

A tangent vector to the circle S^1 at point Q (associated to the complex z) can be written as

$$\mathbf{X} = \alpha\ zi = \alpha\ iz\ \alpha \in \mathbf{R} \tag{23}$$

In the same way, each tangent vector $\mathbf{X}$ to the sphere S^3 at a point Q associated to the quaternion q can be expressed as a quaternion (non necessarily unit) perpendicular to q. One can easily show that such a quaternion reads[19]:

$$\mathbf{X} = q\mathrm{V} \tag{24}$$

where

$$\mathrm{V} = \alpha i + \beta j + \gamma k \tag{25}$$

Hence

$$\mathbf{X} = \alpha(qi) + \beta(qj) + \gamma(qk) \tag{26}$$

The set of the three unit quaternions (qi, qj, qk) forms an orthonormal frame $\{\mathbf{e}_i, \mathbf{e}_j, \mathbf{e}_k\}$ tangent to S^3 at point q. In the same way as the tangent space to the usual sphere S^2 is isomorphic to $\mathbf{R}^2$, the tangent space to S^3 is isomorphic to $\mathbf{R}^3$.

Displacements in S^3

We can now exhibit a simple method to move in S^3 and in its tangent space using the quaternionic notation. We are interested in *isometric* displacements in S^3. This means that the distance between points is conserved. For the circle S^1, an isometric motion is a simple rotation $\mathcal{R}$ which can be described by a unit complex number z_o such as:

$$z \xrightarrow{\mathcal{R}} z' = z_o z = z z_o \tag{27}$$

In the same way, any isometric motion in S^3 can be described by two unit quaternions q_1 and q_2:

$$q \rightarrow q' = q_2 q q_1^{-1} \tag{28}$$

In fact we shall only use particular motions in S^3 corresponding to the following values of q_1 and q_2:

a) $q_1 = 1$, q is just left multiplied by q_2. In this transformation, no point is invariant. In the following it will be denoted as a left translation. (It is also often called left screw).
b) $q_2 = 1$, q is right multiplied by q_1^{-1}. This operation will be denoted as a right translation (also called right screw).
c) $q_1 = q_2$. All the quaternions commuting with q_1 are invariant, i.e. all the linear combinations of 1 and q_1. This transformation is similar to a rotation.

Let us consider the case of a left translation. Let **X** be a tangent vector to S^3 at point Q represented by the unit quaternion q. **X** can be written as $\mathbf{X} = q\mathrm{V}$. The point Q is transformed into the point Q′ (represented by q') through a left translation:

$$q' = q_o q \tag{29}$$

What happens to the tangent vector **X**? It is transported into a tangent vector **X**′ at point Q′. Let us write **X**′ as $\mathbf{X}' = q'\mathrm{V}'$[20]:

$$\mathbf{X}' = q'\mathrm{V}' = q_o X = q_o(q\mathrm{V}) = (q_o q)\mathrm{V} = q'\mathrm{V} \tag{30}$$

Equation (30) shows that V is invariant through a left translation (V′ = V). This important property enables us to build left invariant vector fields. Let us consider a tangent frame of S^3 at point $\mathrm{P} = \mathbf{1}$, for instance the frame (i, j, k). The left product by q carries the point $\mathrm{P} = \mathbf{1}$ onto the point $\mathrm{Q} = q$ and the vectors **i**, **j**, **k** onto the vectors $\mathbf{e}_i = qi$, $\mathbf{e}_j = qj$, $\mathbf{e}_k = qk$. Such operations generate a frame at each point Q *i.e.* a frame field. A vector field which has constant coordinates in this frame field is left invariant.

Notice that right translations generate another frame field $\mathbf{e}'_i = iq$, $\mathbf{e}'_j = jq$, $\mathbf{e}'_k = kq$ which is in coincidence with $\{\mathbf{e}_l\}_{l=i,j,k}$ only at the two points $q = \pm 1$.

Double twisted director field in S^3

In this paragraph, we shall prove that a left (resp. right) invariant director field verifies the left (resp. right) double twist condition and then will allow to construct a texture of Blue Phase. Let us consider the vector field $\mathbf{e}_i = qi$. We have to compare $\mathbf{e}_i$ at two neighboring points q and $q + \delta q$ of S^3. Let us choose $\delta q = qj\,\delta t$. This implies:

$$\begin{aligned} (qi)|_{q+\delta q} &= (q + \delta q)_i \\ &= (qi)|_q + \delta q i \\ &= (qi)|_q + q\,ji\,\delta t \\ &= (qi)|_q - qk\,\delta t \end{aligned} \tag{31}$$

Hence

$$(qi)|_{q+\delta q} - (qi)|_q = -qk\,\delta t$$

and

$$\partial_j \mathbf{e}_i = -\mathbf{e}_k \tag{32}$$

Equation (32) also reads:

$$\partial_j \mathbf{e}_i + \epsilon_{ijk}\,\mathbf{e}_i = 0 \tag{33}$$

This proves that the vector field $\mathbf{e}_i$ verifies the double twist condition (6) with a pitch equal to 1.

Despite a less mathematical construction the frame field $\mathbf{e}_i$ satisfying the double twist was already given by Sethna.[14] Nevertheless the presentation in this paper gives a more general and complete analysis. More precisely it will allow to describe any kind of blue phase textures and configurations with defects.[19]

Texture of Blue Phase

In a more general way any director field of the type $\mathbf{X} = q\mathrm{V}$, where V is constant and does not depend on q, satisfies the double twist rule and then describes a texture of Blue Phase. V is the value of the director at the origin $\mathrm{P} = \mathbf{1}$.

This is very similar to the prescription of a perfect nematic phase in $\mathbf{R}^3$. A perfect nematic configuration in $\mathbf{R}^3$ corresponds to a uniform, constant, orientation $\mathbf{n}$ of the molecules. In other words, if one knows the orientation $\mathbf{n}_o$ of the director at some reference point, the origin, one deduces its orientation at any other point: $\mathbf{n}$ has constant components in a frame field (i, j, k) built by translation of a given frame defined at the origin. This presentation may seem a little cumbersome to describe a constant director field in $\mathbf{R}^3$ but its interest is to introduce the analogy with the construction of the director field in S^3. Indeed the left translations we introduced in S^3 are analogous to usual translations in $\mathbf{R}^3$. Then both perfect nematic and Blue Phase can be described in the same way. One prescribes the orientation $\mathbf{n}_o$ or V at some specific point, the origin, of $\mathbf{R}^3$ or S^3. The perfect phase is then defined by a director $\mathbf{n}$ having constant components in a frame field transported either by classical translation in $\mathbf{R}^3$ or by left translation in S^3. The double twist, in the case of the Blue Phase in S^3, is introduced by the rule of transport of the frame field. This frame field when left transported performs the double twist.

6. SHORT GEOMETRICAL DESCRIPTION OF S^3 AND DIRECTOR FIELD LINES

We now want to give a rapid geometrical description of the hypersphere S^3. To allow a better understanding we shall first consider the pedagogical example of the sphere S^2. The classical 2d-sphere can by chance be visualized in our physical space $\mathbf{R}^3$. Every one has been at least once in physical contact with a ball. This reveals the concrete embedding of the sphere S^2 in our physical space $\mathbf{R}^3$. Unfortunately there is a lack of such a perception for the hypersphere S^3.

The sphere S^2

The shortest formulation could be: points at equal distance R of a given point O. This definition, which uses the embedding of S^2 in $\mathbf{R}^3$, does not make explicit interesting geometrical features we shall now specify. Indeed some special lines can be visualized on the sphere. More precisely circles of different sizes can be drawn on the sphere. A small circle appears, Figure 17, as the intersection of a 2d-plane with the S^2 sphere. When the 2d-plane passes through the origin O of the sphere it defines a great circle C_0. Points are spread over all the surface of the sphere. Special configuration of points corresponds

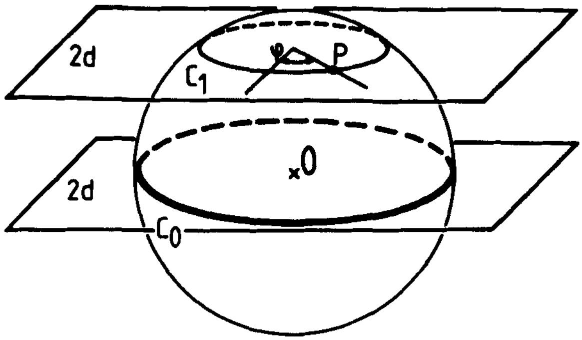

FIGURE 17 2d-sphere. Circles are intersection of 2d-plane with the sphere. Great circles C_o correspond to plane passing through the origin O.

to antipodal points A and B as shown in Figure 18. A circle C_1 can be seen as the points at a constant distance $d_1(A)$ and at a constant distance $d_2(B)$ of two antipodal points A,B. The choice of the antipodal points A and B defines a series of parallel circles, Figure 18. Another choice of antipodal points would have led to another, but equivalent, family of covering circles. Coordinates of a point P can be obtained with use of such a family. A point P is then defined by the knowledge of one circle of one family and of one angle on that circle, Figure 17.

The sphere S^3

Following the same presentation, S^3 appears as the set of points of $\mathbf{R}^4$ at equal distance R_0 of a given point O. But since we are now playing with a 3d-surface we can exhibit on it not only special lines but also special surfaces.

Circles are intersections of 2d-planes with the hypersphere S^3. Here again great circles are obtained when the 2d-plane passes through the origin. An important property is that, on S^3, two great circles are either interlaced or crossing in two points. Furthermore if one considers one great circle, it always exists another great circle perpendicular to the first one.

Spheres are intersections of 3d-planes with the hypersphere. A plane passing through the origin defines a great sphere S^2.

Tori. These surfaces can be described in the same spirit as circles on the sphere S^2. The rôle of the antipodal points A and B is now played by two specific lines: two perpendicular, interlaced great circles C_1 and C_2. A torus is a surface defined by the points which are

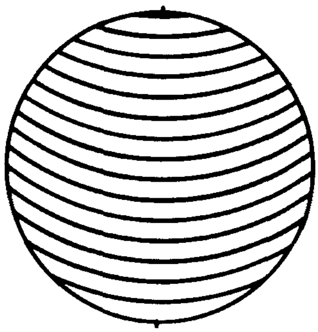

FIGURE 18 The sphere S^2 can be covered by a series of parallel circles, lines at constant distances of two antipodal points A and B.

at a constant distance $d_1(C_1)$ of the circle C_1 and at a constant distance $d_2(C_2)$ of the other limit circle C_2. The spherical torus corresponds to $d_1 = d_2$.

We are now able to give a description of S^3 as covered by a family of parallel tori embedded in one another, Figure 19. Each torus is itself covered by a family of parallel great circles, whose orientation is given by the choice of C_1 and C_2. A point P of S^3 is defined by the knowledge of one torus, one great circle C_p on that torus and one angle on that great circle, Figure 20.

In order to draw director field lines, one needs a tool to visualize S^3 just described above. One is already familiar with stereographic projection by reading maps on the roads. In the same way one can, by stereographic representation, project the hypersphere S^3 on $\mathbf{R}^3$.

Stereographic projection

We recall that stereographic projection defines a map of S^2 (without the pole of the projection) into the plane $\mathbf{R}^2$. In the same way, the stereographic projection defines a map of S^3 (without the pole of the projection) into the space $\mathbf{R}^3$. Some properties of the stereographic projection will be useful in the following:

The projection of a circle is a circle (or a straight line if the pole of the projection lies on the circle).

The projection of a sphere S^2 is a sphere (or a plane if the pole lies on the sphere).

The projection is conform i.e. preserves angles between curves.

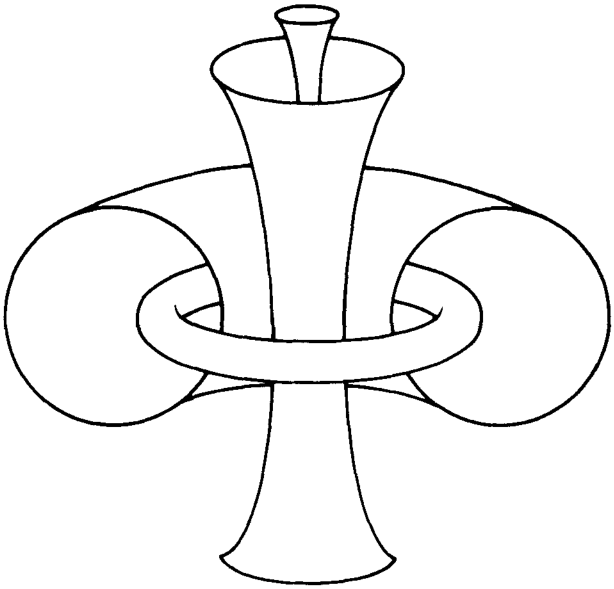

FIGURE 19 The sphere S^3 can be covered by a series of tori (surfaces) nested in one another. The drawing is a stereographic projection of $S^3 \to \mathbf{R}^3$.

Director field lines

The description of a texture of Blue Phase requires the specification of a director or a vector in each point of the space. A vector is defined in the tangent space of S^3 (isomorphic to $\mathbf{R}^3$) at each point P. The director field, satisfying everywhere the double twist condition, is obtained in the following manner. As we have seen, each point P

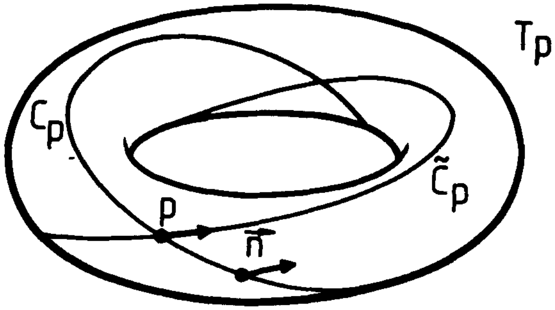

FIGURE 20 Coordinates on S^3. A point P is defined by one Torus, one great circle C_p on that torus and one angle on that circle.

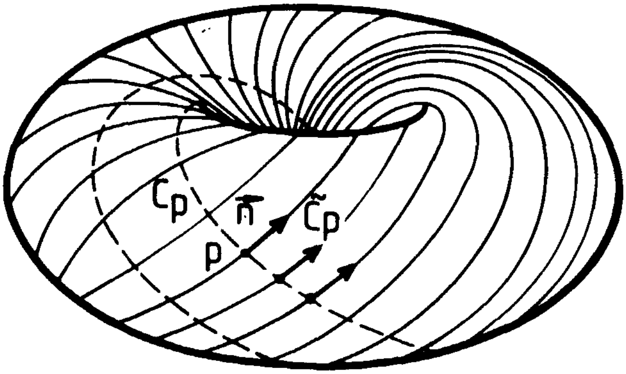

FIGURE 21 Director field lines on one torus. At each point P, the director **n** is tangent to one great circle of the family $\tilde{C}_p$ passing through P.

can be seen as lying on one great circle C_p, lying itself on one torus T_p. Furthermore, through each point P passes another great circle $\tilde{C}_p$, lying on T_p, the orientation of which is also fixed by the two limit circles C_1 and C_2. At each point P the tangent vector-**n**-to circles $\tilde{C}_p$ defines the orientation of the molecules of the Blue Phase, Figure 21. Director field lines are given by the family of great circles $\tilde{C}_p$. The double twist is clearly revealed on Figure 22. Let us point out that the choice of the family of great circles $\tilde{C}_p$ defines the sense of the twist. An opposite twist could be realized by choosing the director field as lying on the other family C_p.

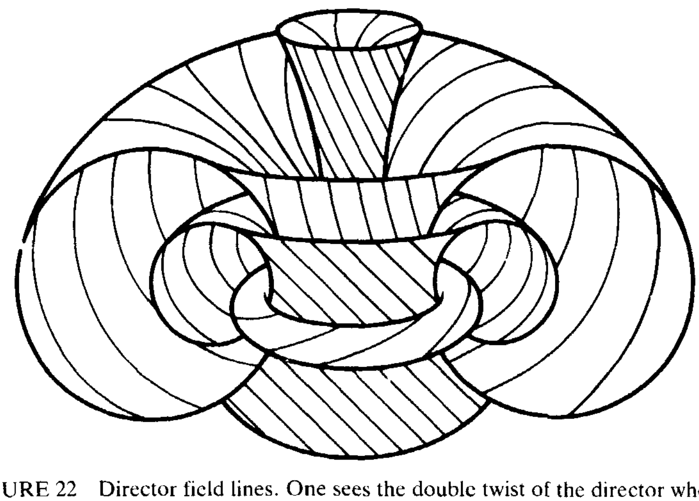

FIGURE 22 Director field lines. One sees the double twist of the director when one moves from one torus to another one of the family.

7. CONCLUSION

We have focused the presentation of this paper to geometrical aspects of some Blue Phase models. The main point is that the local constraint of minimum energy or double twist rule leads to frustration. This means that the prescription, step by step, of the molecular orientation does not allow ascribing a well defined orientation at long distances. This orientation is not uniquely defined but depends on the path chosen to go from one point to another one. This frustration, inherent to the double twist constraint, denies the existence of a well ordered phase in the physical space $\mathbf{R}^3$. We first present the description of Blue Phases as cubic arrays of disclination lines. The spirit of these descriptions is to realize a compromise between the double twist condition and long range order. Since this double twist rule cannot be fulfilled everywhere, it is satisfied in an approximate way and only in some finite regions of the space. The periodic organization of such nearly perfect regions takes into account optical experimental results. The quasi-perfect ordered domains are then directed along symmetry axes of cubic cells. Disorder and more precisely defects are necessary to fill up the remaining space. These phases, composed of defect arrays, are stabilized by the proximity of the isotropic liquid phase where the cost of energy due to disclinations is the lowest.

We have also given in this paper an alternative approach, fixing our mind to the description of a perfect phase satisfying everywhere the double twist rule. We show that the double twist can be expressed in terms of a mathematical connection i.e. a transport rule of vectors. The main argument is that this transport rule differs in a curved space such as S^3 from that on a flat space. It results that the double twist condition defining the molecular orientation in Blue Phases can be fulfilled everywhere in the curved space S^3. Textures corresponding to perfect configurations are generated in S^3 by analogy with nematics in $\mathbf{R}^3$. A perfect ordered nematic phase is characterized by the knowledge of one director orientation $\mathbf{n}_o$ at some reference point and by a rule of transport (translation) for this director. In the same manner the Blue Phase is also defined by one vector V in some specific point of S^3 and a rule of transport which performs naturally the double twist.

The advantage of this approach is to describe in a very simple way a perfect ordered phase. This description only allows local comparison with $\mathbf{R}^3$. Due to the curvature of S^3 one cannot do a global one with $\mathbf{R}^3$ but only compare the topology of the director field in finite regions of the space. The next step would be to introduce disclinations in S^3

in order to decrease its curvature. Introduction of an isolated disclination is already described in Ref. 19. Comparison of a defect in a perfect S^3 Blue Phase with models in $\mathbf{R}^3$ shows similar configurations close to the line. The interest of the description in S^3 is that the director orientation is known everywhere and not only in finite tubes as in the models in $\mathbf{R}^3$. The limit of this description is that it does not lead up to now to the prediction of cubic phases. In any case the determination of the precise structure would require energetical considerations. This is a complex problem in these phases where numerous defects are present.

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20. One could have written **X** as:

$$\mathbf{X} = \mathrm{V}'q$$

with

$$\mathrm{V}' = \alpha' i + \beta' j + \gamma' k$$

Since the product is not commutative, V′ and V are generally different:

$$\mathrm{V}' = \bar{q}\mathrm{V}q$$

21. For a review of Landau theory of Blue Phases, see the paper of Hornreich and Shtrikman *p*: of this book.