ON DEFECTS IN BIAXIAL NEMATIC LIQUID CRYSTALS

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ABSTRACT

We discuss some of the interesting aspects of the topological defects in biaxial nematic liquid crystals.

INTRODUCTION

CLASSICAL nematic liquid crystals are optically uniaxial and are cylindrically symmetric about the preferred direction of alignment given by a dimensionless unit vector **n** referred to as the director. In recent years nematic liquid crystals with optical biaxiality have been discovered in lyotropic[1] and thermotropic[2] systems. Theoretical studies on the defects in biaxial systems have gained a lot of relevance and significance in view of these experimental findings. Some of the topological aspects of defects in such phases have been discussed earlier[3–6]. We shall present, without going into their energetics, the salient features of the defects which have many curious and interesting properties.

We shall confine our attention only to the simplest of the biaxial nematic phases. This has an orthorhombic symmetry and can be looked upon as being made up of molecules which are like rectangular boxes. There are three unique directions **a**, **b** and **c** which are mutually perpendicular and the structure has a two-fold symmetry about each of them. In other words we have a trihedron of nematic directors **a**, **b** and **c**.

CLASSICAL DISCLINATIONS

We can create disclinations in any pair of the orthogonal director fields through the familiar Volterra process. In principle we can create disclinations in $\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$ and $\mathbf{c}-\mathbf{a}$ fields. We show in figure 1a, $s = \frac{1}{2}$ wedge disclination in $\mathbf{a}-\mathbf{c}$ fields.

(i) *Defect classification*: Though these disclinations are like uniaxial nematic disclinations there are some important differences. For example, disclinations of strength $|s| = \frac{1}{2}$ in $\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$ and $\mathbf{c}-\mathbf{a}$ fields cannot be transformed into one another by any topological process. Thus they belong to three distinctly different classes[5]. However, disclinations of strength $|s| = 1$ are mutually interconvertible in the same three pairs of fields. For example, by allowing the $s = +1$ structure to escape in the third dimension as in uniaxial nematics, we can transform a $s = +1$ defect in $\mathbf{a}-\mathbf{b}$ to a $s = +1$ defect in the $\mathbf{b}-\mathbf{c}$ or $\mathbf{a}-\mathbf{c}$ fields (figure 1b). We find the interesting result that unlike in uniaxial nematics $|s| = 1$ defects are singular and that disclinations $\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$ and $\mathbf{c}-\mathbf{a}$ are topologically indistinguishable[6] i.e. they all belong to one and the same class. But this class is different from the three previous classes. There are thus four distinct classes of line singularities.

(ii) *Coalescence between disclinations*: A direct coalescence between two wedge (or twist) disclinations of the same class but of different strength s_1 and s_2 results in a wedge (or twist) disclination of strength $s_1 + s_2$, as in uniaxial nematics. This law of algebraic addition breaks down in the presence of a $|s| = \frac{1}{2}$ disclination of another class. If we take any one of the partners of the pair once round the third defect, belonging to a different class, it gets converted into its antidefect i.e. s_1 (or s_2) $\rightarrow -s_1$ (or $-s_2$). Thus in the coalescence of the pair the end result depends upon the path chosen[4–6].

(iii) *Disclination decay*: One important consequence of the above result is that $|s| = 1$ defect or any integral defect for that matter, decays into a uniform state[5,6] in the presence

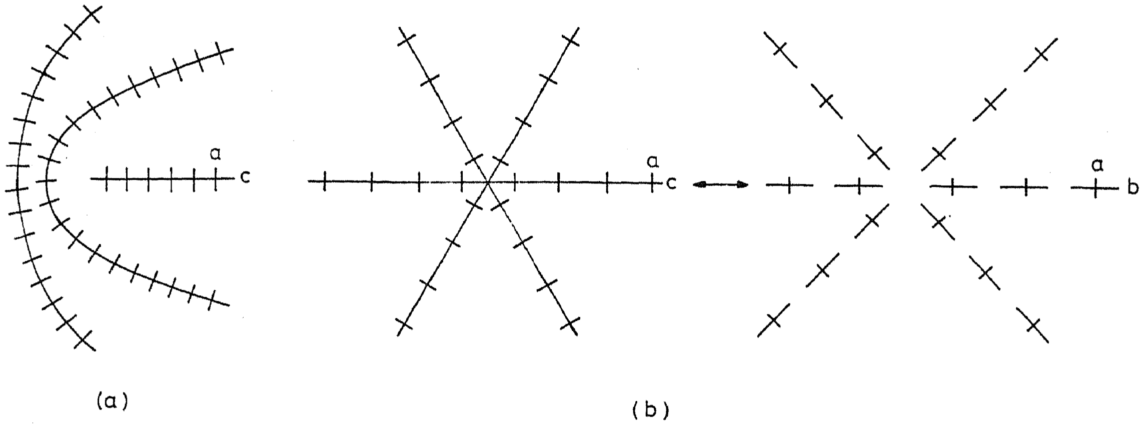

Figure 1a, b. **(a)** $s = +\frac{1}{2}$ wedge disclination in **a** − **c** fields; **(b)** $s = +1$ wedge disclination in **a** − **c** fields can be transformed into an $s = +1$ wedge disclination in **a** − **b** fields by allowing the **c** director to escape in the third dimension.

of a half disclination line of any class. This can be clearly seen by splitting $|s| = 1$ into two identical half disclinations of a class different from the class of the given half disclination. We recombine them by taking one of the partners once round the given half disclination. In this process it gets converted into its antidefect which, on recombination, completely annihilates the other partner of the identical pair.

(iv) *Disclination entanglement*: A surprising result was discovered in biaxial phases by Toulouse[7]. This pertains to the crossing of one disclination by another, which is topologically equivalent to a single twist between them. Two disclinations of the same class can cross one another without any obstruction i.e. they can pass through one another merely by local fluctuations. A disclination with $|s| = 1$ can cross a half disclination of any class. But this is not so, for two half disclinations of different classes. There will be a topological obstruction and one cannot pass through the other without a connecting disclination line which will have a strength of $|s| = 1$. Since the energy of this connection increases with its length i.e. the distance between the two half disclinations, there will be a considerable physical barrier for further separation. They act like rubber strings. However, if the two disclinations were to twist round each other an even number of times then they can be disentangled though they belong to different classes[6]. In the case of odd number of twists they cannot be disentangled since the problem gets reduced to one of single twist i.e. a crossing between the partners[6]. It has been speculated that such a biaxial phase, with many line defects that can entangle, may behave like a polymer type structure and one will observe topological rigidity in elastic and flow properties.

(v) *Non-singular disclinations*: The A phase of ^{3}He is again described by a local trihedron as in biaxial nematics excepting for the fact that one of the axes transforms as a pseudovector as it represents the angular momentum. It was established by Anderson and Toulouse[8] that in this phase disclination lines of $s = \pm 2$ are non-singular. Exactly the same argument has been put forward[4] for $s = \pm 2$ lines in biaxial nematics. We give in figure 2 the three-dimensional distortion that eliminates the singularity. Here the **c**-director bends through $\pm\pi$ as $r \to 0$ and the singularity at $r = 0$ is removed.

It must be remarked that one can even get rid of the singularity through a twist instead of bend. We also notice that this distortion is very different from director escape in $s = 2$ of uniaxial nematics. In uniaxial nematics the director rotates through $\pm\pi/2$ as $r \to 0$.

HYBRID DISCLINATIONS

The symmetry of the biaxial phase permits us to construct again through a Volterra process, another type of defect[9] which can be

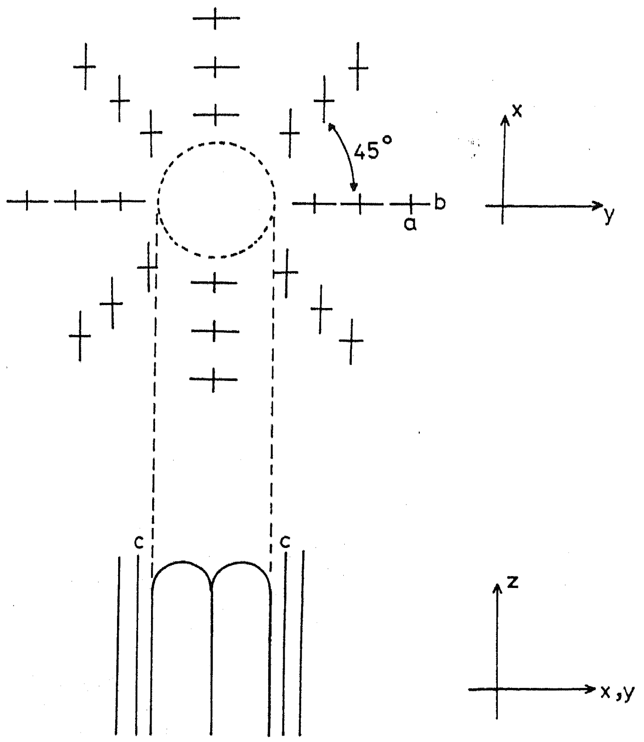

Figure 2. $s = +2$ disclination in $\mathbf{a}-\mathbf{b}$ fields. Inside the region indicated by the circle the $\mathbf{c}$ director escapes through π as shown in the meridional section.

termed an hybrid disclination for reasons that will be clear soon. The Volterra process for creating one such defect (figure 3a) is given below:

(1) Let the plane of cut $\mathbf{b}-\mathbf{c}$ be limited by a line L perpendicular to $\mathbf{c}$ and $\mathbf{a}$ i.e. parallel to $\mathbf{b}$, (2) the two faces of the cut are rotated by a relative angle $\pm 2\pi s_1$ about the $\mathbf{c}$ director i.e. the two faces of cut will now have $\mathbf{b}$ or $\mathbf{a}$ director field. (3) These faces are further rotated through a relative angle $\pm 2\pi s_2$ about the line L. The empty space is filled up with material or overlapping regions are removed and the system is allowed to relax. Steps (2) and (3) can be interchanged. The object so created is a hybrid of two types of disclinations: a twist disclination of strengths $\pm s_1$, and a wedge disclination of strength $\pm s_2$. This may be called a wedge-twist hybrid. In figure 3(b) we show two such hybrids. Another type of hybrid disclination can be created if instead of step (3) we turn the cut surfaces through a relative angle $\pm 2\pi s_2$ about an axis perpendicular to $\mathbf{c}$ and L. This gives a twist-twist hybrid.

When biaxiality disappears the above hybrid disclinations go respectively over to the classical wedge and twist disclinations of uniaxial nematics.

(i) *Interaction between hybrids*: A wedge-twist hybrid disclination can be looked upon as a combination of a twist disclination of one class with a wedge disclination of another class. In a simple theory we can employ this model to predict possible interactions between the hybrids. For instance, consider two parallel hybrids whose wedge components are of the same sign and class, and whose twist components are of opposite signs but of same class. Then the wedge components will repel and twist compo-

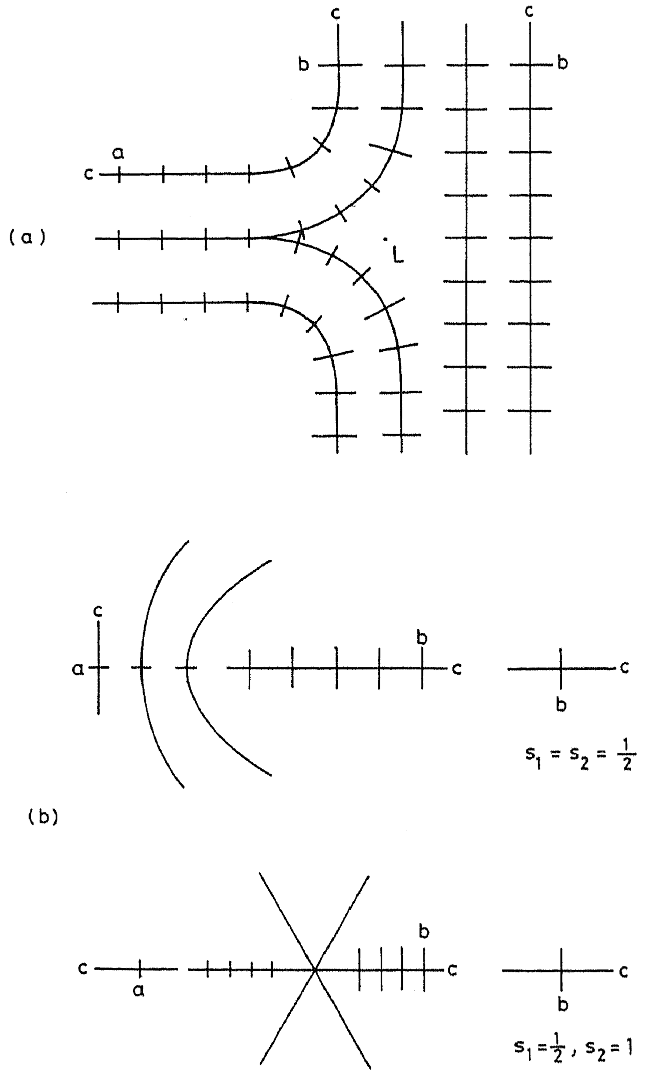

Figure 3a,b. **(a)** Volterra process for creating a hybrid disclination; **(b)** Two hybrids with $s_1 = s_2 = \frac{1}{2}$ and $s_1 = \frac{1}{2}$, $s_2 = 1$. Only the vectors in the plane of the figure have been shown.

nents will attract and depending upon their strengths the hybrids may either repel one another or end up in a bound state.

In the same way we can argue that interaction between two such hybrids will be different from what the above process predicts in the presence of a half defect which may or may not belong to any of the two component classes of the hybrid. If it belongs to one of the component classes then the other component of the hybrid will change sign when it loops once around this half defect. If it does not belong to either class then both the components will change sign. Thus interaction will be path-dependent. Very similar arguments hold for twist-twist hybrids.

(ii) *Non-singular hybrids:* Consider a wedge-twist hybrid with $s_1 = s_2 = 1$ and allow the nematic-like planar director field of the wedge component to escape through $\pm \pi/2$ in the third dimension (through a bend for all radial or a twist for all circular configuration) so that at $r = 0$ it is vertical. That is it escapes

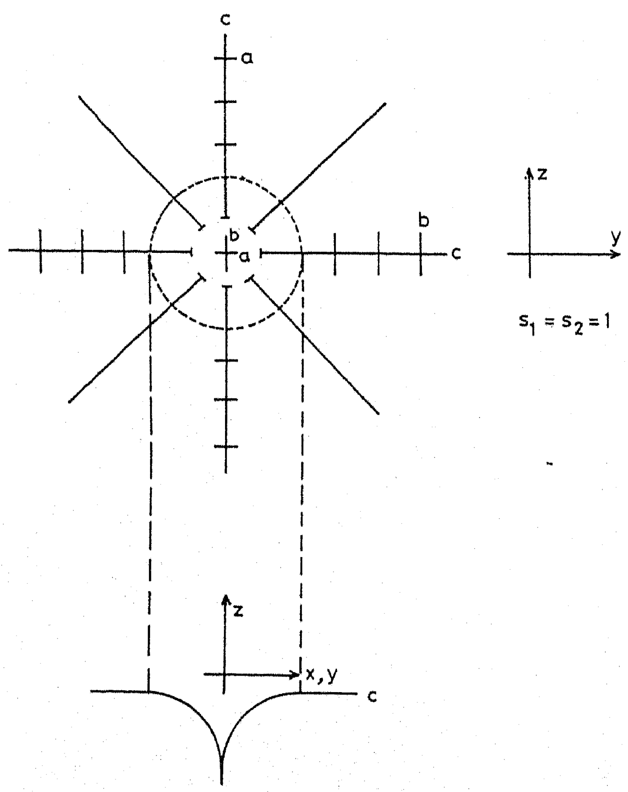

Figure 4. Removal of singularity in a hybrid with $s_1 = s_2 = 1$ by an escape in the **c** director through $\pi/2$.

as in uniaxial nematics. This is depicted in figure 4. In this process the twist component also loses its singularity at $r = 0$. Thus we find a singularity-free configuration of $\mathbf{a}-\mathbf{b}$ orientation at $r = 0$. Therefore such hybrids are truly non-singular. It must be remarked that exactly the same process was suggested many years ago by Mermin and Ho[10] for ^{3}He in the A phase in an experimental geometry that simulates the all radial wedge-twist hybrid structure with $s_1 = s_2 = 1$. However, the singularity will not disappear if the twist component is half integral. In fact in such hybrids we have at $r = 0$ a pure wedge disclination of strength $|s| = \frac{1}{2}$. Thus such a hybrid with one integral component and another of strength $|s| = \frac{1}{2}$ is topologically equivalent to one of the three half disclinations. Only when both components of the hybrid are integral we find it to be non-singular.

POINCARÉ CONFIGURATIONS

In classical nematics we can have half integral point defects[11] which are not isolated defects but the end points of disclinations of strength ± 1. These can be obtained by a technique employed long ago by Poincaré and for this reason we call them Poincaré defects. For example, one of the simple ones has $a + \frac{1}{2}$ wedge structure in the meridional plane. And in every case the director turns through $\pm \pi/2$ when we go round the defect from the $-z$ direction to the $+z$ direction in any meridional plane, and $+z$ direction is singularity-free. Along $-z$ direction, we have a disclination of strength ± 1.

We can construct similar objects even in biaxial nematics. We saw earlier that in a hybrid with $s_1 = s_2 = 1$ the wedge component is exactly like that in uniaxial nematics. If this is folded up smoothly and continuously (i.e. a rotation through $\pm \pi/2$) so that it goes from the xy plane to the $+z$ axis, then not only does the wedge singularity in this director but also the singularity in the other director disappears along $+z$. Thus $s_1 = s_2 = 1$ hybrid can terminate in a Poincaré half-defect point. However, if we impose the Poincaré configuration on a

$|s| = 1$ wedge disclination in one pair of fields, it gets transformed into a $|s| = 1$ wedge disclination in another pair of fields.

MONOPOLES AND BOOJA

One can have isolated point defects in uniaxial nematics. For instance, inside a spherical nematic drop with the director being normal at the surface, we get a hedgehog configuration. In every meridional plane it has the $s = 1$ all radial structure. However point defects are not possible in biaxial nematics[4,5]. If we attempt to construct an hedgehog then we have to replace each radiating line of cylindrical symmetry by a rectangular strip. One of the three vectors, say the **c** director, will be radiating out, while the other two, viz. **a** − **b** will be always locally normal to the radiating lines (figure 5a). Thus at all values of r the directors **a** and **b** always get mapped on to a sphere of radius r surrounding the central part. In any such mapping we always get wedge singularities (figure 5b). In principle the total strength of the wedge singularity is $+2$. We can have the singularity at a single point with strength $+2$ or two diametrically placed points with defect strength $+1$ each or even four symmetrically placed points each of strength $+\frac{1}{2}$. Therefore we end up with a hedgehog point defect in the **c** vector associated with (a) a wedge line of strength $+2$ in **a** − **b** running from the centre to the surface, (b) two wedge lines of strength $+1$ each (figure 5c) or (c) four wedge lines of strength $+\frac{1}{2}$ each. Thus it is very similar to the Dirac monopole defect structure of smectic C: a point defect in the layer normal **n** associated with strings (i.e. disclinations) or filaments in the projection vector **t**.

In the case of (a) if we shift the central point defect to the point singularity on the surface where the string or the $+2$ wedge line starts, then we get a Boojum. This exactly is like the Boojum suggested by Mermin[12] for ^{3}He-A drops. But this calls for a bend in the **c**-vector while the Dirac monopole structure has only splay.

SOLITONS

So far we have considered only singular-distortions i.e. ones that have singularities in the director fields. The singularities in these distortions cannot be removed by local fluctuations which will bring the distortion to a uniform state. However, there are also non-singular distortions[6] which again will not relax to the uniform ground state due to the constraining boundary conditions. They have been termed as solitons.

(i) *Planar solitons or domain walls:* The twist or bend or splay walls of a uniaxial nematic in a magnetic field are good examples of planar solitons[3]. Far away from a given plane the director is uniform. Most of the distortion, which is non-singular, is confined to a field-dependent characteristic thickness.

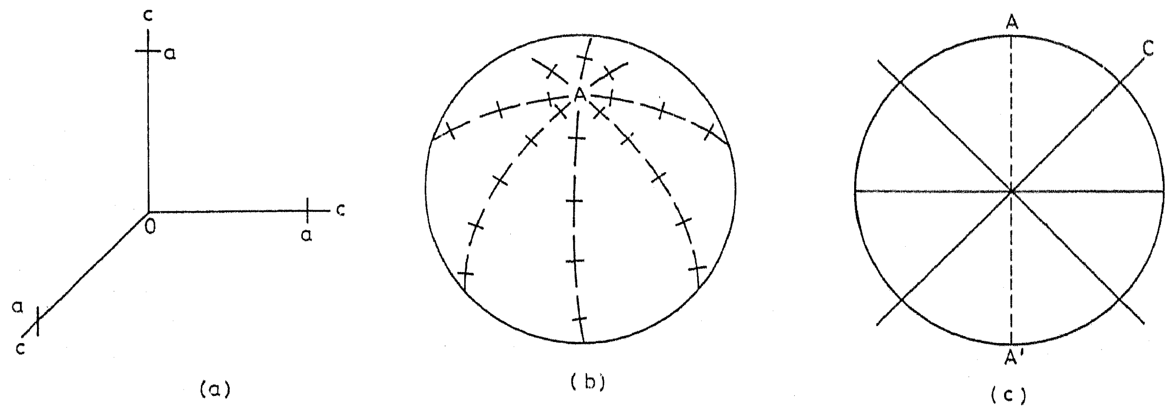

Figure 5a-c. **(a)** **c** director radiating out from 0 with **a** being normal to it everywhere; **(b)** Mapping of **a** − **b** fields on a sphere resulting in $s = 1$ defect at A and its antipode A'; **(c)** A meridional section with point defect in **c** and string in **a** − **b** denoted by the dotted line.

Very similar structures can be constructed and hopefully stabilized by the same process in a biaxial nematic as well. For example, the **c**-director can be along the z-axis far from the wall. Inside the wall it can have a bend in the zx plane or a twist distortion about x axis through an angle $\pm\pi$ (of course, this will require **a** or **b** director to have a splay or twist inside the wall). One axis of the trihedron will remain distortion-free in the configuration (figure 6). Such walls, as in uniaxial nematics, can end in half wedge or twist disclinations.

The symmetry of the biaxial phase also permits us to think of walls wherein **a** – **b** director rotates locally about **c** (which itself is bent or twisted inside the wall) through $\pm\pi$ so that we again have a uniform state far from the wall. We can call them hybrid walls. They can end in hybrid disclinations of half strength.

(ii) *Linear solitons or cylindrical domains:* Here we demand that the phase be in a uniform state far from a given line with non-singular distortions being confined mostly to a cylinder around the line. In uniaxial nematics[3] we get it by radially buckling or twisting the director which is parallel to the given line, through $\pm\pi$ as $r \to 0$. Of course, at half the radius of the cylinder, we get $s = +1$ director configuration which is perpendicular to the uniform state. By analogy we can get a linear soliton in biaxial nematics by allowing one of the directors, say **c**, of the uniform state to radially bend or twist through $\pm 2\pi$ as $r \to 0$. At half the radius we get a $s = +2$ director configuration in the **a** – **c** or **b** – **c** fields. Outside the cylinder the trihedron is in a uniform state with **c** parallel to the cylinder axis and at $r = 0$ there is no singularity. This configuration can probably be stabilized again with a magnetic field.

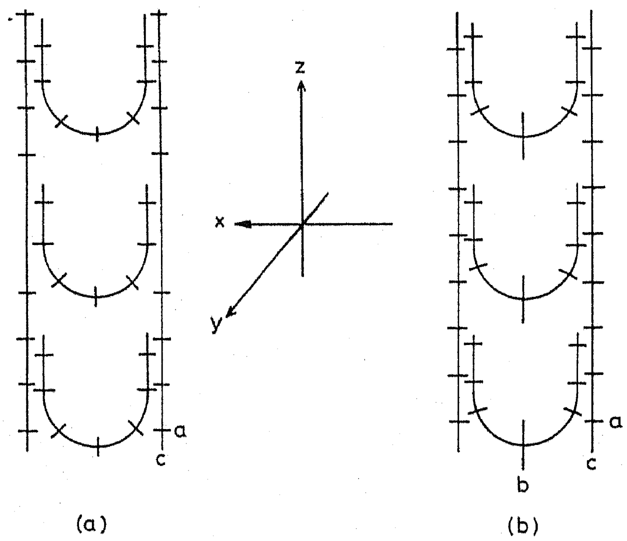

Figure 6a,b. **(a)** Soliton in **a** – **c** fields. **c** director bends through π; **(b)** Hybrid soliton having bend in **c** and twist about **c**.

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