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The Topological Microstructure of Defects in Nematic Liquid Crystals

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We study the core of line and point defects in nematic liquid crystals. The topological theory of defects allows us to prove that a uniaxial nematic has two ways to avoid a topologically stable defect: either it melts, by becoming isotropic on the putative defect, or a complex biaxial structure arises, that we describe in the paper.

Keywords: Nematic liquid crystals; defects; topology

1. INTRODUCTION

The understanding of defects – both lines and points – in liquid crystals has a long history. Oseen [1] in the 1930s, and Frank [2] in 1958, sketched the director configurations of what Frank called *disclinations*, as opposed to the *dislocations* he was used to in the study of defected solids. Frank identified disclination lines along which the nematic order parameter could no longer be defined. The disclination lines could be indexed according to the number of times the director turned as the defect line was circumnavigated. Thus an index $m = 1/2$ line indicated that the director made a 1/2 turn or a turn of $\theta = 2\pi \times 1/2$ in going around the disclination line. Defects of half integer index were admissible; the half integer (as opposed to only whole integer) being a feature peculiar to liquid crystals due to the symmetry of the molecules that makes the director n equivalent to $-n$.

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Frank further subclassified the disclination lines into *wedge* and *twist* disclination lines, depending on the angle between the plane of rotation of the director and the plane perpendicular to the defect line. This particular classification was also borrowed from the dislocations of material science. The wedge disclinations have the director always in the plane perpendicular to the defect, whereas in the twist disclinations the director, unsurprisingly, twists its way around the defect line. A further interesting feature of defect lines which was noticed relatively early is that the defects of integer index are not *real* defects, for the director can *escape*. Taking as an explicit case the wedge disclination of index 1, in which the director points radially away from the defect line, close to the defect line the director simply bends out of the plane perpendicular to the disclination, and on the defect line itself (or what we thought was the defect line) the director points along the line. Hey presto, the defect has disappeared!

The topological classification of defects elucidated this initially surprising conclusion [3, 4, 5]. It now became clear that when the order parameter manifold $\mathscr{R}$ is topologically trivial the system is able to avoid defects, where defects can now be explicitly identified as discontinuities of the application that assigns an order parameter to every point of the body. This classification was extremely useful in liquid crystals. There is now only *one* topologically independent type of disclination line. All of Frank's examples of apparently different disclination lines can be continously twisted, distorted or otherwise deformed into the same unique object.

This all follows from the topological theory. The inputs here are: (a) the *order parameter manifold*, which in the case of strictly uniaxial liquid crystals is equivalent to the real projective plane $\mathscr{P}^2$; and (b) its *fundamental group* - that is, the group of homotopy classes of closed paths of the order parameter, which in the uniaxial case is the cyclic group $\mathscr{Z}_2$. This group has just two elements: $\{1, x\}$, with $x^2 = 1$. These elements identify the topologically distinct defects; the unit element identifying the *lack* of a defect. Putting two index 1/2 wedge disclinations together is equivalent to combining two elements x; $x^2 = 1$ indicates that the disclination (now of index 1) disappears.

And yet, we are still missing something. What has happened to the former menagerie of disclination types? And what happens in the *immediate* region of the disclination line? It is the latter question which we address in this paper. These are questions for which topology does not provide all the answers; we shall nevertheless use topology to delve inside the defect core.

In order to describe the kind of problem we have to face and the way we overcome it by means of the embedding of $\mathscr{P}^2$ in an appropriate manifold, we focus our attention on a simple example. Let us consider an $m = -1/2$

wedge defect along the z-axis (see Fig. 1). Far from the defect, the degree of order $\bar{P}_2$ attains a constant value, and the director is given by $(\cos\frac{1}{2}\varphi, -\sin\frac{1}{2}\varphi, 0)$, where φ is the usual polar azimuthal variable. Now what happens on the z-axis? Clearly the fluid is no longer nematic, because it is impossible to define the director consistently. If it is not *nematic*, it is presumably isotropic - locally the phase loses its ordered configuration and becomes disordered. And if it is disordered, the degree of order $\bar{P}_2$ vanishes, and increases smoothly as the distance from the defect line increases.

Actually this picture is not entirely correct, although of course it contains more than a grain of physical truth. Versions of this picture have been put forward by Fan [6] and Ericksen [7]. The crucial question, again, concerns the order parameter manifold. The manifold of equilibrium states is indeed $\mathscr{P}^2$, and the macroscopic topological signature of the defects is determined by this manifold. But close to a defect the system is locally forced out of this manifold, and the question is – to what ?

We shall digress for a moment in order to inquire about the implicit prejudices which govern the belief that the core of a wedge disclination might be isotropic. The archetypal example of an ordered system which sustains line defects is the XY magnet. This system has low temperature phase governed by a complex order parameter $\eta = \rho e^{i\varphi}$, or equivalently an order parameter with magnitude ρ and director $\mathbf{n} = (\cos\varphi, \sin\varphi)$. The macroscopic order parameter manifold is S^1, and the fundamental group is the integer group Z, which is the topologist's way of saying that disclinations come with integer winding number, and then when you put two of them together, you add the winding numbers. The simplest disclinations are those

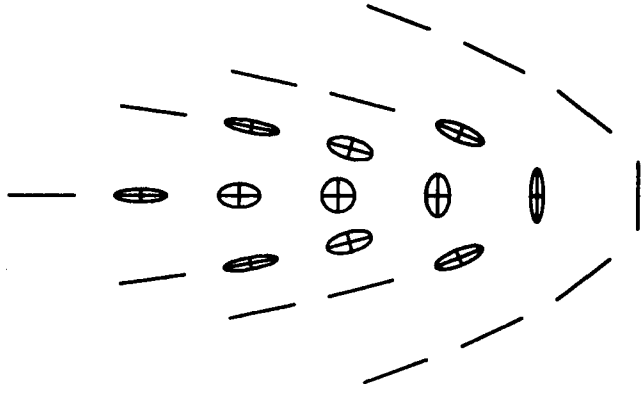

FIGURE 1

of index 1 or -1, and in these the asymptotic angle φ is equal to the azimuthal angle φ (index + 1) or minus the azimuthal angle (index − 1). As one approaches the defect line the magnitude of the order parameter ρ decreases. The core of the defect is truly isotropic. Macroscopically, on the defect line the director cannot be defined. On a microscopic scale, the signature of the defect is a line along which the order parameter is zero.

In the absence of topological insight the temptation is to describe the nematic wedge disclination similarly. Allowing the XY magnet to become a *Heisenberg* magnet (three, rather than two, internal degrees of freedom, S^2 rather than S^1) gives problems, because then the director can escape from integer-indexed defect lines, but changing to the nematic order parameter, and only considering half-inter defects restores the integrity of the disclination line. But otherwise one might think, 'the argument goes through'.

The mathematical formulation of this idea is as follows. The liquid crystal order parameter in a uniform uniaxial system can be described by the Saupe [8] ordering matrix Q_{ij}, where

$$Q_{ij} = S\left(n_i n_j - \frac{1}{3}\delta_{ij}\right), \tag{1.1}$$

where S is the degree of order proprotional to $\bar{P}_2$ and $\mathbf{n}$ is the director.

In a non-uniform system the simplest generalization is to allow the quantity S to be a function of poistion $\mathbf{r}$. The free energy density F becomes a functional of S, and symmetry considerations yield

$$S(\mathbf{r}) = S(r,\varphi) \tag{1.2}$$

where r is the radial distance from the disclinations. Furthermore, $S(\cdot,\varphi)$ is periodic with period $2\pi/3$, and $S(0,\cdot) = 0$ necessarily. This point of view leads naturally to the conclusion that the core of the dislocation contains a line along which the order parameter is strictly zero.

What is wrong with this idea? Mathematically it is fine. Where we find a problem is in the *physics*. The question is as follows: what is the natural mathematical object in which we embed the order parameter manifold $\mathscr{P}^2$ as the defect is approached? The natural object is $\mathscr{Q}$, the set of traceless symmetric second order tensors. A general element of $\mathscr{Q}$ can be written as:

$$Q_{ij} = S\left(n_i n_j - \frac{1}{3}\delta_{ij}\right) + p(l_i l_j - m_i m_j) \tag{1.3}$$

where $\{\mathbf{n}, \mathbf{l}, \mathbf{m}\}$ form an orthogonal set of unit vectors. The quantity p is often known as the *biaxial* order parameter.

There are at least two sensible reasons why this choice of order parameter is to be preferred over that of question (1.1). On a *microscopic* level, we can observe that the order parameter $\bar{P}_2$ only crops up if the director is already known; if it is not, the Saupe ordering tensor is the true order parameter, and

$$Q_{ij} \propto \left\langle \ell_i \ell_j - \frac{1}{3}\delta_{ij} \right\rangle, \tag{1.4}$$

where ℓ is the orientation of a single molecule and the mean is taken over molecules.

In the absence of external fields, Q_{ij} is uniaxial and takes the form given by equation (1.1). But this is primarily and *experimental* fact – justified *ex post facto* by the Landau-de Gennes theory. In fact a more complex set of molecules, with a more complex phenomenological theory, can be shown to exhibit equilibrium biaxial phases, and indeed Al Saupe [9] has been influential in exploring these.

A second reason comes from the macroscopic manifestation of the liquid crystal property form the electric or magnetic *susceptibility tensor*, which is roughly speaking proportional to the liquid crystal order parameter. Some back of the envelope calculations assure us that the energy associated with biaxial fluctuations (*i.e.* p becoming locally non-zero) is of the same order of magnitude as that associated with changes is S; *ergo*, the embedding of equation (1.1) is not physcially justified.

This idea underlies the observation by Lyusyuktov [10] that on shortish length scales close to a defect the energy barrier forbidding biaxiality would be overcome by gradient terms. The order parameter is released to explore a larger manifold – one which has a trivial fundamental group. The defects no longer exist – or at least there is no microscopic signature.

But in fact, this too is an oversimplification. Schopohl and one of the present authors [11], (and even earlier, independently, Meiboom *et al.* [12]) carried out more detailed calculations of the internal structure of wedge disclinations. We concentrate on the behaviour of the eigenvalues of the matrix Q in a slice through the core of the defect, shown in Figure 2. At $x = -\infty$ and $x = +\infty$ the order parameter is *uniaxial* with eigenvalues $\{2/3, -1/3, -1/3\}$ in both cases. As we traverse the defect the eigenvalues exchange, so that a different eigenvalue is the principal eigenvalue on each side of the defect.

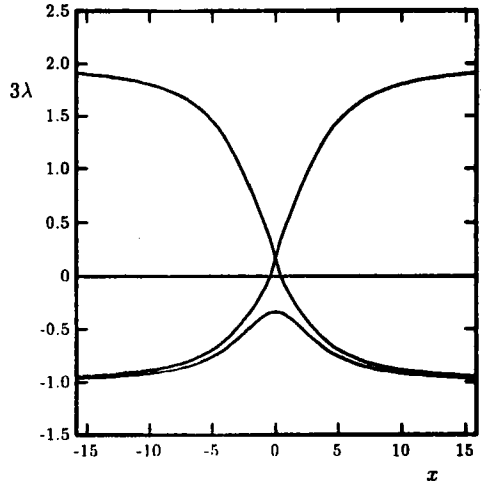

FIGURE 2

Let us examine the features of Figure 2 [11]. In an outer region $r \geqslant 10\xi$ (ξ is the characteristic scale for order parameter changes), the two negative eigenvalues reduce from their bulk value, but hug each other tightly. On this scale, the nematic liquid crystal is indeed uniaxial. Inside this the two negative order parameters part company. One remains negative. The other two exchange places. There are two crucial types of points that we can identify. The point where the eigenvalues change places can be identified with the centre of the defect core. This corresponds to a *line* in three dimensional space, along which the nematic is again uniaxial, but now with *negative* order parameter, for the principal eigenvalue is now negative. The points where one of the eigenvalues cross zero form a *cylinder* in three dimensional space. On this cylinder, which surrounds the defect, $\det(\mathbf{Q}) = 0$. In what follows we shall prove this result rigorously.

In Section 2 we recall the definition and the main properties of the manifold $\mathcal{Q}$. In Section 3 we prove our main theorem, that shows that there are two ways to aviod both points and lines defects in uniaxial liquid crystals. Either the system *melts*, by becoming isotropic on the putative defects, or the following structure arises: a biaxial region surrounds the former defect, which is replaced by uniaxial points where the order parameter s has a negative value (*i.e.* opposite to the sign it attains on the boundary of the system); furthermore there is a biaxial surface, which encloses the new uniaxial points, where one of the eigenvalues of $\mathbf{Q}$ vanishes, so that $\det \mathbf{Q} = 0$.

2. ORDER PARAMETER MANIFOLD OF NEMATIC LIQUID CRYSTALS

The microscopic properties of a nematic liquid crystal are described by the second order tensor [13, 8,7] $\mathbf{Q}(x)$ defined in equation (1.4). The symmetric traceless tensor $\mathbf{Q}$ takes values in the manifold

$$\mathcal{Q} := \left\{ \mathbf{Q} = \sum_{i=1}^{3} \lambda_i e_i \otimes e_i : \sum_{i=1}^{3} \lambda_i = 0,\ \lambda_i \geqslant -\frac{1}{3} \right\}. \tag{2.1}$$

In [14] two of the present authors have studied in detail the topological properties of $\mathcal{Q}$ and its most significant submanifolds, namely

(i) $\mathcal{B} := \{\mathbf{Q} \in \mathcal{Q} : \lambda_i \neq \lambda_j \forall i \neq j\}$, the class of biaxial distributions;
(ii) $\mathcal{U}^* := \{\mathbf{Q} \in \mathcal{Q} : \lambda_i = \lambda_j \neq \lambda_k \text{ for } i \neq j \neq k\} = \{\mathbf{Q} = s(n \otimes n - \frac{1}{3} I),\ s \in [-\frac{1}{2}, 1] \setminus \{0\},\ n \cdot n = 1\}$, the set of anisotropic uniaxial distributions;
(iii) the singleton $\{0\} \subset \mathcal{Q}$, which describes the isotropic distribution.

In the following we will also consider $\mathcal{U} := \mathcal{U}^* \cup \{0\}$, the submanifold of all uniaxial distributions, $\mathcal{U}^+$ (respectively $\mathcal{U}^-$): $= \{\mathbf{Q} \in \mathcal{U} : s > 0$ (respectively $s < 0\}$, the class of prolate (respectively oblate) uniaxial distributions, and $\mathbf{Q}^* := \mathcal{Q} \setminus \{0\} = \mathcal{U}^* \cup \mathcal{B}$, the set of all anisotropic distributions.

3. TOPOLOGICAL MICROSTRUCTURE OF NEMATIC DEFECTS

Before stating Theorem 1 below, we prove two Lemmas, where we illustrate which topological tools are at work here.

LEMMA 1 *A strictly uniaxial liquid crystal can be forced to have isotropic point defects.*

Proof Let us consider the manifolds $\mathcal{U}$ and $\mathcal{U}^*$ introduced above. We want to show that topology can, under some circumstances, dictate the existence of a distribution $\mathbf{Q} = 0$. To do so, we only have to prove that $\mathcal{U}$ is topologically trivial, while $\mathcal{U}^*$ is not. In fact, the former assertion implies that a uniaxial material can never be forced to have discontinuities of the application $\mathbf{Q}(x)$, while the latter tells us that it can be forced to have *defects* (thought of as isotropic points).

In other words, given any continuous boundary condition, the application $\mathbf{Q}(x)$ can always be made continuous in the whole domain where it takes values in $\mathcal{U}$; by constrast, $\mathbf{Q}(x)$ could fail to be so if all its values are in

$\mathcal{U}^*$. Then, when we are considering a uniaxial material, the singular points that we classify by studying $\mathcal{U}^*$ are points belonging to $\mathcal{U}\backslash\mathcal{U}^* = \{0\}$.

To study the topological properties of any manifold it is useful to use its deformation retracts. With them, we can deform (in a continous and homotopy preserving way) the original manifold until we reach some well-known manifold, whose topological properties are already known. We will use this technique in the study of both $\mathcal{U}$ and $\mathcal{U}^*$.

$\mathcal{U}$ can be continously deformed onto the isotropic point, by the continuous application $\mathbf{F}:\mathcal{U}\times[0,1]\to\mathcal{U}$ defined by

$$F\left(s\left(n\otimes n-\frac{1}{3}I\right),t\right):=(1-t)s\left(n\otimes n-\frac{1}{3}I\right); \tag{3.1}$$

note that $\mathbf{F}(\mathcal{U},0)=\mathcal{U}$ and $\mathbf{F}(\mathcal{U},1)=\{0\}$. The topological properties of a point are obviously trivial.

$\mathcal{U}^*$ has two connected components ($\mathcal{U}^*_+$ with positive s, and $\mathcal{U}^*_-$ with negative s). Each component can be continously deformed onto $\mathcal{P}^2$ by means of the applications $\mathbf{F}\pm:\mathcal{U}^*_\pm\times[0,1]\to\mathcal{U}^*_\pm$ such that

$$F_+\left(s\left(n\otimes n-\frac{1}{3}I\right),t\right):=(1-t)s\left(n\otimes n-\frac{1}{3}I\right)+t\left(n\otimes n-\frac{1}{3}I\right),$$

$$F_-\left(s\left(n\otimes n-\frac{1}{3}I\right),t\right):=\left(-\frac{1}{2}-t\right)s\left(n\otimes n-\frac{1}{3}I\right)+t\left(n\otimes n-\frac{1}{3}I\right). \tag{3.2}$$

In fact, F_+ (resp. F_-) deforms $\mathcal{U}^*_+$ (resp. $\mathcal{U}^*_-$) onto its subset characterized by $s=1$ (resp. $s=-1/2$), and both these subsets are equivalent to the real projective plane $\mathcal{P}^2$.

LEMMA 2 *A nematic liquid crystal can avoid any isotropic point by becoming biaxial in a neighbourhood of it.*

Proof We need to show that the manifold $\mathcal{Q}^*$ is topologically trivial, so that all isotropic defects found in $\mathcal{U}^*$ can dissolve in it.

The set $\mathcal{Q}$ is a path-connected and convex five-dimensional manifold, so that it is homotopic to the five-dimensional unit ball $\mathcal{B}^5$. Since $0\in\mathcal{Q}$ is an interior point, from elementary topology [14] we obtain that $\mathcal{Q}^*$ is

homotopic to $\mathcal{S}^4$, the four-dimensional unit sphere which, as far as we are concerned, is topologically trivial, in the sense that its first three homotopy groups are trivial.

The desired conclusion follows from the fact that $\mathbf{Q}(x)$ can then attain all its values in $\mathcal{Q}^*$, which does not contain the isotropic distribution.

We are now in a position to prove our main result.

THEOREM 1 *Let $\mathcal{U}^*$, $\mathcal{U}^*_\pm$ and $\mathcal{B}$ be the manifolds defined above.*

(i) $\mathcal{U}^*_+ \cup \mathcal{B}$ (respectively $\mathcal{U}^*_- \cup \mathcal{B}$) is topologically equivalent to $\mathcal{U}^*_\pm$ (resp. $\mathcal{U}^*_-$). The same isotropic defects that can be found in a uniaxial nematic with only positive or only negative values of s survive if we let it become biaxial; thus, the isotropic points cannot be changed into biaxial distributions. They can only be replaced by uniaxial distributions with inverted sign of s.

(ii) When isotropic defects of $\mathcal{U}^*_+$ or $\mathcal{U}^*_-$ are relaxed in $\mathcal{U}^* \cup \mathcal{B}$, a surface of biaxial tensors with null determinant which surrounds the uniaxial points that replace the original defect always appear.

Proof To prove part (i) of the Theorem we will show that $\mathcal{U}^*_+$ is a deformation retract of $\mathcal{U}^*_+ \cup \mathcal{B}$, so that they share the same homotopy groups. The proof that $\mathcal{U}^*_+$ and $\mathcal{U}^*_- \cup \mathcal{B}$ are topologically equivalent can be constructed almost in the same way, and so it will be omitted.

Every $\mathbf{Q} \in \mathcal{U}^*_+ \cup \mathcal{B}$ can be written as

$$\mathbf{Q} = \sum_{i=1}^{3} \lambda_i \mathbf{e}_i \otimes e_i, \tag{3.3}$$

where either $\lambda_1 > \lambda_2 > \lambda_3$(if $\mathbf{Q} \in \mathcal{B}$) or $\lambda_1 > 0, \lambda_2 = \lambda_3 < 0$ (if $\mathbf{Q} \in \mathcal{U}^*_+$). In any case, let $\mathbf{Q}_f(\mathbf{Q})$ be the tensor

$$\mathbf{Q}_f(\mathbf{Q}) := \lambda_1 e_1 \otimes e_1 + \frac{\lambda_2 + \lambda_3}{2}(e_2 \otimes e_2 + e_3 \otimes e_3); \tag{3.4}$$

note that $\mathbf{Q}_f(\mathbf{Q}) = \mathbf{Q}$ if, and only if, $\mathbf{Q} \in \mathcal{U}^*_+$. A retraction of $\mathcal{B} \cup \mathcal{U}^*_+$ onto $\mathcal{U}^*_+$ is then

$$F(\mathbf{Q}, t) := (1 - t)\mathbf{Q} + t\, \mathbf{Q}_f(Q). \tag{3.5}$$

In fact, $\mathbf{F}$ is continuous, it maps $\mathcal{U}^*_+ \cup \mathcal{B}$ onto $\mathcal{U}^*_+$ and its restriction to $t = 0$ is the identity on $\mathcal{U}^*_+ \cup \mathcal{B}$. Note that the application (3.5), if defined on the whole of $\mathcal{Q}^* = \mathcal{U}^*_+ \cup \mathcal{B} \cup \mathcal{U}^*_-$, is not continuous since $\mathbf{Q}_f(\mathbf{Q})$ fails to be so in all points of $\mathcal{U}^*_-$ (this is why $\mathcal{Q}^*$ is not equivalent to $\mathcal{U}^*_+$).

The second part of the Theorem can be proved by considering the function det **Q**. It is a continuous function which attains positive values far away from the defect (where $\mathbf{Q} \in \mathcal{U}^*_+$) and a negative value at the uniaxial point (s) which has (have) replaced the defect. By the mean value theorem, det **Q** vanishes at a surface that encloses the uniaxial point(s) with negative *s*. Finally, this surface must be biaxial since the only uniaxial distribution with zero determinant is the isotropic one, but our application takes values in $\mathcal{U}^* \cup \mathcal{B}$, thus excluding that possibility.

To illustrate better the Theorem above, we close our paper with an example. Let us consider the class $C_{\mathbf{v}}$ of all distributions that share one fixed eigenvector **v**. This class is very useful in studying the properties of nematic liquid crystals near a bounding surface, where the normal **v** breaks the symmetry among all directions, and so it may well be an eigenvector of **Q**.

$C_{\mathbf{v}}$ is topologically equivalent to a cone [15] similar to that shown in Figure 3. In it, both biaxial and uniaxial distributions are represented, as well as the isotropic one. In particular:

(i) $\{0\}$ is the vertex of the two-fold cone in the figure;
(ii) $\mathcal{U}^*_+ \cap C_{\mathbf{v}}$ consists in the lower part of the two-fold cone and the upper part of the axis (the bold lines in the figure);
(iii) $\mathcal{U}^*_- \cap C_{\mathbf{v}}$ consists in the upper part of the two-fold cone and the lower part of the axis (the dashed lines in the figure), and
(iv) the rest of the cone belongs to $\mathcal{B} \cap C_{\mathbf{v}}$.

Now, consider in $\mathcal{U}^*_+ \cap C_{\mathbf{v}}$ the non-trivial closed loop γ shown in Figure 4: γ cannot be shrunk to a point in $\mathcal{U}^*_+ \cap C_{\mathbf{v}}$ since this latter lacks the

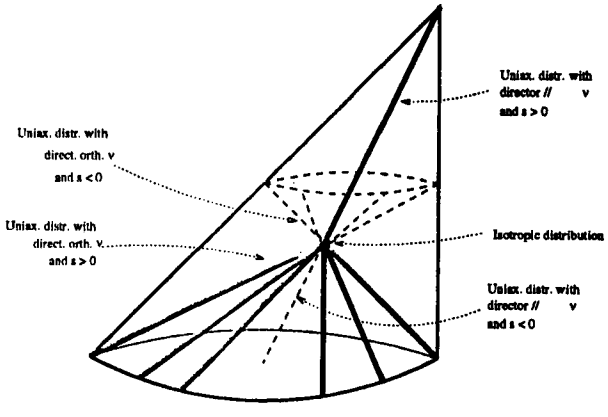

FIGURE 3

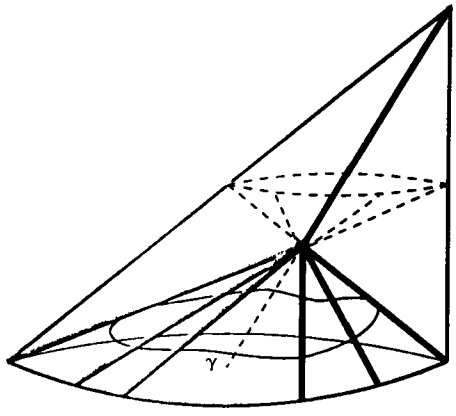

FIGURE 4

isotropic vertex of the two-fold cone. One can easily be convinced, just by looking at the figure, that there are only two ways to shrink γ avoiding the isotropic distribution $\{0\}$: either by touching the lower part of the axis of C_v or by crossing the upper part of the two-fold cone. In both cases some uniaxial distribution with negative s have been traversed.

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