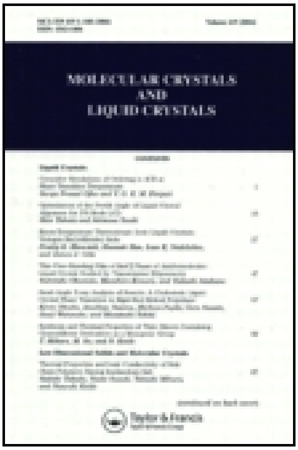

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Interaction Between a Caviy and a Singularity in Nematics

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Interaction Between a Cavity and a Singularity in Nematics

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It is shown that a singularity of strength s interacts with a cylindrical cavity having uniform boundary conditions, as though instead of the cylindrical cavity there is a singularity of strength s at the conjugate point together with one of strength $(1 - s)$ at the centre. At large distances the cavity acts as a disclination of strength $+1$. Disclinations of negative strength form dipoles with the cavity. An extension of this result can account for the interaction between a spherical cavity and a singular point.

INTRODUCTION

Disclinations are line singularities found in an otherwise perfectly aligned liquid crystal. Their structure and properties have been studied in detail in the case of nematic liquid crystals.[1–4] More recently[3,5,6] even point singularities have been found to exist in nematics. In many ways they behave like disclination lines. For instance point singularities of opposite sign attract and of like sign repel one another. Point singularities interact with spherical cavities and in fact -1 singular point forms a dipole with a spherical cavity.[3,6] It has also been noticed that only a $+1$ singular point is found inside a capillary[3] or a nematic drop.[7]

In this paper the problem of the interaction of a line singularity with a cylindrical cavity with its axis parallel to the singular line is considered. It is shown that outside the cylinder a positive disclination is always repelled by the cavity, while a negative singularity forms a dipole disclination. On the other hand if we try to confine a singularity in a cylinder we find that only $s = +1$ singularity can be stabilized. Disclinations with $s \neq 1$ will be considered distorted by the cylindrical boundary. These results can be qualitatively generalized to singular points and many of the experimental observations accounted for.

Theory

In the one elastic constant approximation ($K_{11} = K_{22} = K_{33}$), the equation of elastic equilibrium in cylindrical polars is

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r}\frac{\partial \phi}{\partial r} + \frac{1}{r^2}\frac{\partial^2 \phi}{\partial \alpha^2} + \frac{\partial^2 \phi}{\partial z^2} = 0 \qquad (1)$$

where ϕ is the orientation of the director at (r, α, z), and the distortion is planar. Solutions of this equation describing disclinations with singular lines along z-direction, are[1,3]

$$\phi = s\alpha + c_0 = s \tan^{-1}\frac{y}{x} + c_0 \text{ (arbitrary constant)} \qquad (2)$$

with the singular lines at (0, 0) and $s = \pm n/2$, n being an integer. When a group of singularities are present the director orientation at (x, y) is[3]

$$\Phi = \sum_k s_k \tan^{-1}\left[\frac{y - y_k}{x - x_k}\right] + c. \qquad (3)$$

Here s_k is the strength of the singularity at (x_k, y_k) and c a constant.

Consider a disclination of strength s placed at a distance D from the centre of a cylinder of radius R, i.e., at $r = D$ and $\alpha = 0$ such that the line of singularity is parallel to the axis of the cylinder. Figure 1 gives the (x, y) section of the geometry with $R < D$, i.e., the disclination is outside the cylinder. Let a disclination of strength $(1 - s)$ be at the centre of the cylinder and one of strenght s at a distance D' from the centre at $r = D'$ and $\alpha = 0$. Net orientation at $P(x, y)$ a point on the cylinder according to Eq. (3) is:

$$\Phi = (1 - s)\tan^{-1}\frac{y}{x} + s\tan^{-1}\frac{y}{x - D'} + s\tan^{-1}\frac{y}{x - D} + c$$

$$= (1 - s)\tan^{-1}\frac{y}{x} + s\tan^{-1}\left[\frac{y(2x - D' - D)}{x^2 + D'D - x(D' + D) - y^2}\right] + c.$$

If D' is such that $DD' = R^2$ $(= x^2 + y^2)$ then Φ becomes

$$\Phi = (1 - s)\tan^{-1}\frac{y}{x} + s\tan^{-1}\frac{y}{x} + c$$

or

$$\Phi = \alpha + c, \qquad (4)$$

which implies that there is a uniform alignment on the surface of the cylinder. Therefore assuming uniform boundary conditions (i.e., that on the surface the director is everywhere inclined at the same angle with respect to radius

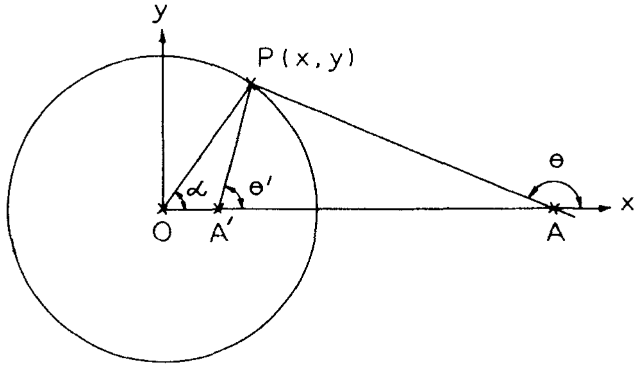

FIGURE 1 A line singularity of strength s at a distance D from the centre of a cylindrical cavity of radius R. $0A = D$, $0A' = D'$ and $0P = R$.

vector) the cylinder can be replaced mathematically by two disclinations, one of strength $(1 - s)$ at its centre and another of strength s at the conjugate point.

Results

1. *Disclination lines* The net force on a singularity of strength s_i due to singularities of strengths s_j kept at vector distances of $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is[3]

$$\mathbf{f}_i = 2\pi K s_i \sum_j s_j \frac{\mathbf{r}_{ij}}{r_{ij}^2}. \tag{5}$$

Using this equation, the net force acting on the disclination is

$$\mathbf{f} = 2\pi K \left[\frac{s(1 - s)}{D} + \frac{s^2}{D - D'} \right] \mathbf{r}_0 \tag{6}$$

$\mathbf{r}_0$ being a unit vector directed away from the centre of the cylinder towards the singularity. At large distances $(D \gg R)$ from the cylinder

$$\mathbf{f} = 2\pi K \frac{s}{D} \mathbf{r}_0. \tag{7}$$

In the neighbourhood of the cylinder $(D \approx R)$

$$\mathbf{f} = 2\pi K \frac{s^2}{D - D'} \mathbf{r}_0. \tag{8}$$

At very small distances $(D \ll R)$

$$\mathbf{f} = 2\pi K \frac{s(1 - s)}{D} \mathbf{r}_0. \tag{9}$$

Hence at far off points, the cylinder behaves as a $s = +1$ disclination located at its centre. At points near the surface it behaves as a disclination of strength s located at the conjugate point. In the limit $D \to R$, i.e., $D \to D'$, **f** becomes the image force. However at very small distances the cylinder behaves as though it had a singularity of strength $(1 - s)$ at its centre. Also the point at which $\mathbf{f} = 0$ is a position of equilibrium for the singularity. The equilibrium point is at

$$D_0 = R(1 - s)^{1/2}. \tag{10}$$

When the *disclination is outside the cylinder*, its interaction with the cylinder can be traced as follows. A negative disclination ($s < 0$) is attracted by the cylinder when it is at large distances and if it moves to distances closer than D_0 it is repelled by it. At D_0 it forms a dipole disclination with the cylinder. A positive disclination ($s > 0$) on the other hand is always repelled by the cylinder at all distances.

When the *disclination is inside the cylinder*, the only values of s resulting in real values of D_0 are $s = +\frac{1}{2}$ and $s = +1$. With $s = +\frac{1}{2}$ a complicated director field results inside the cylinder. However, with $s = +1$ for which $D_0 = 0$, i.e., the centre, the director pattern is unperturbed by the boundary. Hence only $s = +1$ can be stabilized inside the cylinder. If we try to contain singularities with $s > 1$ or $s < 0$ inside the cylinder, it will be strongly attracted by $(1 - s)$ which is at the centre. The singularity finally sits at the centre with its director field considerably distorted to resemble the $s = +1$ pattern. As an example the case of $s = -1$ is shown in Figure 2.

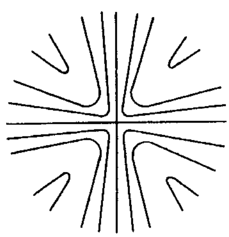

FIGURE 2 Confining a $s = -1$ singularity inside a cylinder with radial boundary conditions.

2. *Singular points* The structure of singular points have been worked out by Saupe[3] and Meyer.[4] Meyer studied in detail the singular points formed at the interface between a nematic and its isotropic phase. $A + 1$ singular point is found to have a director field of $s = +1$ or -1 in the XY plane and of $s = +1$ in the YZ and $s = +1$ or -1 in the ZX planes. Thus one possible structure of $+1$ singular point is a pure radial distribution of molecules. The structure of a -1 singular point can be described as follows. In the XY plane

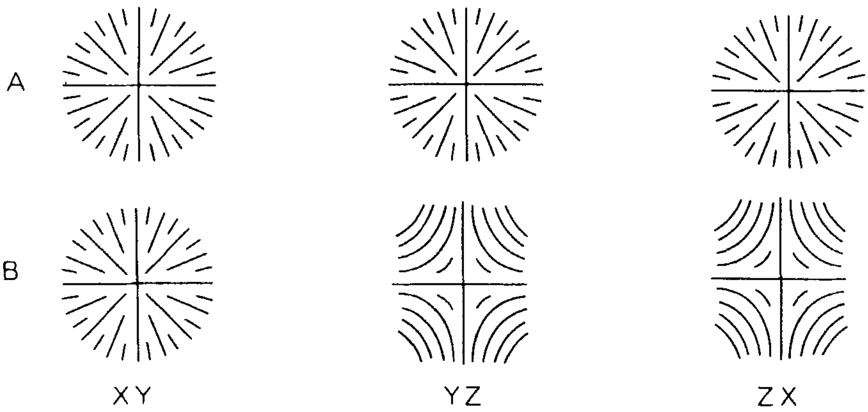

FIGURE 3 Director pattern around (A) + 1 and (B) − 1 point singularities. Both have $s = +1$ pattern in the XY plane. In the other two planes + 1 point has $s = +1$ structure and − 1 point has $s = -1$ structure.

it has a director field corresponding to $s = +1$ disclination. While in YZ and ZX planes it has $s = -1$ pattern (see Figure 3). For all these patterns $c = 0$.

Consider a + 1 point (with radial structure) and a − 1 point placed along the Z-axis at a distance of D apart. Let the X and Y axes of the two structures be made to coincide. Then in any plane passing through both the singularities, + 1 point has the $s = +1$ radial pattern and the − 1 point has $s = -1$ pattern. Hence they attract one another. If instead of the + 1 point we had a spherical cavity with normal boundary conditions on its surface then in any plane containing the centre of the cavity and the − 1 point we meet the problem discussed earlier. Hence the − 1 point is attracted by the cavity at large distances and repelled by it at small distances, thus forming a dipole disclination. Again the equilibrium distance is $R(1 - s)^{1/2} = R(2)^{1/2}$. Also at large distances the cavity will behave like a + 1 point. These conclusions are in good agreement with the observations of Meyer.[5]

The type of singular point that can be stabilized inside a sphere with normal boundary conditions can also be found out easily. In any plane passing through the centre of the sphere only the $s = +1$ director pattern with normal boundary conditions at the circular boundary can be stabilized. Such a structure describes a nematic drop often found in the isotropic phase of nematic liquid crystals.[7]

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