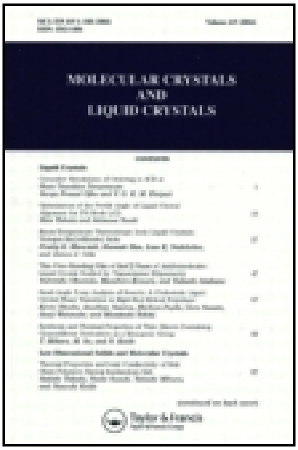

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Disclination Lines in an External Magnetic Field

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The director configuration of disclination lines in the presence of an external magnetic field is evaluated. Applying a polynomial expansion, we obtain approximate analytical solutions for the director field which are discussed for the general case of elastic anisotropy. They point out the possibility of an extended defect core. The actual size of the core is estimated by minimizing the total energy, including both the energy of the nematic phase and the core energy.

Keywords: topological defects

Disclinations are linear sigularities in the director field of nematics. Unlike in spin systems, disclinations of topological charge $\pm\frac{1}{2}$ are possible and stable in nematics. When an external magnetic field is applied perpendicular to such a disclination line, the resulting director configuration can be regarded as a domain wall filling a half-plane which terminates in the disclination line. Such a structure has been denoted a planar soliton.[1]

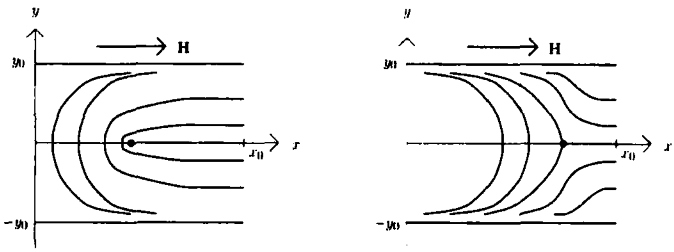

FIGURE 1 Geometry and coordinates for planar solitons in nematics. Left: positive soliton, right: negative soliton.

The geometry for planar solitons in nematic liquid crystals is drawn schematically in Fig. 1. The director field is essentially planar, perpendicular to a disclination line of strength $\pm\frac{1}{2}$ (positive or negative soliton) along the z direction of a Cartesian coordinate frame. Because the structure is independent of z, we restrict ourselves to the x-y plane ($z = 0$). Now we impose a magnetic field in the plane of the director along the x axis. Due to the magnetic anisotropy of the nematic the director tends to align along the magnetic field. The resulting structure is a planar domain wall of Néel type which ends in the disclination line. Locally, close to the disclination, the director field preserves the defect structure. However, in a plane at a finite distance from the disclination line, which is given by the half width y_0 of the planar Néel wall (Fig. 1), the director field is aligned parallel to the external magnetic field.

Due to the translational symmetry along the z axis the director orientation is completely determined by the *tilt angle field* $\Phi(x, y)$, which is measured with respect to the direction of the magnetic field $\mathbf{H}$ (x axis).

$$\mathbf{n} = \cos\Phi(x,y)\,\hat{\mathbf{x}} + \sin\Phi(x,y)\,\hat{\mathbf{y}}, \qquad \mathbf{H} = H_0\,\hat{\mathbf{x}}. \tag{1}$$

The static director orientation inside the soliton corresponds to a configuration minimizing the total free energy F (per unit length in the z direction) which contains both the energy of the nematic phase $F_{\rm nem}$ and the core energy of the disclination $F_{\rm core}$. (Within the defect core local phase transitions may occur.) The nematic energy $F_{\rm nem}$ is the area integral of a free energy density $\mathcal{F}_{\rm nem}$. This free energy density, in turn, consists of the Oseen-Zöcher-Frank elastic energy density and of the coupling to the external magnetic field $\mathbf{H}$ via the anisotropy of the magnetic susceptibility

$\Delta\chi$.

$$\mathcal{F}_{\rm nem} = \frac{1}{2} K_{11} \, (\operatorname{div} \mathbf{n})^2 + \frac{1}{2} K_{33} \, (\mathbf{n} \times \operatorname{curl} \mathbf{n})^2 - \frac{1}{2} \mu_0 \, \Delta\chi \, (\mathbf{n} \cdot \mathbf{H})^2 \qquad (2)$$

In (2) K_{11} and K_{33} denote the elastic constants for *splay* and *bend* deformations in the nematic. Due to the restriction to planar director fields according to (1) there are no *twist* deformations and the elastic constant K_{22} does not enter the calculations. When inserting the ansatz for the planar director field (1) into (2), we obtain the free energy density $\mathcal{F}_{\rm nem}$ of the nematic phase as a functional of the tilt angle.

The director configuration for the planar soliton, which minimizes the energy of the nematic phase, follows as a solution of the corresponding Euler-Lagrange equation

$$\frac{\delta \mathcal{F}_{\rm nem}}{\delta n_i} \equiv \frac{\partial \mathcal{F}_{\rm nem}}{\partial n_i} - \partial_j \left(\frac{\partial \mathcal{F}_{\rm nem}}{\partial \left(\partial_j n_i \right)} \right) = 0. \qquad (3)$$

The boundary conditions are an essential feature of the planar solitons. According to Fig. 1 the defect structure is surrounded by a homogeneous director field and by a planar Néel wall. Thus the boundary conditions are

$$\Phi(x,\, y = y_0) = 0, \qquad \Phi(x,\, y = -y_0) = \pm\pi, \qquad \Phi_y(x,\, y = \pm y_0) = 0, \qquad (4)$$

$$\Phi(x = 0,\, y) = \pm\frac{\pi}{2} \mp \frac{3\pi}{4} \frac{y}{y_0} \pm \frac{\pi}{4} \left(\frac{y}{y_0} \right)^3, \qquad \Phi(x = x_0,\, y) = 0. \qquad (5)$$

where the different signs are valid for the positive and negative soliton, respectively. (Φ_y means partial derivative along y.) Whereas the half width of the domain wall is given by

$$y_0 = \frac{3\pi}{4H_0} \sqrt{\frac{K_{\rm Neel}}{\mu_0 \Delta\chi}}, \qquad K_{\rm Neel} = \left(1 + \frac{32}{9\pi^2} \right) K_{33} - K_{11}, \qquad (6)$$

it is important to note that the soliton length x_0 is yet unknown at this stage.

Our strategy for solving the non-linear partial differential equation (3) for the tilt angle $\Phi(x,y)$ proceeds in two steps. First we apply a polynomial expansion[2] of the tilt angle field in the y coordinate. After separating the y dependence, we are left with a set of ordinary differential equations which can be solved, approximately, analytically. Of course, the polynomial expansion in y must satisfy the boundary conditions (4). Therefore, up to third order it reads

$$\Phi(x,y) = \left(\pm\frac{\Phi_0(x)}{y_0^2} + C(x)\,y\right)(y \mp y_0)^2 \bmod \pi, \qquad \text{for } y \geq 0,\ y \leq 0 \text{ resp.} \tag{7}$$

Our ansatz (7) is continuous everywhere apart from the x axis ($y = 0$). When crossing the x axis between $x = 0$ and $x = x_0$, a jump in the director orientation from $+\Phi_0(x)$ to $-\Phi_0(x)$ occurs. This is connected to the physical singularity of the disclination line in the center of the defect. Most significantly, due to the influence of the external magnetic field the cross-section of the defect core is no more a point-like object in the x-y plane, but it is extended to a segment of a straight line of length x_0.

When inserting the third order polynomial expansion (7) into the equation (3), by comparison of the coefficients for the first two powers in the y coordinate (*i.e.* y^0, y^1) we obtain two ordinary differential equations for the unknown expansion coefficients $\Phi_0(x)$ and $C(x)$. An approximate analytical solution for them can be achieved, which turns out to be quite accurate, as being revealed by a comparison with numerical solutions. This solution, in turn, is then inserted into the free energy density (2). After integrating (2) over the area covered by the soliton ($0 \leq x \leq x_0$, $-y_0 \leq y \leq y_0$), we obtain the total energy of the nematic phase, which still depends on the reduced length $\overline{x}_0 \equiv x_0/y_0$ of the soliton.

$$F_{\text{nem}} = \frac{1}{2}(K_{11} + K_{33})\left[\frac{0.58}{\overline{x}_0} - 0.72\,\overline{x}_0 + \overline{K}\left(\frac{0.19}{\overline{x}_0} + 0.93 - 11.69\,\overline{x}_0\right)\right] \tag{8}$$

In (8), $\overline{K} = (K_{33} - K_{11})/(K_{11} + K_{33})$ denotes the elastic anisotropy.

The expression (8) would suggest that $\overline{x}_0$ should be as large as possible – then F_{nem} would be minimal. In fact, this is *not* the case, due to the very large free energy stored in the defect core, where local transitions into disordered phases may occur. The energy of the core is due to large gradients in the orientational order, which appear on a *molecular* length scale σ_0. A rough estimate of the core energy is

$$F_{\text{core}} \approx \frac{1}{4}(K_{11} + K_{33})\,\Phi_y^2\,x_0\frac{\sigma_0}{\sqrt{2}} = \frac{\pi^2}{8\sqrt{2}}(K_{11} + K_{33})\,\frac{y_0}{\sigma_0}\,\overline{x}_0. \tag{9}$$

The total energy of the planar soliton is then $F = F_{\text{nem}} + F_{\text{core}}$. We now insert (8), (9) and then minimize F with respect to the reduced core length $\overline{x}_0$. It is easy to find out that the $\overline{x}_0$ corresponding to the minimum total energy is given by

$$\overline{x}_0^2 = \frac{0.58 + 0.19\,\overline{K}}{1.74\,y_0/\sigma_0 - 0.72 - 11.69\,\overline{K}}. \qquad (10)$$

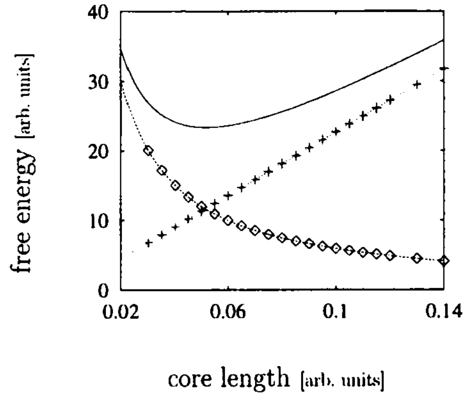

FIGURE 2 Free energy (per unit length) vs. reduced core length.
Dashed line and rhombs: nematic energy (analytically and numerically), dotted line and crosses: core energy (analytically and numerically), solid line: total energy.

Let us compute $\overline{x}_0$ for a particular nematic material. For N-(p-methoxybenzylidene)-p-buthylaniline (MBBA) at 25°C[3] the elastic constants are $K_{11} = 6.0 \cdot 10^{-12}$ N and $K_{33} = 7.5 \cdot 10^{-12}$ N. The magnetic anisotropy is $\mu_0 \Delta\chi = 9.7 \cdot 10^{-8}$ Vs/Am, the molecular length $\sigma_0 = 30$ Å. The magnetic field strength H_0 is chosen 500 Oersted, according to a magnetic flux density $B_0 \equiv \mu_0 H_0 = 0.05$ T. Then, the elastic anisotropy is $\overline{K} = 0.11$. Equation (6) yields $y_0 = 3900$ Å. Finally, $\overline{x}_0^2 \approx 0.0027$, and $x_0 \approx 202$ Å. The resulting physical length of the core x_0 is relatively large and it probably could be seen in appropriate experiments. Disclination lines in thin nematic films are directly observable under a polarizing microscope, from singular points that are connected by dark brushes of *Schlieren* textures. A possible elongated shape of the defect core under the influence of a strong magnetic field should be expected to affect these textures. This should give rise to their distortion close to the singular points, which could be investigated by a high-resolution microscope.

The dependence of the nematic, core and total energies on the reduced length of the defect core is plotted in Fig. 2. This reveals most clearly, that the actual core length emerges as a compromise from the competition between the opposite tendencies in the nematic and the core energy.

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