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Structure of the core of a screw dislocation in smectic A liquid crystals

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The structure of the core region of a screw dislocation in smectic A liquid crystals is investigated by a Ginzburg–Landau type expansion of the smectic order parameter. The core radius and the energy of a screw dislocation are discussed.

Smectic A liquid crystals are fluids composed of (typically) rod-shaped molecules showing a density modulation in one direction. They can be regarded as one-dimensional solids or layered structures. In equilibrium the layers are flat and their normal $\hat{\mathbf{n}}$ is constant ($\hat{\mathbf{n}}^0$). The layer spacing d_0 is only a very weak function of temperature and pressure and given approximately by the length of the molecules (e.g. 30 Å) [1].

A screw dislocation is a line defect in the layer structure characterized by [2]

$$\oint_C \nabla_\perp u \cdot d\mathbf{s} \;=\; md_0 \equiv b, \tag{1}$$

where u is the displacement of a layer along its normal $\hat{\mathbf{n}}$ (in equilibrium $u \equiv 0$). Equation (1) means that while encircling the screw dislocation on a layer one ends up at a point which is displaced along $\hat{\mathbf{n}}$ by md_0. The integer m is then called the strength of the defect and b is the absolute value of the appropriate Burgers' vector.

In the simplest model the screw dislocation is described as a straight line (the z axis in the following) with a layer structure [2]

$$u \;=\; \bar{b}\theta, \tag{2}$$

where θ is the angle in cylindrical coordinates (ϱ, θ, z) and $\bar{b} \equiv b/2\pi$. Equation (2) describes a layer structure consisting of one simply connected layer wound around the line defect. The layer is a minimal surface, i.e. without curvature or $\operatorname{div}\hat{\mathbf{n}} \equiv 0$ ($\hat{\mathbf{n}}$ is related to u by $\hat{\mathbf{n}} = (\hat{e}_z - \nabla u)/|\hat{e}_z - \nabla u|$ and is not parallel to the z axis). This simple model of a screw dislocation, is however, insufficient for mathematical and physical reasons, since u is ill-defined for $\varrho = 0$ (screw line) and the elastic energy due to the distortion of the layers diverges (see later). These difficulties are avoided by introducing a core region, in which the smectic order (i.e. modulus ψ_0 of the smectic order parameter

$$\Psi \;=\; \psi \exp\left(i\frac{2\pi}{d_0}[z - u]\right),$$

decreases from its constant value ψ_0 outside the core to zero at $\varrho = 0$. Thus, any singularity and non-physical divergence is removed.

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It is the aim of the present paper to investigate the structure of the core by a continuum approach. Assuming a Ginzburg–Landau expansion to exist (and still to make sense within the core) the energy density is written as [3]

$$\varepsilon_{\mathrm{GL}} = -\frac{a}{2}|\Psi|^2 + \frac{c}{4}|\Psi|^4 + \left(\frac{1}{2M}\right)_{ij}(D_i\Psi)^*(D_j\Psi) + \frac{K}{2}(\operatorname{div}\hat{\mathbf{n}})^2, \tag{3}$$

where

$$\mathbf{D} = \nabla - i\frac{2\pi}{d_0}\hat{\mathbf{n}}$$

and

$$\left(\frac{1}{2M}\right)_{ij} = \frac{1}{2M_1}n_i n_j + \frac{1}{2M_2}(\delta_{ij} - n_i n_j).$$

The equilibrium smectic order is given by $\psi_0 = a/c$ (a, c positive), while $M_{1,2}$ (positive) describe the stiffness of both the order and the structure against spatial inhomogeneities. The curvature energy ($\sim K$) is related to the nematic order and not to the smectic order, but has been added to equation (3) for completeness. In terms of ψ and u equation (3) reads explicitly

$$\begin{aligned}\varepsilon_{\mathrm{GL}} = &-\frac{a}{2}\psi^2 + \frac{c}{4}\psi^4 + \frac{1}{2M_2}(\nabla_\perp\psi)^2 + \frac{1}{2M_1}(\nabla_z\psi)^2 \\ &+ \frac{4\pi^2\psi^2}{2d_0^2M_1}(1 - F(u))^2 + \frac{K}{2}\left(\nabla\cdot\frac{\hat{\mathbf{e}}_z - \nabla u}{F(u)}\right)^2 \\ &- \frac{1}{2}\left(\frac{1}{M_1} - \frac{1}{M_2}\right)(\nabla_\perp u\cdot\nabla_\perp\psi)(2\nabla_z\psi[1 - \nabla_z\psi] - \nabla_\perp u\cdot\nabla_\perp\psi)F(u)^{-2},\end{aligned} \tag{4}$$

with

$$F(u)^2 = 1 - 2\nabla_z u + (\nabla u)^2$$

and

$$\nabla_\perp = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, 0\right).$$

In a region where ψ is constant equation (4) reduces to the well-known covariant elastic energy [4]

$$\varepsilon = \frac{B}{2}\left(\frac{d - d_0}{d}\right)^2 + \frac{K}{2}(\operatorname{div}\hat{\mathbf{n}})^2, \tag{5}$$

with $d = d_0F(u)^{-1}$ and $\hat{\mathbf{n}} = (\hat{e}_z - \nabla u)F(u)^{-1}$ and the elastic modulus B is given by $\psi_0^2 4\pi^2(d_0^2M_1)^{-1}$. Note that $u = \not{b}\theta$ is an exact equilibrium solution of equation (5).

In the general case where ψ is not constant, minimization of $\int\varepsilon_{\mathrm{GL}}\,dV$ with respect to ψ and u leads to two coupled non-linear partial differential equations, which have to be solved under the conditions of equation (1) (with the path C outside the core) together with $\psi(\varrho = 0) = 0$ and $\psi(\varrho \to \infty) = \psi_0$. The solution of these equations is facilitated by assuming $\psi = \psi(\varrho)$, i.e. the core region has the same cylindrical symmetry as the original line singularity (another possibility will be discussed later). Then $u = u(\theta)$ follows immediately, which means $u = \not{b}\theta$ everywhere. The remaining equation for $\psi(\varrho)$ then reads

$$-a\psi + c\psi^3 - \frac{1}{M_2}\Delta\psi + \psi\frac{4\pi^2}{d_0^2M_1}\left(1 - \left(1 + \frac{\not{b}^2}{\varrho^2}\right)^{1/2}\right)^2 = 0. \tag{6}$$

In the interior of the core, i.e. for small $\varrho(\varrho \ll \hbar)$, ψ is expected to be very small, so that the cubic non-linearity can be neglected; then

$$-a\psi - \frac{1}{M_2}\left(\psi'' + \frac{1}{\varrho}\psi'\right) + \frac{m^2}{M_1}\psi\frac{1}{\varrho^2} = 0 \tag{7}$$

whose appropriate solution is the Bessel function

$$\psi = AJ_\nu[\varrho\sqrt{(aM_2)}] \tag{8}$$

of index $\nu = m(M_2/M_1)^{1/2}$. Since I expect $M_2 \gg M_1$ (inhomogeneous order parameter fluctuations along the layer normal should cost more energy than in the transverse direction) ν is a large number and $\psi \sim \varrho^\nu$ for $\varrho \to 0$ is a flat function of ϱ. Thus the core region is rather more nematic (or isotropic) than smectic. This is even truer for screw dislocations with large Burger's vectors or large defect strength m. The function $J_\nu[\varrho\sqrt{(aM_2)}]$ reaches its first maximum at $\varrho_{\max} \approx \nu(aM_2)^{-1/2} = m(aM_1)^{-1/2}$, which serves as a characteristic length scale of this solution.

In the opposite case, far away from the core, $\varrho \to \infty$, the smectic order ψ should deviate only slightly from its constant value ψ_0 (obtained in a defect-free sample), i.e. $\psi = \psi_0 + \Delta$ with $\Delta \ll \psi_0$. Linearizing in Δ gives

$$\Delta \sim K_0[\varrho\sqrt{(2aM_2)}], \tag{9}$$

where K_0 is a modified Bessel function. Since Δ constitutes an exponentially small correction only to ψ_0 (even for $\varrho = \varrho_{\max}$) it can be neglected in comparison with ψ_0 for most purposes. Then the two limiting cases can be combined to give an approximate solution $\psi(\varrho)$ for all ϱ by

$$\psi(\varrho) = \begin{cases} \psi_0 \dfrac{J_\nu[\varrho\sqrt{(aM_2)}]}{J_\nu[\varrho_c\sqrt{(aM_2)}]} & \text{for} \quad \varrho \leqslant \varrho_c, \\ \psi_0 & \text{for} \quad \varrho > \varrho_c, \end{cases} \tag{10}$$

with the core radius ϱ_c chosen as

$$\varrho_c = \varrho_{\max} = m(aM_1)^{-1/2}. \tag{11}$$

Thus ϱ_c increases with the defect strength and increases near the smectic–nematic phase transition, where a is expected to vanish with some power law $(T_c - T)^\gamma$.

Instead of choosing ϱ_c by matching the two solutions $\psi(\varrho)$ for small and large ϱ at the characteristic length $\varrho_{\max}$ the core radius ϱ_c can be determined by a different procedure. Taking the solution (10) with ϱ_c as an adjustable parameter the total energy of the screw dislocation $E = \int \varepsilon \, dV$ can be calculated, with

$$\varepsilon = \varepsilon_{\mathrm{GL}} - \varepsilon_{\mathrm{GL}}^{\mathrm{eq}}, \quad \left(\varepsilon_{\mathrm{GL}}^{\mathrm{eq}} = -\frac{a^2}{4c}\right);$$

minimizing E with respect to ϱ_c leads to ϱ_c.

Outside the core ($\varrho > \varrho_c$) the screw dislocation energy is purely elastic, since ψ_0 is constant and $\operatorname{div}\hat{\mathbf{n}} = 0$ (no curvature energy). Using equation (5) the energy per unit length is found to be

$$E_{\mathrm{el}}^{>} = \pi B\left[\hbar^2 \ln\frac{1}{2}\left(1 + \left(1 + \frac{\hbar^2}{\varrho_c^2}\right)^{1/2}\right) + \varrho_c^2\left(\left(1 + \frac{\hbar^2}{\varrho_c^2}\right)^{1/2} - 1\right) - \frac{1}{2}\hbar^2\right], \tag{12}$$

which reduces for $\varrho_c \gg b$ to the known result [5]

$$E_{el}^{>} = \frac{\pi B b^4}{8\varrho_c^2}. \tag{13}$$

For $b = \varrho_c$ the approximate result (13) differs from (12) only slightly (by a factor of 5/4) and is still a reasonable approximation. For $b \gg \varrho_c$ the exact result (12) shows that $E_{el}^{>}$ diverges for $\varrho_c \to 0$

$$E_{el}^{>} = \pi B b^2 \ln \frac{b}{\varrho_c}. \tag{14}$$

This divergence is the physical reason for introducing a finite core radius ϱ_c.

Inside the core ($\varrho < \varrho_c$) the simplest approximation is $\psi \equiv 0$. Then, the screw dislocation energy is $\varepsilon = \varepsilon_{GL}^{eq} = (a^2/4c)$ (which should be equal to the thermodynamic result [6] $\varepsilon = k_B \Delta T v_{mol}^{-1}$ where v_{mol} is the molecular volume and ΔT the temperature difference to the nematic–smectic A transition temperature) and

$$E_{core}^{<} = \frac{a^2}{4c}\pi\varrho_c^2. \tag{15}$$

Minimizing the sum of (13) and (15) with respect to ϱ_c leads to

$$\varrho_c^2 = b m (aM_1)^{-1/2}. \tag{16}$$

Equation (16) is compatible with equation (11), if $(aM_1)^{-1/2}$ is of the order of d_0; then $\varrho_c \approx b$, which is quite reasonable [7].

The smallness of ϱ_c is connected with the weakness of the (logarithmic) singularity of the elastic energy which a coreless screw dislocation would have (equation (14)). The relation $b = m(aM_1)^{-1/2}$ breaks down near the smectic A–nematic phase transition (because d_0 is a geometrical constant), since the crude approximation leading to (15) then becomes invalid.

In this treatment we have assumed cylindrical symmetry of the core region, for example, no z dependence of ψ or u. However, a periodic z dependence is still compatible with the notion of an overall straight (infinite) screw dislocation. Indeed there is such a model with two helical singular lines spiralling around the z axis [8]. It is obtained, if a parent surface (generated by a straight line which is perpendicular to the z axis and which rotates with pitch $b \gg d_0$) is enveloped by a family of surfaces all having constant distance from each other; for details and illustration see [5]. By construction there is no elastic energy involved but only curvature energy. The total curvature energy diverges logarithmically [9] and the singular lines (the cuspidal edge of the focal surface connected with the family of surfaces) form a double helix of wedge disclinations [5]. Again the introduction of a finite core removes singularities and divergences. The core region in this case is a double helical tube of radius ϱ_c. This core region, however, is characterized by the decrease of nematic order (not smectic order), since the curvature energy ($\sim K$) vanishes with the nematic order. Thus, to obtain a quantitative picture of this core region one should use a Ginzburg–Landau type expansion for the nematic order parameter, which goes, however, beyond the scope of this paper.

A Ginzburg–Landau type expansion has been used to investigate the core structure. Although the results are quite reasonable, this procedure is not rigorous for the following reasons. Because of the smallness of the core radius any continuum description of the interior of the core is debatable. An expansion in Ψ (if it exists at all) is believed to be correct for small Ψ only and is less accurate for finite Ψ (i.e. $\psi = \psi_0 =$ constant). Instead of expanding in Ψ, ψ and u could be used separately giving rise to additional coupling terms between the gradients of ψ and u in equation (4) (which are, however, probably rather small). Nevertheless the results derived concerning core radius and screw dislocation energy are believed to be correct qualitatively, and it is hoped that they can be verified experimentally.

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