Nematic liquid crystals between antagonistic cylinders: Spirals with bend-splay director undulations

D. R. M. Williams*
Laboratoire de Physique de la Matière Condensée, Collège de France, 75231 Paris Cedex 05, France

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We reexamine the problem of a nematic fluid trapped between two concentric cylinders with different anchoring conditions on each of the cylinders. If the splay constant K_s is less than the bend constant K_b, the director varies monotonically between the plates. If, however, $K_s > K_b$, the director can undergo a series of spatial oscillations. Observation of these oscillations may allow measurement of K_s/K_b. For semiflexible polymer liquid crystals the oscillations should be readily observable and very sensitive to temperature changes.

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A nematic fluid is contained between two concentric cylinders of radii r_1 and r_2. The anchoring conditions at each cylinder are such that the nematic director is perpendicular to the cylinder axes. On the inner cylinder the angle made by the director with the radial direction is 0 and on the outer cylinder α. What is the director field inside the cylinders? This problem was first proposed by Meyer, solved in a special case by Padrodi, and is discussed in the book by de Gennes [1]. The interest lies in the case $\alpha \neq 0$. The director is then forced to traverse the cylinder between two boundaries offering different anchoring conditions and must therefore distort.

The special case studied in [1] is the so-called one-constant approximation where the elastic constants for splay, K_s, and bend, K_b, are set equal to one another. In that case the angle made by the director with the radial direction $\psi(r)$ varies monotonically with radius, $\psi(r)=\alpha \ln(r/r_1)\ln(r_2/r_1)$ (Fig. 1). In many problems the one-constant approximation is a reasonable simplification and captures the essential physics of the system. The magic spiral problem is a counterexample. By setting $K_s \neq K_b$ we find an interesting, nonmonotonic, change in ψ.

To see this we write the director in cylindrical coordinates (r,θ,z) as $n=(n_r,n_\theta,n_z)=(\cos\psi,\sin\psi,0)$. Note that as in the previous treatment of this problem we assume the director has no z component [2]. This could be forced upon the system by application of a strong field favoring alignment perpendicular to the cylinder axis. To make the system mathematically tractable we make a small distortion assumption, $\psi \ll 1$.

The total nematic energy per unit length of the cylinder is then [1]

$$F=\pi\int_{r_1}^{r_2} dr (K_b-K_s)r^{-1}\psi^2+K_b r\left[\frac{d\psi}{dr}\right]^2 . \tag{1}$$

In problems with cylindrical symmetry it is useful to introduce the transformation $t=\ln(r/r_1)$. The free energy then has the form

$$F\propto\int_{\ln r_1}^{\ln r_2} dt\left[\frac{d\psi}{dt}\right]^2-\psi^2\left[\frac{K_s}{K_b}-1\right] . \tag{2}$$

Note that the first term has exactly the same form as that for director distortions between two *flat* plates. The second term is a potential induced by the curved geometry. This second term vanishes if $K_s=K_b$. If t is interpreted as a time, then the free energy (2) is the same as the action for a particle with displacement ψ moving in a parabolic potential well. The free energy minimum can thus be found directly from the equation of motion

$$\frac{d^2\psi}{dt^2}=-k\psi \tag{3}$$

with $k\equiv K_s/K_b-1$. Three regimes are then possible.

(i) If $K_s=K_b$ then the one-constant approximation is strictly valid and we obtain the Padrodi result:

$$\psi(r)=\alpha\ln(r/r_1)/\ln(r_2/r_1) , \tag{4}$$

i.e., a monotonic variation with distance. In this case the potential vanishes.

(ii) If $K_s>K_b$ then the director moves in a potential

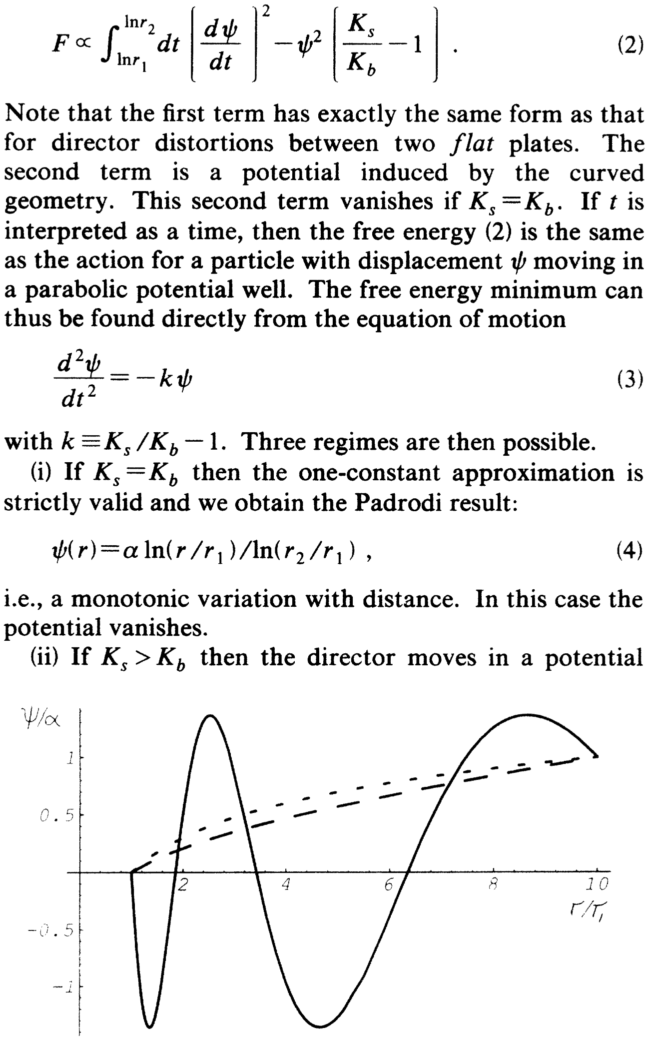

FIG. 1. Plot of the radial dependence of the angle (normalized to α) made by the director with the radial direction, as a function of r/r_1. Here we choose $r_2/r_1=10$. We show the three possible scenarios. (i) (dotted line) $K_s=K_b$, (ii) (full line) $K_s/K_b=26>1$, (iii) (dashed line) $K_s/K_b=0.5<1$. In (ii) the director undergoes spatial oscillations of amplitude larger than α.

*Present address: The Harrison M. Randall Laboratory of Physics, The University of Michigan, Ann Arbor, MI 48109-1120.

well and the solution is oscillatory,

$$\psi(r)=\alpha \sin[\sqrt{k}\ \ln(r/r_1)]/\sin[\sqrt{k}\ \ln(r_2/r_1)] \ . \quad (5)$$

(iii) If $K_s < K_b$ the solution is again monotonic,

$$\psi=\alpha \sinh[\sqrt{-k}\ \ln(r/r_1)]/\sinh[\sqrt{-k}\ \ln(r_2/r_1)] \ . \quad (6)$$

In this case the particle moves in an inverted potential "well."

Case (ii) is the one of most interest. Provided $k \ln(r_2/r_1) > 2\pi$ the director makes one or more oscillations in traveling between the plates. In t space these have period

$$2\pi(K_2/K_b-1)^{-1/2} \ . \quad (7)$$

The period is independent of any dimensional parameters and depends only on K_s/K_b. The number of complete oscillations is the largest integer not greater than

$$n \equiv (2\pi)^{-1}\ln(r_2/r_1)(K_s/K_b-1)^{1/2} \ . \quad (8)$$

Physically, the oscillations occur because or large K_s/K_b it costs less free energy for the director to bend than to splay. By oscillating splay is avoided at the expense of bend. If $K_b > K_s$ it is no longer favorable to bend and we have case (iii).

We can plot the "nematic trajectory" in each case, i.e., the curve with tangent following the local nematic director. These follow from the geometrical relation $\tan\psi\, dr/d\theta \approx \psi\, dr/d\theta = r$ along with the equation of motion (3). Here θ is the usual polar angle in cylindrical coordinates. Integrating once gives

$$\theta(r)=\theta(r_1)+g(r)-g(r_1) \ , \quad (9)$$

where $g(r) \equiv -(r/k)d\psi/dr$. The curves $\theta(r)$ are plotted in Fig. 2.

Two things are to be noted. First, the oscillations do not occur between two flat plates. In that case $r_2=r_1=\infty$. With two flat plates the free energy has the same form as (2) but without the potential term. The cylindrical geometry induces this term. Second, the amplitude of the oscillations can be much larger than α. The maximum is $\psi_m=\alpha/\sin(\sqrt{k}\ \ln r_2/r_1)$. For $2n=m$, with m an integer, the oscillations diverge. We then need to include nonlinear corrections, which were ignored in deriving (1) [3]. For many small molecule nematics $K_s/K_b<1$, and there will be no oscillations. However, for rigid polymeric nematics the splay constant can become very large [4]. It is governed by the constant density constraint which forces the chain ends to arrange in an entropically unfavorable way [5]. The splay constant then diverges as the length of the molecule, whereas the bend constant depends on the rigidity of the molecule. We can thus expect $K_s > K_b$ for such systems. For *semiflexible* polymer nematics some novel effects can occur due to the presence of hairpins [6]. These rapid bends in the chain each have associated energy penalty U_h. Thus the number of hairpins per chain of length L is $(L/l)\exp(-U_h/kT)$, here l is a microscopic length. Each hairpin acts like a chain end and $K_s/K_b \propto (U_h/kT)^{7/4}\exp(U_h/kT)$ [5,7,2]. Thus K_s/K_b is large and grows rapidly with decreasing temperature. This implies that the number of oscillations should be very temperature dependent.

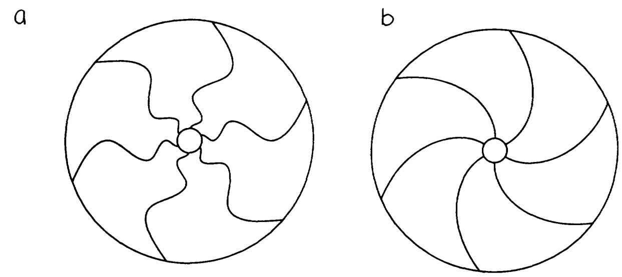

FIG. 2. The director orientation between the cylinder in the two cases. (a) $K_s/K_b=26>1$, so the bends to escape splay. (b): $K_s/K_b=0.5<1$; there are no oscillations. We have chosen $r_2/r_1=10$ and the anchoring angle $\alpha=1$, to make the oscillations clear. The director is tangent to the curves at each point.

The oscillations predicted here should be visible under polarized light, using the optical birefringence of nematics, and may provide a method of directly measuring K_s/K_b.

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