Saddle-splay elasticity and field induced soliton in nematics

O V Manyuhina

Nordita, Royal Institute of Technology & Stockholm University, Roslagstullsbacken 23, SE-10691 Stockholm, Sweden

E-mail: oksanam@nordita.org

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Abstract

The symmetry breaking Fréedericksz transitions, when a uniformly aligned nematic state is replaced by a homogeneously or periodically distorted state, have been extensively studied before. Here we analyse the influence of the saddle-splay elasticity on the non-linear ground state of a nematic liquid crystal in the presence of a magnetic field above the Fréedericksz threshold. We identify the bifurcation point when the localized soliton-like state is linearly unstable with respect to the perturbations of the wavevector in the direction perpendicular to the initial plane of the soliton. This instability occurs only if the ratio of the saddle-splay elastic constant to the elastic modulus of nematics in the one-constant approximation is above the critical value $|K_{24}/K| \geq 0.707$.

1. Introduction

A nematic liquid crystal is an anisotropic fluid, composed of rod-like molecules, characterized by a unit vector $\mathbf{n}$ called the director, pointing along the averaged orientation of molecules [1]. Since the pioneering work of Zolina and Fréedericksz [2] the field induced Fréedericksz transition is one of the most studied and most useful phenomena in the physics of liquid crystals. When the magnetic (or electric) field is applied perpendicular to the uniformly aligned nematic, confined between two parallel plates, above a certain threshold the director experiences deformations and tends to align along the field. The critical threshold is inversely proportional to the thickness of the nematic sample $d$, and quantifies the competition between the magnetic field $B$ and the boundary effects mediated by elastic forces, given by

$$B_c = \frac{\pi}{d} \sqrt{\frac{K}{\chi_a}},$$  \hspace{1cm} (1)

where $\chi_a$ is the magnetic susceptibility and $K$ is the elastic constant. The symmetry breaking in classical Fréedericksz transitions happens in one direction along the thickness of the nematic sample and the observed distortions can be explained within a continuum theory of liquid crystals [3]. The discovery of a periodic splay–twist Fréedericksz transition by Lonberg and Meyer [4], when homogeneous distortions are replaced by a spatially periodic pattern of stripes at even lower threshold value than $B_c$, posed new questions on the equilibrium structure of the nematic in the presence of the magnetic field. Taking into account more realistic boundary conditions, namely a finite anchoring strength [5] and the saddle-splay elastic term [6], would influence the critical threshold and result in the periodic saddle-splay Fréedericksz transitions [7].

The problem of finding the critical threshold in different classes of Fréedericksz transitions was formulated in terms of linear perturbation theory, assuming a uniformly aligned ground state. In this paper we consider the nematic liquid crystal in the presence of high magnetic fields $B \gg B_c$, when the ground state is initially distorted: more precisely, in the bulk the director is aligned parallel to the field, and in the boundary layer at the surfaces the director reorients rapidly. The equilibrium configuration found within the boundary layer is the kink-like soliton, because magnetic energy enters the Lagrangian of the system in a non-linear way. To our knowledge, the influence of the saddle-splay elastic constant on this non-trivial localized ground state in the presence of high magnetic field $B \gg B_c$ has not been considered theoretically before. In essence the boundary layer can be conceived as a thin nematic film spread on a liquid substrate, subjected to the antagonistic boundary...
conditions [8]. Nevertheless, in this case the ground state depends linearly on the coordinate along the thickness, a so-called hybrid aligned nematic, because there is no non-linearity entering the free energy. It has been shown that the saddle-splay term plays an important role for thin nematic films with weak anchoring conditions, when the instability towards a periodically distorted stripe phase was found [9–11].

In the present paper we treat the problem within the Oseen–Zocher–Frank continuum theory of liquid crystals, assuming the one-constant approximation of the elastic free energy [1]. Starting from the non-linear ground state of the nematic director in the presence of high magnetic field, we consider the onset of instability towards a periodically deformed state, with stripes parallel to the direction of the field. As a result, the stripe phase can be energetically favoured if the absolute value of the saddle-splay elastic constant is higher than \( K/s_1 \). The found analytic expression for the critical wavenumber as a function of the control parameter suggests a new experimental way to identify simultaneously the anchoring strength and the saddle-splay elastic constant.

2. Soliton solution

Let us consider a nematic liquid crystal constrained between two glass plates, separated by distance 2\(H\) along the \(z\) axis, and subjected to the magnetic field \(B\) parallel to the \(x\) axis as shown in figure 1. We assume that glass surfaces impose a homeotropic anchoring, favouring director alignment along the normal to the surface, and the positive magnetic susceptibility of molecules \(\chi_m\), so that \(n\) tends to align along the field. Above the Fréedericksz threshold \(B \gg B_c\) (1) we get \(n\) parallel to the field in the bulk, and two regions in the vicinity of glass surfaces, known as boundary layers, where the reorientation of \(n\) takes place. The equilibrium configurations of nematics minimize the total free energy, written as the sum of the Frank free energy in the one-constant approximation and the magnetic energy

\[
\mathcal{F}_b = \frac{1}{2} \int_V dV \left[ K|\nabla n|^2 - K_{2a} \nabla \cdot [(\nabla \cdot n)n + n \times \nabla \times n] \right] - B^2 \chi_a (n \cdot e_x)^2.
\]  

(2)

Figure 1. Schematic representation of the director \(n \leftrightarrow -n\) configuration in the presence of magnetic field \(B\) in a cell of 2\(H\) thickness. In the boundary layer with dimensionless thickness \(\epsilon_\theta \ll 1\) (4), \(n\) changes from the orientation parallel to the field, along the \(x\) axis, towards the one imposed by the glass surface through the boundary condition (6). The equilibrium angle \(\theta\) (8), between the director \(n\) and the \(z\) axis, is a function of the scaled coordinate \(\zeta\), where \(\zeta \to \infty\) corresponds to the inner border of the boundary layer.

The second divergent term, where \(K_{2a}\) is the saddle-splay elastic constant,\(^1\) can be transformed into a surface integral, entering boundary conditions in the case of non-planar geometry. Moreover, at the glass surface we introduce the additional energy associated with the anchoring, which we write in the Rapini–Papoular form as

\[
\mathcal{F}_s = \frac{1}{2} \int dS \{ W_0 - W_a (n \cdot e_z)^2 \},
\]  

(3)

where \(W_a > 0\) is the anchoring strength and the minus sign reflects that anchoring favours director alignment parallel to \(e_z\).

We are looking first for the equilibrium configuration of the nematic director in the 2D case with the parametrization \(n = \sin \theta(z) e_x + \cos \theta(z) e_z\), so that \(|n|^2 = 1\) and \(\theta\) is the angle which the director makes with the \(z\) axis. Introducing the dimensionless coherence length and the scaled coordinate \(\zeta\)

\[
\epsilon_\theta = \frac{1}{H} \sqrt{\frac{K}{\chi_a B^2}}, \quad \frac{z}{H} = 1 - \epsilon_\theta \zeta,
\]  

(4)

the Euler–Lagrange equation for \(\theta\) associated with (2) takes the form

\[
\partial_\zeta \theta + \sin \theta \cos \theta = 0.
\]  

(5)

Without loss of generality we consider the upper half-plane, and the boundary conditions in the bulk (\(\zeta \to \infty\)) and at the glass surface (\(\zeta \to 0\)) are respectively

\[
\theta|_{\zeta \to \infty} = \frac{\pi}{2}, \quad \partial_\zeta \theta|_{\zeta \to \infty} = 0,
\]

\[
\rho (\partial_\zeta \theta)|_{\zeta = 0} = (\sin \theta \cos \theta)|_{\zeta = 0},
\]  

(6)

\(\rho\) is the density of nematic director and \(\theta\) is the angle of the director with the \(z\) axis.

\(\epsilon_\theta\) is the anchoring strength, which we assume to be constant in the bulk and to decay exponentially near the glass surfaces.

\(\chi_m\) is the magnetic susceptibility of the molecules.

\(B\) is the magnetic field.

\(H\) is the thickness of the cell.

\(\theta\) is the angle of the director with the \(z\) axis.

\(\zeta\) is the scaled coordinate.

\(\rho\) is the density of nematic director.

\(\sin \theta\) and \(\cos \theta\) are trigonometric functions.

\(\partial_\zeta \theta\) is the derivative of \(\theta\) with respect to \(\zeta\).

\(\mathcal{F}_b\) and \(\mathcal{F}_s\) are the Frank free energy and the surface integral, respectively.

\(W_0\) is the Frank free energy.

\(W_a\) is the anchoring energy.

\(K\) is the Frank elastic constant.

\(K_{2a}\) is the saddle-splay elastic constant.

\(\chi_a\) is the Frank elastic constant.

\(\chi_m\) is the magnetic susceptibility of the molecules.

\(H\) is the thickness of the cell.

\(\theta\) is the angle of the director with the \(z\) axis.

\(\zeta\) is the scaled coordinate.

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\(\partial_\zeta \theta\) is the derivative of \(\theta\) with respect to \(\zeta\).

\(\mathcal{F}_b\) and \(\mathcal{F}_s\) are the Frank free energy and the surface integral, respectively.

\(W_0\) is the Frank free energy.

\(W_a\) is the anchoring energy.
where \( \rho \equiv \sqrt{K B^2 X_a/W_a} \) is the dimensionless parameter relating the strength of the magnetic field to the anchoring. The first integral of (5), satisfying (6) in the bulk, is
\[
\partial_\xi \theta = \cos \theta, \tag{7}
\]
which can be integrated again yielding
\[
\theta(\xi) = \arcsin \left( \frac{Ae^{2\xi} - 1}{Ae^{2\xi} + 1} \right), \tag{8}
\]
where the integration constant \( A \) satisfies the boundary condition at the interface (6), yielding
\[
A(\rho) = \frac{1 + \rho}{1 - \rho}. \tag{9}
\]
In order to have a non-trivial solution \( \rho \leq 1 \) should hold. In the case of infinite anchoring \( W_a \to \infty (\rho \to 0) \) we get \( A = 1 \) and thus \( \theta(\xi) = \arcsin(\tanh \xi) \). The obtained soliton-like solution is due to non-linearity in (5), resulting in the localization of the distortion of \( n \) within the boundary layer of thickness \( \varepsilon_0 H \).

### 3. Linear stability analysis

Let us consider a small perturbation of the director in the \( yz \) plane
\[
n = \sin(\theta + \psi) \cos \phi e_x + \sin(\theta + \psi) \sin \phi e_y + \cos(\theta + \psi) e_z, \tag{10}
\]
where \( \phi(y, z) \) and \( \psi(y, z) \) are assumed to be small \( O(\varepsilon) \) and periodic functions with respect to the variable \( y \). Then, expanding the free energy density up to \( O(\varepsilon^2) \) we find the perturbed bulk \( f_b^{(2)} \) and the surface \( f_s^{(2)} \) contributions, respectively,
\[
f_b^{(2)} = \frac{K}{2} ([\partial_\xi \psi]^2 + (\partial_n \phi)^2 + (\partial_n \phi)^2 + (\partial_n \phi)^2) \tag{11}
\]
\[
f_s^{(2)} = \frac{W_a}{2} (\cos 2\psi \sqrt{\omega^2 - \sin^2 \theta \phi^2}) |_{\xi=0} - K_{2a} (\sin^2 \theta \phi \partial_\xi \psi) |_{\xi=0} \tag{12}
\]
where the saddle-splay term favours non-zero distortions of \( \phi \) and \( \psi \). To characterize the instability of the planar solution (8) with respect to the perturbation of wavevector \( q \) in the \( y \) direction we are searching for the periodic solution in the form
\[
\phi(z, y) = g(z) \cos(qy), \quad \psi(z, y) = f(z) \sin(qy). \tag{13}
\]
The variational problem for \( f \) and \( g \) associated with (11), given the solution of \( \theta(\xi) \) (8), leads to the differential equations
\[
\partial_\xi f - f \left( \frac{\omega^2 - \frac{8Ae^{2\xi}}{(Ae^{2\xi} + 1)^2}}{1 + Ae^{2\xi}} \right) = 0, \tag{14}
\]
\[
\partial_\xi g + \partial_\xi g \frac{8Ae^{2\xi}}{Ae^{2\xi} + 1} - g \omega^2 = 0, \tag{15}
\]
written in terms of the scaled variable \( \xi \) (4), and another dimensionless variable \( \omega^2 \equiv 1 + q^2 \varepsilon_0^2 H^2 \) is introduced. The resulting solutions, vanishing in the bulk (\( \xi \to \infty \)), can be cast into the form
\[
f(\xi) = C_1 e^{-i(\omega(1 + \omega) + \omega - 1)} \left( 1 + Ae^{2\xi} \right) \tag{16}
\]
\[
g(\xi) = C_2 A^{(1-\omega)} e^{-i(\omega(1 + \omega) + \omega - 1)} \left( (\omega - 1)(Ae^{2\xi} - 1) \right), \tag{17}
\]
where the integration constants \( C_1 \) and \( C_2 \) should satisfy the following boundary conditions at the glass surface \( \xi = 0 \):
\[
\partial_\xi f(0) = \left( \frac{1}{\rho} - 2\rho \right) f(0) - \tau \sqrt{\omega^2 - 1} g(0), \tag{18}
\]
\[
\partial_\xi g(0) = -\tau \sqrt{\omega^2 - 1} f(0), \quad \tau \equiv K_{24}/K. \tag{19}
\]

The resulting system of linear equations \( \sum M_i C_i = 0 \) with respect to unknowns \( C_1 \) and \( C_2 \) has a non-trivial solution if and only if the determinant of the \( 2 \times 2 \) matrix of the coefficients is zero, \( \det M = 0 \). This condition yields the implicit relationship between the dimensionless parameters of the system \( \rho, \omega \) and \( \tau \); the latter should satisfy Ericksen’s inequalities for nematic liquid crystals [12], which in the one-constant approximation reduce to \( |\tau| \leq 1 \). If \( \det M > 0 \) the 2D non-linear state (8) is stable (\( C_1 = 0 \)), otherwise an instability towards the periodically distorted state occurs, with a wavevector \( q \) determined at the bifurcation point \( \det M = 0 \). In section 4 we analyse the instability threshold and identify the associated critical parameters.

### 4. Periodic solution

We make use of Mathematica 7 to compute the determinant of the matrix
\[
det M = \frac{4(1 + \rho)^2(1 + \rho - 2\rho(\rho + \omega)^2}{(1 - \rho)^2 \rho^4(\omega - 1)^2} \omega^2(1 + 2\rho \omega) - \rho^2(\tau^2 - 1)\omega^2(\omega - 1) - \rho^3 \omega(1 - 2\tau^2) + (1 + 2\tau^2) \omega^2 - \rho^4(\omega^2(1 + \tau^2 - \tau^2)) \tag{20}
\]
and to plot the curves \( \det M = 0 \) in the \( \omega-\rho \) parameter space for a given value of \( \tau \), as shown in figure 2. The minimum of every curve gives the critical values of the governing parameter \( \rho_c \), characterizing the relative strength of magnetic field compared to the anchoring of the surface, and the corresponding scaled wavenumber \( \omega_c \) of the perturbed state. We notice that not all the considered values of the saddle-splay elastic constant, satisfying Ericksen’s inequalities, result in a real value for the critical wavenumber. In figure 2(a) \( \omega_c < 1 \) and the corresponding wavenumber \( q_c = \sqrt{\omega_c^2 - 1/(\varepsilon_0 H)} \) is complex and physically irrelevant; therefore, the periodically modulated state is not feasible. In contrast, in figure 2(b) the curves reach their minimum at \( \omega_c > 1 \), corresponding to real values of \( q_c \), thus dividing the parameter space into two regions: (i) below the curve (\( \rho < \rho_c \)) the 2D base state (8) is stable (\( \det M > 0 \)); (ii) above \( \rho_c \) the periodically modulated state is the energetically preferred one. The underlying picture can be understood in terms of the control parameter \( |\tau| \), which being below its critical value \( \tau_c \) results in the stability of the unperturbed 2D state, and above \( \tau_c \) one may find a
The solution of the equation $\det M = 0$ (20) for different values of the saddle-splay constant, given by $\tau = K_{24}/K$: (a) $|\tau| < \tau_c$, (b) $|\tau| > \tau_c$ with $\tau_c = 1/\sqrt{2}$. The minima of the curves in (b) define the critical wavenumbers $q_c$ related to $\omega$, which occur at the critical ratio of the magnetic energy to the anchoring energy, given by $\rho_c$.

Let us plot in figure 3 the critical parameters $\omega_c$ and $\rho_c$ at the bifurcation point as a function of the saddle-splay elastic constant $\tau$. The curves show that the perturbation with a finite wavelength, when $\omega_c > 1$, appears only for $|\tau| > 0.7$. The critical value of $\tau$ is defined by taking the limit $\lim_{\rho \to 1, \omega \to 1}$ of (20), which exists if and only if $|\tau_c| = 1/\sqrt{2} \simeq 0.7$. For the saddle-splay elastic constant, which does not satisfy Ericksen’s inequalities, namely $|\tau| > 1$, there is no critical point. Requiring the determinant (20) to vanish in the limit $|\tau| \to 1$ and $\omega \to \infty$, we find $\rho_c = \sqrt{2}/3 \simeq 0.82$. Therefore, the instability threshold between the soliton-like ground state (8) and the periodically distorted state (13) with finite wavelength exists for the following range of parameters: $1/\sqrt{2} < |\tau| < 1$ and $1 > \rho_c > \sqrt{2}/3$.

According to the plotted critical curves, for a magnetic field of the order of Tesla we may find a periodicity of the stripes of the order of microns if the anchoring strength $W_a \sim 10^{-6}$ J m$^{-2}$. These values are experimentally accessible. Therefore, if we know the strength of the magnetic field and can measure the periodicity of the stripes, we can identify the saddle-splay elastic constant $\tau$ from figure 3(a), and consequently estimate the anchoring strength $W_a$ from figure 3(b). The strong homeotropic anchoring ($\rho < 1$) leads to smaller wavelength of the distorted stripe state, compared to the weak anchoring ($\rho \simeq 1$), yielding the long-wavelength periodic pattern. In figure 4 we show the equilibrium nematic state with periodic distortions along the $y$ axis for typical values of the parameters $\rho, \omega, \tau$ slightly above the critical threshold. The resulting stripes are formed in the vicinity of the glass surface along the direction of the applied magnetic field or the $x$ axis, which is not shown.

5. Conclusions

The intrinsic anisotropy of nematic liquid crystals leads to a non-linear elastic response to the applied magnetic field, and therefore the equilibrium state is described by a localized soliton (8). Nevertheless, this localized ground state can become unstable with respect to the perturbations of the wavevector $q_c$, when the saddle-splay elastic term
becomes important. Within the linear stability analysis we examined the onset of stripe instability, arising due to the interplay between the elastic and magnetic forces in the bulk versus the anchoring and saddle-splay forces, favouring the undulations at the surface. The bifurcation to the periodically deformed stripe state with a finite wavelength happens only if $1/\sqrt{2} < |\tau| < 1$. Moreover, the threshold is characterized by the critical ratio of the magnetic energy to the anchoring energy, which falls into the range $\sqrt{2}/3 < \rho_c < 1$. If we know the parameters such as anchoring at the glass surface together with the saddle-splay and elastic moduli of the nematic, we can estimate, assuming the one-constant approximation, the critical value of the magnetic field and the corresponding critical wavelength of the stripes. On the other hand, varying the magnetic field and observing the periodic deformations of the nematic in the vicinity of the surface, we can identify simultaneously the anchoring strength and the poorly studied saddle-splay elastic constant, by comparing experimental data with theoretical predictions (20) based on the analytic solutions. To account for the difference in splay, twist and bend elastic constants would require numerical analysis for solving non-linear partial differential equations. We believe that considering a ground state different from the widely explored planar nematic is important for analysing experimental observations. Moreover, studying competing interactions between the surface effects and high magnetic fields above the Fréedericksz threshold may give insight into fundamental physics of liquid crystals as well as contributing to practical applications.

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References

[1] de Gennes P G and Prost J 1993 The Physics of Liquid Crystals (Oxford: Clarendon)
[2] Fréedericksz V and Zolina V 1933 Trans. Faraday Soc. 29 919
[3] Stewart I W 2004 The Static and Dynamic Continuum Theory of Liquid Crystals (London: Taylor and Francis)
[4] Lonberg F and Meyer R B 1985 Phys. Rev. Lett. 55 718
[5] Napoli G 2006 J. Phys. A 39 11
[6] Napoli G 2010 Europhys. Lett. 92 46006
[7] Kralj S, Rosso R and Virga E G 2005 Eur. Phys. J. E 17 37
[8] Cazabat A-M, Delabre U, Richard C and Yip Cheung Sang Y 2011 Adv. Colloid Interface Sci. 168 29
[9] Sparavigna A, Lavrentovich O D and Strigazzi A 1995 Phys. Rev. E 51 792
[10] Lavrentovich O D and Pergamenshchik V M 1995 Int. J. Mod. Phys. B 9 2389
[11] Manyuhina O V, Cazabat A M and Ben Amar M 2010 Europhys. Lett. 92 16005
[12] Ericksen J L 1966 Phys. Fluids 9 1205