Boundary-roughness effects in nematic liquid crystals

The Mathematics of Liquid Crystals - Young Researchers Meeting

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Overview

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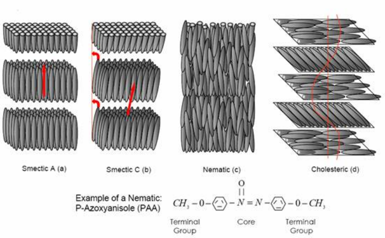
Nematic liquid crystals

- Different liquid crystal phases [1]



- We consider nematic liquid crystals: they consist of rod-like molecules, oriented along a preferred direction, but without ordering of centers of mass. In the Oseen-Frank theory, the average orientation is given by the unit director field, $\vec{n}$.

[1] http://www.laynetworks.com/images/Molecular-Orientation-in-Liquid-Crystal-Phases_clip_image002_0000.jpg

Landau - De Gennes theory 1

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- In the following, we use the Landau-de Gennes Q-tensor theory to model the nematic configurations.
- The free-energy functional has two components, elastic f_{el} and bulk f_{LdG}:

$$f_{el}(Q) = \frac{1}{2}K|\bigtriangledown Q|^2, \tag{1}$$

$$f_{LdG}(Q) = A\,\mathrm{tr}Q^2 - B\,\mathrm{tr}Q^3 + C\,\mathrm{tr}Q^4, \tag{2}$$

with K a typical elastic constant, and $A = A(T)$, $B > 0$, $C > 0$ material parameters.

Landau - De Gennes theory 2

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- Furthermore, we consider the uniaxial symmetry, with two equal eigenvalues of Q. Then,

$$Q = s\left(n \otimes n - \frac{1}{3}I\right), \qquad s \in \left[-\frac{1}{2}, 1\right], |n| = 1.$$

- In this case, we can rewrite the energies (1) and (2) as

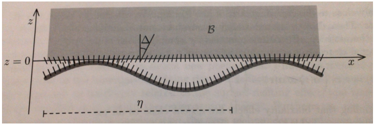
$$f_{el}(s,n) = K\left(s^2|\nabla n|^2 + \frac{1}{3}|\nabla s|^2\right),$$

$$f_{LdG}(s) = \frac{2}{3}As^2 - \frac{2}{9}Bs^3 + \frac{2}{9}Cs^4.$$

- The total free-energy density is given then by $f := f_{el} + f_{LdG}$.

Problem description

Consider one boundary to be a corrugated plate such that n is perpendicular to the surface, Equivalently, the undulating boundary can be described as a flat surface with an undulating b.c.:



with Δ the amplitude and η the wave length. We assume that a uniform configuration in y so that

$$n = (\sin\theta, 0, \cos\theta).$$

Note that $|\bigtriangledown n|^2 = |\bigtriangledown \theta|^2$. With the second point of view, we can write $\theta(x, y, 0) = \Delta \cos\frac{x}{\eta}$ (b.c.).

Two-scale analysis (P. Biscari, S. Turzi)

- In their paper [2], P. Biscari and S. Turzi derive the Euler-Lagrange equations associated to f:

$$s^2 \triangle \theta + 2s \triangledown s \cdot \triangledown \theta = 0, \qquad \triangle s - 3s|\triangledown \theta|^2 - 3\frac{\sigma(s)}{\xi^2} = 0,$$

with $\sigma = \sigma(s, s_{pr})$, s_{pr} the preferred degree of orientation, and $\xi = \sqrt{\frac{9K}{C}}$ the nematic coherence length (comparing the strength of the contributions by f_{el} and f_{LdG} to f_b).

- Through a two-scale analysis, a particular method in singular perturbation theory, they approximate θ by a function G, i.e.

$$\theta = \theta(x, z) = G(x, z, \eta).$$

[2] Boundary-Roughness Effects in Nematics, 2007, SIAM J. Appl. Math 67.2

Limit question

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What happens when $\eta \to 0$?

The function $\cos \frac{x}{\eta}$ increasingly oscillates. As the oscillation period gets very small, the wave length and the distance between top & bottom plates have different length scales. From the macroscopic perspective, the fine structure may appear as homogeneous.

Different approach

Treat the problem in terms of calculus of variations: Instead of analyzing the Euler-Lagrange equations, analyze the minimizers of the energy.

Idea of Γ-convergence

- What can we say about the limit for the family of energies (f_η) as $\eta \to 0$?
- What can we say about the limit of minimizers as $\eta \to 0$?

Γ-convergence is the tool to answer this question.

Gamma Convergence: Definition

Let (X, d) be a metric space with distance d. We say that a sequence $F_j : X \to \mathbb{R}$ Γ-converges in X to $F : X \to \mathbb{R}$ if for all $x \in X$, we have

1. (lim inf inequality) for every sequence (x_j) converging to x:

$$F(x) \leq \liminf_j F_j(x_j),$$

2. (lim sup inequality) there exists a sequence (x_j) converging to x such that

$$F(x) \geq \limsup_j F_j(x_j).$$

Gamma Convergence: Our Case

Find a functional F such that the sequence (F_η) Γ-converges to F, Then, by definition, the minimizers of (F_η) converge to the minimizer of F.

Summary

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- Nematic liquid crystal with undulating boundary.
- Γ-convergence to study minimizer as wave length $\eta \to 0$.

Thank you!