Short-Term Scientific Mission (STSM) Report for "Nematic-Smectic Pattern Formation in Confined Geometries" Action TD1409 - 39215

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1 Purpose of the STSM

I am a Reader (Associate Professor) in applied mathematics at the University of Bath, United Kingdom. I specialize in the mathematics and modelling of nematic liquid crystals and their applications in science and technology. I was awarded a STSM grant on "Nematic-Smectic Pattern Formation in Confined Geometries" to initiate a new collaboration with Professor Angel Manuel Ramos del Olmo and his research group at the Departamento de Matemtica Aplicada, Facultad de Matemticas, Universidad Complutense de Madrid, Spain. As stipulated in my STSM award, I was hosted by Professor Ramos during my research visit to work on this new collaborative project. My research visit had two main outcomes -

- I delivered two lectures as part of a graduate mini-course on "Mathematics and Modelling for Nematic Liquid Crystals for New Applications" on the 15th December 2017 intended as introductory material for the collaborative project.
- I started a new collaborative project on "Nematic-Smectic Pattern Formation in Square Geometries" with Professor Ramos and Professor Jose Maria Rey (Modelos Matemticos en Ciencia y Tecnologa, Universidad Complutense de Madrid). This collaboration also involves scientific exchanges (and potential collaborations) with Dr Ian Griffiths (Mathematical Institute, University of Oxford), Professor Dirk Aarts (Department of Chemistry, University of Oxford) and Dr Maria Crespo Moya (Montpellier, France). We also expect to forge new scientific connections with Professor Francisco Guillen-Gonzalez (Instituto de Matemticas Univ. Sevilla (IMUS)) , who has worked on the analysis of mathematical models for Smectic-A liquid crystals, as part of this collaboration.

2 Scientific Description

Our new collaborative project is motivated by the experimental work in [2], on colloidal liquid crystals in square confinement. Liquid crystals are mesophases which have physical properties intermediate between those of conventional liquids and conventional solids [3]. Nematics and smectics are perhaps the two commonest types of liquid crystals [1]. Nematic liquid crystals (NLCs) are simply put, anisotropic liquids wherein the constituent rod-like molecules align along certain locally preferred directions i.e. they are directional liquids. Smectic liquid crystals (SLCs) combine the orientational order of NLCs with partial positional ordering i.e. the molecules are typically arranged in layers and the layers can slip past each other.

In [2], the authors experiment with colloidal silica rods in water, confined to square chambers treated to induce planar degenerate anchoring. In other words, if we look down at the bottom cross-section, the cross-section is a square and the square edges are treated so that the silica rods on the edges are tangent to the edges. In [2], the authors observe isotropic disordered rod phases near the top of the chamber, nematic-like orientationally ordered profiles towards the center of the chamber and layered smectic-like rod profiles near the bottom of the chamber. The authors typically work with silica rods of length 5 μm, aspect ratio in the range of $9 - 15$ (rod length/rod diameter) and square chamber widths of about $75 - 100$ μm [2]. Professor

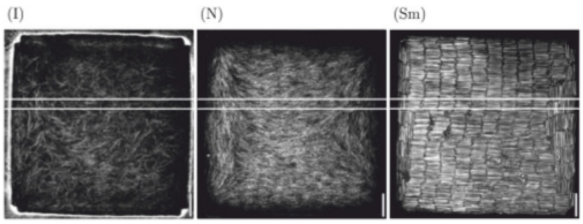

Figure 1: Figure from [2] where the authors observe (a) disordered isotropic rod phases, (b) nematic rod phase and (c) layered smectic-bridge phases

Aarts and his group are very much interested in developing a mathematical model for these experiments. During my STSM, we proposed a simple but promising model for smectic pattern formation, using an idea informally suggested to me by Dr Canevari (Basque Centre for Applied Mathematics, Spain). The celebrated Oseen-Frank theory for NLCs describes the nematic state by a unit-vector field $\mathbf{n}$, whose physical interpretation is that it represents the locally preferred direction of average molecular alignment [3, 4]. We work with a square domain, $\Omega = \{(x, y) \in \mathbb{R}^2 : 0 \leq x, y \leq 1\}$ and take $\mathbf{n} = (\cos\theta, \sin\theta)$, where θ depends on x and y. The planar degenerate conditions require that $\mathbf{n} = (\pm 1, 0)$ on the edges $y = 0, 1$ and $\mathbf{n} = (0, \pm 1)$ on the edges $x = 0$ and $x = 1$ i.e.

$$\begin{aligned} \theta &= (2n+1)\frac{\pi}{2} \quad x = 0,1 \\ \theta &= m\pi \quad y = 0,1 \end{aligned} \tag{1}$$

for some integers n and m. The experimentally observed states correspond to minimisers of the Oseen-Frank functional in this framework [3, 5]

$$I_{OF}(\theta) := \frac{K_3}{2}\int_{\Omega} |\nabla\theta|^2 - \delta\left(\theta_y \cos\theta - \theta_x \sin\theta\right)^2 \ dxdy \tag{2}$$

where $\theta_x = \frac{\partial\theta}{\partial x}$ etc., $\delta = 1 - \frac{K_1}{K_3}$ is the scaled elastic anisotropy parameter and $K_1, K_3 > 0$ are material-dependent elastic constants. The energy minimisers are solutions of the associated Euler-Lagrange equation for θ as shown below.

$$-\Delta\theta = \delta\left[\frac{\sin(2\theta)}{2}\left(\theta_y^2 + 2\theta_{xy} - \theta_x^2\right) + \theta_x\theta_y\cos(2\theta) - \theta_{xx}\sin^2(\theta) - \theta_{yy}\cos^2(\theta)\right]. \tag{3}$$

This problem has been studied in detail in [5, 6] for $\delta = 0$. **Indeed, the observed nematic textures near the square centre can be captured in terms of the "diagonal" and 'rotated' solutions reported in [5, 8].**

We propose to study smectic pattern formation by studying energy minimizers of (2) for $\delta \to 1$ or equivalently for large K_3 and fixed K_1. As $K_3 \to \infty$, energy minimizing unit-vector fields are expected to have curl$\mathbf{n} \to \mathbf{0}$ almost everywhere, so that $\mathbf{n} \to \nabla\phi$ for some scalar function ϕ, where the contours of ϕ model the smectic layers and the corresponding $\mathbf{n}$ is oriented along $\nabla\phi$ or the layer normals.

3 Results

In what follows, Professor Ramos, Professor Rey and I numerically solved the elliptic PDE (3) on the square domain, for different choices of the integers n and m in (1), for different choices of δ, using a Finite Element commercial solver, COMSOL [7]. COMSOL is widely used to solve systems of partial differential equations that arise in the context of the physical and applied sciences and we thought this was a first good step to test our conjecture that we should numerically observe layered smectic profiles as δ approaches unity. We did indeed observe some layered profiles for certain choices of the boundary conditions and δ as illustrated below. I am not including all the numerical experiments since we tried at least six different choices of boundary conditions and three different initial conditions, for the Newton iterations as part of the COMSOL numerical algorithm.

Our main conclusions so far are:

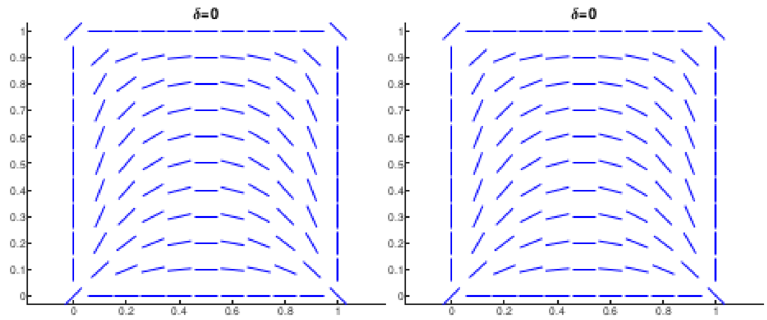

Figure 2: The simplest rotated case with $\theta(0,y) = \frac{\pi}{2}, \theta(1,y) = -\frac{\pi}{2}$, $\theta = 0$ on $y = 0, 1$

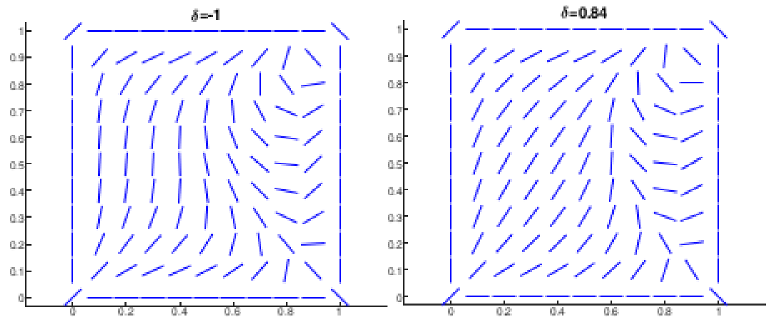

Figure 3: A non-trivial case with $\theta(0,y) = \frac{\pi}{2}, \theta(1,y) = \frac{3\pi}{2}$, $\theta = 0$ on $y = 0, 1$. We see a diagonal profile in the left-hand side of the square followed by a boundary layer-like structure near the right edge; as δ approaches unity, the boundary layer is sharper and pushed towards the edge $x = 1$.

- **we can use different choices of n and m in (1) to generate configurations with boundary layers** which, to some extent, mimic the layered smectic profiles;
- **as δ increases or equivalently, as K_3 increases, there is numerical evidence of sharper interfaces** or well-partitioned sub-domains again consistent with the smectic picture and
- **this relatively simple approach is a novel way of exploiting boundary conditions and the elastic anisotropy parameter, δ, to generate layered structures which has not received much attention in the literature.**

A number of open questions remain - $\theta = \frac{\pi}{2}$ and $\theta = \frac{5\pi}{2}$ correspond to $\mathbf{n} = (0, 1)$ and the values of n and m in (1) determine the number of turns that the unit-vector field makes in the square interior - what actually dictates the number of turns in the square interior? We propose to do the following to better understand this problem -

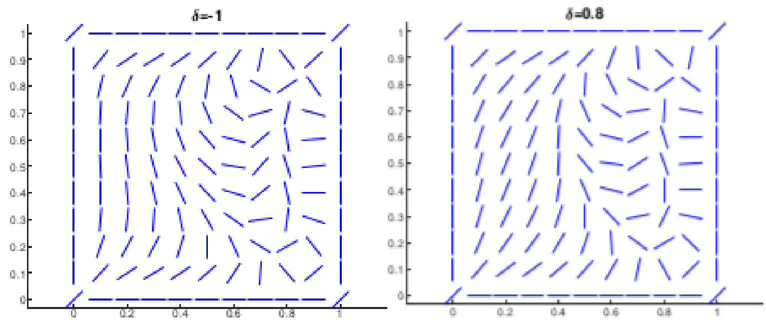

Figure 4: A non-trivial case with $\theta(0,y) = \frac{\pi}{2}, \theta(1,y) = \frac{5\pi}{2}$, $\theta = 0$ on $y = 0, 1$. We see evidence of three ordered regions for this choice of boundary conditions and the interfaces do indeed get sharper as δ approaches unity.

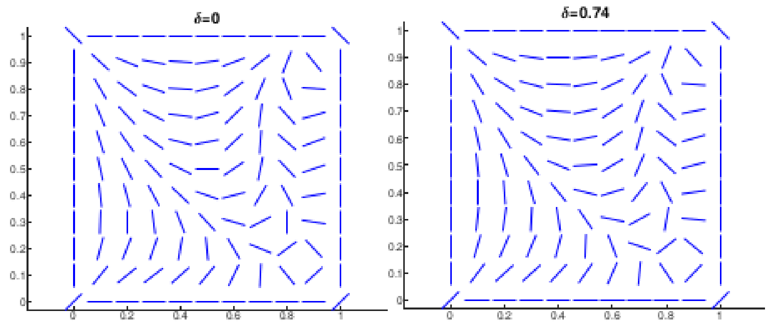

Figure 5: A non-trivial case with $\theta(0,y) = \frac{\pi}{2}, \theta(1,y) = \frac{5\pi}{2}$, $\theta(x,0) = 0$ and $\theta(x,1) = \pi$. We see clear evidence of a boundary layer near $x = 1$ and a boundary layer is reminiscent of the experimentally observed smectic-like profiles but this does not seem to be strongly dependent on δ.

- **improve the numerical resolution of our existing results and also write a finite-difference based code in Matlab** ;
- **numerically check that the large K_3 limit indeed enforces curln → 0 almost everywhere** for energy minimizers.
- **We conjecture that as δ increases, the energetic penalty for large values of n and m in (1) decreases so that we can experimentally see layered profiles qualitatively similar to Figures 3, 4** and we will check this conjecture numerically.
- **We will compare this new model with other models for Smectic-A liquid crystals, such as**

$$I[\theta,\phi] := \int_\Omega \frac{1}{2}|\nabla\theta|^2 + \frac{B}{2K}\left(\phi_x - \sqrt{\phi_x^2+\phi_y^2}\cos\theta\right)^2 + \frac{B}{2K}\left(\phi_y - \sqrt{\phi_x^2+\phi_y^2}\sin\theta\right)^2\,dxdy \tag{4}$$

where θ is defined as above, $\phi(x, y) = 0$ characterizes the smectic layers, B and K are material-dependent constants (see [9] for more discussion). The resulting Euler-Lagrange equations for the energy minimizers are a highly nonlinear coupled system of partial differential equations for θ and ϕ.

4 Future Collaborations

This collaborative project is part of a relatively new research network spanning the University of Bath, University of Oxford and the Universidad Complutense de Madrid, created in 2016. We will co-author a research paper on the work carried out during this STSM in the near future, which will be submitted to an international peer-reviewed journal and forge new connections with the Department of Mathematics at the University of Sevilla.

References

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