ICMS RESEARCH IN GROUPS ON "MINIMIZERS IN THE LANDAU-DE GENNES THEORY FOR NEMATIC LIQUID CRYSTALS: REGULARITY, SINGULARITIES AND GENERALIZATIONS" SCIENTIFIC REPORT

Scientific Team: A team of three researchers spent an intensive research period from 1st - 15th September at the International Centre for Mathematical Sciences, Edinburgh to exclusively focus on a new research project. The team members are named below.

- Team Leader: Dr Apala Majumdar (Reader in Applied Mathematics, University of Bath)
- Team Members: Dr Giacomo Canevari (Postdoctoral Fellow in Applied Analysis, Basque Centre for Applied Mathematics, Bilbao, Spain); Professor Bianca Stroffolini (Associate Professor in Analysis, Università Federico II, Naples, Italy).

The team has complementary and diverse expertise. Dr Majumdar specialises in the mathematics and applications of nematic liquid crystals and has worked on multiple aspects of liquid crystal research: foundational and analytical issues, analysis of stable equilibria and stable singularities, bifurcations and dynamical systems approaches and detailed numerical studies in collaboration with mathematicians, physicists, chemists and engineers. Dr Canevari specialises in the analysis of partial differential equations, with a background in Ginzburg-Landau theory for superconductivity which is particularly relevant to the Landau-de Gennes theory for nematic liquid crystals. Professor Stroffolini has extensive expertise in regularity theory for problems in the calculus of variations and this is particularly useful for new liquid crystal energies which might exploit novel notions of convexity or singular potentials. The team essentially focussed on a variant of a commonly used version of the Landau-de Gennes energy functional that presents new analytical challenges and may be better tailored to describe higher-dimensional defects and complex spatial patterns.

Scientific Summary: Nematic liquid crystals are classical examples of *directionally ordered* complex liquids intermediate in character between solids and liquids. Loosely speaking, they combine the translational freedom of liquids with the orientational ordering of solids and are characterised by "nematic directors" or distinguished directions of averaged molecular alignment. This orientational anisotropy makes them the working material of choice for a range of optical devices, notably they form the backbone of the multi-billion dollar liquid crystal display (LCD) industry. The mathematics of nematic liquid crystals is undergoing a modern day renaissance as analysts, applied modellers, numerical analysts come together to ask fundamental questions about the derivation and validity of continuum macroscopic theories for nematic liquid crystals, the relation between mathematical and physical singularities and the universal features of different variational theories of material science.

This project focussed on the analysis of variants of the celebrated Landau-de Gennes theory for nematic liquid crystals. The Landau-de Gennes (LdG) theory is one of the most powerful and general continuum theories for nematics. Indeed, de Gennes was awarded the Nobel Prize in physics in 1991, partly because of the LdG theory and its widespread applications. The LdG theory describes the state of a nematic by a macroscopic order parameter, the $\mathbf{Q}$-tensor order parameter, which is a symmetric traceless 3×3 matrix with five degrees of freedom [8]. The eigenvectors of the LdG $\mathbf{Q}$-tensor represent the special directions of preferred molecular alignment and the corresponding eigenvalues measure the degree of orientational order about these directions. As with most variational theories in materials science, the LdG theory assigns a stored free energy to a confined nematic system and there are multiple choices of the LdG free energy, including elastic terms that penalize spatial inhomogeneities, bulk potentials that dictate the preferred degree of orientational order as a function of the temperature and material parameters, surface energies that encode the effect of boundary conditions and external field energies [14]. The simplest form of the LdG energy is

$$I[\mathbf{Q}] = \int_{\Omega} W(\mathbf{Q}, \nabla \mathbf{Q}) + f_{\mathrm{B}} \left(\operatorname{tr} \mathbf{Q}^2, \operatorname{tr} \mathbf{Q}^3 \right) \, \mathrm{d}V \tag{1}$$

where W is an elastic energy density *quadratic and convex* in $\nabla\mathbf{Q}$ and $f_{\rm B}$ is typically a quartic polynomial in $\mathbf{Q}$ whose eigenvalues dictate the "preferred bulk order" as a function of the temperature [13]. In [13, 10, 5], the authors work with the Dirichlet elastic energy density i.e. $W(\nabla\mathbf{Q}) = \frac{L}{2}|\nabla\mathbf{Q}|^2$ and prove strong results about global LdG minimizers on two-dimensional and three-dimensional bounded domains, Ω with Dirichlet boundary conditions, in the asymptotic limit of vanishing elastic constant, relevant for macroscopic domains where the elastic constant L is typically very small compared to other material parameters and the domain size (to be interpreted in dimensionless terms). In [13], the authors prove that global LdG minimizers on three-dimensional domains with Dirichlet boundary conditions, converge uniformly to a *limiting minimizing harmonic map* away from the singularities of the harmonic map. A minimizing harmonic map can be understood in terms of a unit-vector field, $\mathbf{n}^*$, that is a minimizer of the Dirichlet energy, $I[\mathbf{n}] = \int_\Omega |\nabla\mathbf{n}|^2 \, {\rm d}V$, subject to appropriate Dirichlet conditions, in the class of S^2-valued maps or unit-vector fields. It is well known, from the pioneering work of Schoen and Uhlenbeck [15], that the singular set of a minimizing harmonic map, in three dimensions, is a discrete set of isolated points. In other words, in [13], the authors are able to provide an approximate description of the global LdG energy minimizers away from a finite set of singular points of a minimizing harmonic map. In [10], the authors prove some rigorous results about the structure of defect cores i.e. they show that, for a set of physically relevant hypotheses in the low-temperature regime, defect cores have sets of "maximal biaxiality" where the LdG $\mathbf{Q}$-tensor has a zero eigenvalue and "uniaxial sets" for which the LdG $\mathbf{Q}$-tensor has two degenerate non-zero eigenvalues.

However, these results strongly rely on the isotropic quadratic nature of the Dirichlet energy density and it is not at all clear if elastic energy densities have such regular mathematical structures in the vicinity of defects, interfaces or critical temperatures. The state-of-art experimental techniques do not allow us to measure the exact structure of the elastic energy density near defects. Equally importantly, the LdG energy density is derived on the assumption that macroscopic variables change very slowly compared to molecular length scales or are regular at small length scales and this assumption does not really hold for nano-sized defect cores. This is corroborated by the fact that quadratic elastic energy densities impose a relatively high energetic penalty for line and surface defects whereas line defects are actually common in confined nematic systems, suggesting that the real energetic penalty for such higher-dimensional defects may be lower than what is suggested by the quadratic LdG elastic energy densities. It was once suggested by Professor Sir John Ball [1] to Majumdar that one could perhaps use a subquadratic elastic energy density in regions of high distortion i.e. an energy density of the form

$$W^*(\nabla\mathbf{Q}) = \begin{cases} \dfrac{L}{2}\,|\nabla\mathbf{Q}|^p & \text{for } |\nabla\mathbf{Q}| > G_0, \quad \text{with } 1 < p < 2 \\ \phi(|\nabla\mathbf{Q}) & \text{for } G_1 < |\nabla\mathbf{Q}| < G_0 \\ \dfrac{L}{2}\,|\nabla\mathbf{Q}|^2 & \text{for } |\nabla\mathbf{Q}| \leq G_1 \end{cases} \tag{2}$$

where G_0, G_1 are empirical positive constants and ϕ is a convex interpolation between a subquadratic elastic energy density with $1 < p < 2$ and the usual Dirichlet energy density. The main benefit of this modified elastic energy density is that it should mathematically tame higher-dimensional singularities i.e. reduce the energetic penalty associated with higher-dimensional defects and hence, one might expect to see defects of higher dimensionalities (such as line defects) more easily within such a description. Of course, these notions need to be carefully defined and studied but given that there is no affirmative information about energy densities near defect cores where the underpinning assumptions of a quadratic elastic energy break down, Equation (2) is a reasonable suggestion whose merits are yet to be tested and verified.

The ICMS research-in-groups project focussed on qualitative properties of global energy minimizers of the following modified LdG energy on three-dimensional bounded domains with Dirichlet boundary conditions:

$$I^*[\mathbf{Q}] = \int_\Omega W^*(\mathbf{Q}, \nabla\mathbf{Q}) + f_{\rm B}\left({\rm tr}\,\mathbf{Q}^2,\, {\rm tr}\,\mathbf{Q}^3\right) \, {\rm d}V \tag{3}$$

where W^* is defined in (2) and $f_{\rm B}$ is the usual quartic bulk potential. The corresponding global minimizers

are classical solutions of the following system of coupled, nonlinear partial differential equations:

$$\operatorname{div}\left(|\nabla \mathbf{Q}|^{p-2}\,\nabla \mathbf{Q}\right) = \left(\frac{\partial f_{\mathrm{B}}}{\partial \mathbf{Q}_{ij}} - \frac{\partial f_{\mathrm{B}}}{\partial \mathbf{Q}_{kk}}\frac{\delta_{ij}}{3}\right) \tag{4}$$

which is considerably more complicated than the Euler-Lagrange equations associated with (1), since the system (4) is nonlinear in the gradient terms itself. The research team made substantial progress on this problem and their key results are described below.

- The team could adapt methods in [16], [4] and [13] to establish three technical tools. The first and the second tool are a maximum principle argument which guarantees boundedness of the norm of a minimizer, and an energy monotonicity inequality. These two results collectively are enough to establish the strong convergence of global energy minimizers, in an appropriately defined Sobolev space $W^{1,p}$ where p is defined in (3), to a **p-minimizing** harmonic map defined in terms of minimizers of the p-harmonic energy, in the space of all S^2-valued maps on Ω:

$$I_p[\mathbf{u}] := \int_{\Omega} |\nabla \mathbf{u}|^p \, \mathrm{d}V, \quad \text{with } 1 < p < 2. \tag{5}$$

  The team could then adapt arguments in [16] to prove a Böchner inequality for the energy density in (3) away from the singularities of the p-minimizing harmonic map, which is enough to prove that *global minimizers of the modified LdG energy in* (3) *converge uniformly to a* **p-minimizing harmonic map** *away from the singularities of the p-minimizing harmonic map.* The team will write a co-authored publication on this work since this result is of sufficient interest and novelty to warrant publication.

- The team studied the modified functional (3) in the low-temperature regime. For the usual quadratic Dirichlet elastic energy densities, it is known from the work of Canevari [4] (in the two-dimensional setting) and Contreras & Lamy [6], Henao, Majumdar & Pisante [10] (in the three-dimensional setting) that there are no isotropic points (with $\mathbf{Q} = 0$) in global minimizers for sufficiently low temperatures, largely because these isotropic points are energetically expensive. This excludes certain types of point defects, such as radial hedgehog point defects, for low temperatures. A preliminary study indicates that the same result will also hold for the modified LdG energy in (3), at least for two-dimensional domains. This is somewhat unexpected because the modified elastic energy density in (2) is expected to tame singularities and energetic penalties of isotropic points, so this is also worth reporting in the literature.

- The team studied an exact solution of the system (4), namely the p-variant of the radially symmetric radial hedgehog solution [12, 7, 11]. They established the existence of such a solution and will study its qualitative properties, namely, the location and multiplicity of the zeroes and its stability in future work.

- The team would also like to consider the question of regularity for local minimizers of a continuum model derived from Maier-Saupe mean-field theory. The model was derived by Ball & Majumdar in the paper [2]. The Ball-Majumdar functional is a costrained one; the admissible class $\mathcal{M}$ consists of an open, bounded and convex set of traceless symmetric matrices $\mathbf{Q}$ whose eigenvalues satisfy the constraint $\lambda_i(\mathbf{Q}) \in (-\frac{1}{3}, \frac{2}{3})$. In the special case where the liquid crystal occupies a cylindrical region in $\mathbb{R}^3$ with cross section $\Omega \subset \mathbb{R}^2$, Bauman & Phillips [3] considered a material whose tensor $\mathbf{Q}(x_1, x_2)$ is a 3×3 matrix that does not depend on the transversal variable, x_3. They proved, using the harmonic replacement and properties of harmonic mappings in the plane, that finite-energy local minimizers are C^∞-smooth and cannot touch the boundary of $\mathcal{M}$. From the physical point of view, this result implies that a nematic liquid crystal cannot assume a configuration of perfect nematic order. The team would like to consider the p-harmonic energy (3), with f_{B} replaced by the Ball-Majumdar potential, and look for a regularity result for local minimizers, which would also imply that local minimizers have eigenvalues strictly within the physical range $(-\frac{1}{3}, \frac{2}{3})$. We expect that techniques devised in the regularity theory for other variational problems, e.g. in [9], might play a rôle in this analysis.

Future plans. The ICMS provided an excellent, stimulating and very hospitable working environment for the research team for two weeks, which was much needed to explore an entirely new research project. The research team would like to express their gratitude to the ICMS and its staff for supporting them at every step. This short stay has resulted in one completed piece of research which will be written up for publication in an internationally leading mathematics journal. The team also benefitted from a very enjoyable public lecture on the life of Mary Somerville during their stay, which was timely since it was the penultimate day of their stay! The team plan to continue their collaboration; they will meet again at Banff Research Station in Canada in November 2017 where Majumdar is the principal organizer of a research workshop. Majumdar is also the Bath representative of a LMS South-West network for "Generalized Solutions for Nonlinear Partial Differential Equations" which regularly organizes meetings, which can provide another meeting point for further collaboration and completion of the research initiated during the ICMS Research in Groups scheme. The team expects to co-author two publications as an immediate consequence of this scheme and ICMS support and hospitality will be gratefully acknowledged in all related publications, research outputs and grant applications.

References

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