Modelling Nematic Liquid Crystal Defects in Landau-de Gennes Theory

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Background

The use of Liquid Crystals (LCs) in everyday life is virtually unavoidable, spanning applications from the all-too-familiar use in Liquid Crystal displays (LCDs) in smartphones, to more unusual applications such as in the pharmaceutical industry [1]. Following the discovery of the cholesteric LC in 1888 by the botanical physiologist Friedrich Reinitzer, many more types of LCs have been identified since and closely studied by chemists, physicists and mathematicians. It is, therefore, not surprising that mathematical models, which can predict how these materials behave are of particular interest, one of which is the Landau-de Gennes theory, which this project will consider.

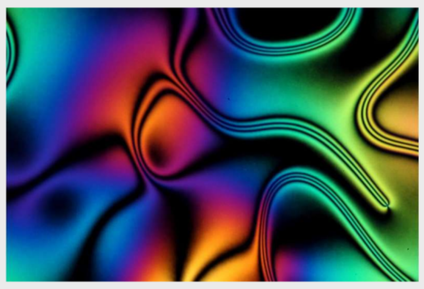

Figure 1: Liquid Crystal viewed through polarised light [3].

Liquid Crystals and the Q-Tensor

A LC describes a type of material which has an intermediate state lying between the solid and liquid phases. Because of this unique property, LCs behave interestingly: they flow as liquids, but yet preserve properties unique to crystalline solids (e.g. optical properties).

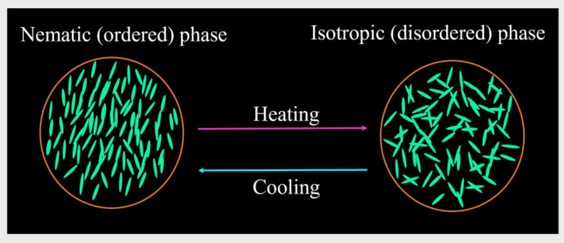

Figure 2: Schematic diagram of the transition between phases.

There is a wide variety of types of these materials, such as lyotropic LCs which depend on the concentration in a solution to trigger a phase transition; an example of this is a simple mixture of soap and water! Thermotropic, temperature-dependent, nematic LCs are another type on which we will focus. Thermotropic LCs are the simplest to model, mathematically speaking, since the constituent molecules are rod-like in shape and mathematicians exploit this fact. Due to the symmetric structure, a matrix, the Q-Tensor, can describe the orientations of the molecules. In 2 dimensions it is defined as:

$$Q := \int_0^{2\pi} \left(\begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} \otimes \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} - \frac{1}{2}\mathbb{I}_{2\times 2} \right) F(\theta)\, \mathrm{d}\theta,$$

where $F : [0, 2\pi) \to [0, 1]$ is the probability distribution function (PDF) defined on the unit circle. This essentially tells us how likely one is to find a molecule pointing in the θ-direction.
Now, Q can not be any matrix – it must obey the following conditions:

- $Q^T = Q$ (symmetric),
- $\mathrm{tr}(Q) = Q_{11} + Q_{22} = 0$ (traceless),
- $-\frac{1}{2} \leq \lambda(Q) \leq \frac{1}{2}$ (bounded eigenvalues).

Formally, $Q \in \mathscr{S}_0 := \left\{ Q \in \mathbb{R}^{2\times 2} : Q^T = Q,\ \mathrm{tr}(Q) = 0,\ -\frac{1}{2} \leq \lambda(Q) \leq \frac{1}{2} \right\}$.

Defects in Nematic LCs

One of the special properties LCs possess is that they can exhibit defects. Many exist, but we shall focus on one specific type: hedgehog-type defects.

As the name suggests, these defects are in a way "spiky", that is, the orientations of molecules within a hedgehog are pointing towards the core. Take the $Q \in \mathbb{R}^{2\times 2}$ to be the zero matrix: this is the isotropic Q-tensor. All other Q-Tensors are representative of the nematic phase.

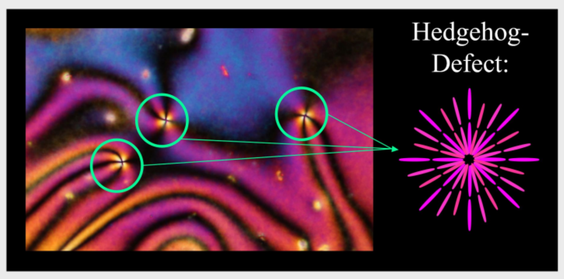

Figure 3: Schematic diagram to help visualize hedgehog defects [2].

Varying orientational order within a liquid crystal manifests itself in the coloured regions in the image above. Black regions represent the isotropic regions.

The associated Q-Tensor field of this defect is given (in cartesian co-ords):

$$Q(x) = s \begin{pmatrix} \frac{1}{2}(x_1^2 - x_2^2) & x_1 x_2 \\ x_1 x_2 & \frac{1}{2}(x_2^2 - x_1^2) \end{pmatrix},\ s \in \mathbb{R}. \tag{1}$$

The Landau-de Gennes Energy and the Euler-Lagrange Equation in 2D

The Landau-de Gennes (LdG) energy describes the free energy of nematic liquid crystals, specifically, their equilibrium properties. It is defined as:

$$E[Q] := \int_\Omega \underbrace{\frac{L}{2}|\nabla Q(x)|^2}_{\text{Elastic energy}} + \underbrace{\frac{a}{2}\mathrm{tr}(Q(x)^2) + \frac{c}{4}(\mathrm{tr}(Q(x)^2))^2}_{\text{Bulk energy}}\, \mathrm{d}x, \tag{2}$$

where $a, c, L \in \mathbb{R}$, $(L > 0)$.

The LdG energy expression is derived via methods found in group theory: we say that $\Psi(Q, D)$ is isotropic if and only if $\Psi(RQR^T, D^*) = \Psi(Q, D)\ \forall\ R \in SO(2)$, where $D^* = R_{il}R_{jm}R_{kp}D_{lmp}$. This tells us that the value observed is independent of the reference frame used. Now, recall the bulk term above, and set $a := a_0(\theta - \theta_c)$ for some constants $a, \theta, \theta_c \in \mathbb{R}$. We then have:

$$f_B(Q) = \frac{a_0(\theta - \theta_c)}{2}\mathrm{tr}(Q^2) + \frac{c}{4}(\mathrm{tr}(Q^2))^2 \Longrightarrow \tilde{f}_B(\lambda) = a_0(\theta - \theta_c)\lambda^2 + c\lambda^4$$

is written in terms of the eigenvalues, λ, of Q. $\tilde{f}_B$ has roots: $\bar{\lambda} = 0$, (AM=2), $\bar{\lambda}^2 = \frac{-a_0(\theta-\theta_c)}{c}$.

Taking $c, a_0 > 0$, $\theta_c \in \mathbb{R}$ and varying θ we consider the three case for which $\frac{-a_0(\theta-\theta_c)}{c}$ is positive, zero and negative.

Suppose we want to find the equilibrium equation of a nematic LC. What we do is minimize (2) using methods from variational calculus; this gives us the expression below:

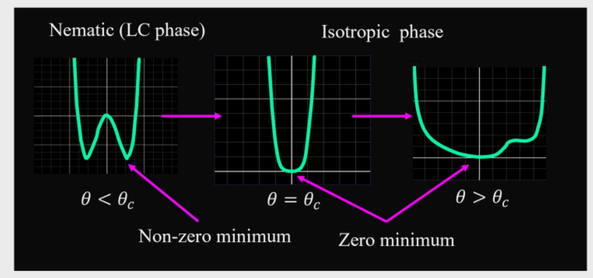

Figure 4: The three cases for the quartics. θ denotes the varied temperature, θ_c denotes the critical temperature.

$$-L\Delta Q(x) + aQ(x) + c\mathrm{tr}(Q(x)^2)Q(x) = 0 \in \mathbb{R}^{2\times 2}. \tag{3}$$

It can be shown that the defect seen in (1) is a solution of this Partial Differential Equation (PDE).

Future work: The Beris-Edwards Equations

The Beris–Edwards Model is:

$$(\mathcal{S}) \begin{cases} \frac{\partial Q}{\partial t}(x,t) + \big(u(x,t).\nabla\big)Q(x,t) - S\big(Q(x,t), \nabla u(x,t)\big) = -\Gamma\, \frac{\delta E}{\delta Q}\big(Q(x,t)\big), \\ \frac{\partial u}{\partial t}(x,t) + \big(u(x,t).\nabla\big)u(x,t) = \nu\Delta u(x,t) - \nabla p(x,t) + \mathrm{div}(\tau(x,t) + \sigma(x,t)), \\ \nabla.u(x,t) = 0, \end{cases}$$

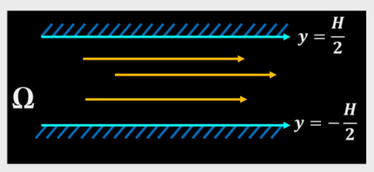

Figure 5: Flow of LCs through a channel Ω.

where $\Gamma, \nu \in \mathbb{R}$, $\frac{\delta E}{\delta Q}$ is the LHS of equation (3), and τ, σ are the stress tensors. S denotes to what degree the flow, u, locally rotates and dilates Q. The task we will consider is to investigate the stability of time-independent (equilibrium) solutions to $(\mathcal{S})$ in the following geometry Ω.

Summary

To quickly summarize what we have covered, we began by introducing liquid crystals and the history behind them. We saw that for one type, the nematic LC, there exists a matrix, the Q-Tensor, which models the orientations of the molecules. Formally, Q is an element of $\mathscr{S}_0$. Next we considered defects, specifically, hedgehog defects, which have their own matrix representation, seen in (1). These defects are a solution of the PDE which was derived by minimizing the energy expression $E[Q]$. We have visualized the three cases that arise when we vary θ in the second root of $\tilde{f}_B(\lambda)$. Lastly, we briefly introduced the future topic of the project which will concern the stability of equilibrium solution to $\mathcal{S}$.

References

[1] Imran Tadwee, Dr.Sadhana Shahi , Vivek Ramteke , Iftequar Syed, 2012, Liquid Crystals Pharmaceutical Application, Volume 1, Issue 2 (2012), 06-11. [online] [Accessed 7 March 2022].

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[3] SOFT MATTER LABORATORY, Nematic 8CB thin layer on a glass [online]. Available at: https://softmatter.si/gallery [Accessed 8 March 2022] [ill.].