NPDE PROJECT
MULTISTABILITY IN LIQUID CRYSTALS

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This document presents a look into the multistability of liquid crystals. I provide a brief peep into the physics of liquid crystals. The equations from which the basic analysis stems are assumed to hold good. Finite elements method for numerical analysis of partial differential equations has been implemented to find out the solutions of the mathematical equations.

Introduction To Liquid Crystals

Liquid Crystals are matter in a state which has properties between those of conventional liquids and those of solid crystals. A liquid crystal may flow but its molecules may be oriented in a crystal like way. Liquid crystals may be of different types depending on whether the phase transition occurs on the basis of temperature or concentration change.

1. Thermotropic: They exhibit a liquid-crystal phase transition as temperature is changed.

2. Lyotropic: They exhibit the transition as both temperature and concentration change.

3. Metallotropic

Thermotropic phases are those that occur in a particular range of temperatures. On the basis of

positional and orientational order the liquid crystal exist in various phases. At higher temperature they are mostly isotropic, and closer to the properties of a liquid. At lower temperatures however due to temperature changes the Thermotropic liquid crystals do exist in a number of changes being differentiated on the grounds of how the orientation varies across the different phases.

1. **Nematic phase**: Long range orientational order without any positional order. In nematic liquid crystals the molecular orientation of the rod like molecules is roughly in the same direction. They can flow freely. This gives rise to anisotropicity. They exhibit uniaxiality (only one axis, the other two being equivalent) and hence useful in LCD applications Optical properties are also present (due to polarized light).

2. **Smectic phase**: Found at lower temperatures than the nematics, they form well defined layers.

3. **Chiral phase**: Chiral molecules (molecules with no internal planes of symmetry) give rise to this phase.

4. **Blue phase**: Found in the temperature range between the chiral nematic (a type of chiral phase) and the isotropic phase.

Some Definitions

The director: The liquid crystals have a macroscopic order in place. The cylindrical molecules of the liquid crystal are oriented in a particular manner leading to the various interesting properties. This orientation is what gives rise to positional and orientational long range order in liquid crystals. The direction of the preferred order of orientation gives the director n (**n** and **-n** are equivalent).

The order parameter s: Gives a measure of the order present in the liquid crystal varying from

1 in solid crystal to 0 in isotropic liquids. It is defined as

$$s = \frac{< 3\sin^2\theta - 1 >}{2}$$

where θ is the angle between the molecular axis and the director **n**.

Remarks

Generally, the nematic liquid crystals that are in use today are unistable. They have just one stable state (which is the ground state) and energy is required to keep them in the ground state. In multistable liquid crystals theoretically speaking no energy is required to maintain an image in the ground state. Energy is only required to move from one state to the other. This decreases the power consumption. How are these stable states and hence ground states decided? Through free energy calculations. What is free energy? Free energy is that portion of any first law- energy that is available to perform thermodynamic work; i.e., work mediated by thermal energy. The minima wells in the free energy diagram constructed for the liquid crystals give the ground state configuration for the liquid crystals. The probability for the liquid crystal molecules to be in that state will be the maximum.

MULTISTABILITY

As mentioned earlier due to power consumption issues the need for multistable liquid crystals is rising. In a paper by Tsakonas et al the introduction to multistability through the use of liquid crystal wells was made. Nematic crystals were used and the temperature was held fixed to prevent the change in the phase of the liquid crystal due to changes in temperature.

Aim:

1. Physical;

a. Understanding the different theories used for arriving at the results and their drawbacks.

b. Finding the ground states solutions

c. Findin g the transition pathways between the different ground states.

2. Mathematical:

a. Numeric al methods to arrive at the results

b. Finite element method for one and two dimensional differential equations.

The planar device consists of small micrometer sized wells. Suitable substances and chemicals are used for ensuring multistability and homeotropic (tangent to the surface) Dirichlet boundary conditions. Depending on the strength of the anchoring the energy profile of the nematic liquid crystals consist of 6 wells or 2 wells. In the strong anchoring case 6 ground states exist- 4 rotated and 2 diagonals. In the weak anchoring case only two stable states exist the 2 diagonal states. These results are verified both experimentally and theoretically. Experimental results have been gotten through observing the liquid crystal sample through crossed polarizers. Experimental observations are validated through the Landau de Gennes free energy framework.

In the diagonal state the molecules are oriented along the diagonal of the wells. In the rotated state the orientation of the molecules changes through π along the cell. The walls of the cell are less than half the cross sectional length of the cell. Due to this a 2 dimensional approach to the problem can be made ignoring the 3^{rd} dimension completely. The entire mathematical calculation follows from a 2 dimensional approach to the Landaus de Gennes treatment.
There exists a critical value of the anchoring strength at which the bifurcation occurs. So for $W>W_c$ there exist 6 solutions but for $W<W_c$ there exist only the two diagonal solutions. Two different approaches have been studied and their drawbacks listed. The strong and the weak anchoring case have been dealt with separately. It turns out that the weak anchoring case converges to the strong anchoring case as the anchoring tends to infinity.

For finding out the stable states the anchoring strength is constant along the 4 edges. However, for studying the switching between two stable states a change in the anchoring strengths

along the four edges must be made. This is because we are studying the switching due to dielectric causes. We are ignoring flexoelectricity. The multistability of liquid crystals is being studied solely for the fluctuations in dielectric conditions. These changes affect the way the liquid crystal behaves in the presence of polarized light (due to changes in the optical properties).

The Two Theories- A brief Overview

OSEEN FRANK FRAMEWORK:

Its the simplest continuum theory available for nematic liquid crystals. A very important assumption is that of uniaxiality. It talks of a director **n** of the liquid crystal and assigns a free energy for each admissible **n**. The free energy under the one constant approximation is given by:

$\varepsilon_{OF}[\mathbf{n}]=\int\int_{\Omega} \frac{1}{2}\mathrm{K} \, \|\nabla \mathbf{n}\|^2 \, dA$

where K is the common value for the Frank constants K_1, K_2,and K_3 which are the constants that appear in this framework dependent on the liquid crystal itself.In this case $\Omega \subseteq \mathbb{R}^2$is the physical domain and **n** belongs to the Sobolev space $H^1(\Omega, S^1)$which is the space of unit vector fields with square integrable derivatives. In this framework owing to uniaxiality, there exists a homeotropic director direction along each surface. This leads to discontinuity in **n** at the vertices where two edges meet. However, it has been shown discontinuous **n** do not belong to the Sobolev space and hence this leads to infinite Oseen Frank energy. This problem is resolved by removing the assumption of uniaxiality and moving to the next viable theory, namely the Landau de Gennes theory of free energy.

LANDAU DE GENNES FRAMEWORK

This free energy model removes the assumption of uniaxiality and instead considers a symmetric traceless matrix of order 2 (assumption of 2 dimensionalities for the problem in hand), namely **Q**. The matrix **Q** contains the information about the degree of order and the anisotropy of the liquid crystal. The eigenvectors of this matrix give the direction of the director and hence biaxiality is built in this matrix. The Eigen values give the order of directionality present in the liquid crystal.

$$\boldsymbol{Q} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \tag{1}$$

and s=s(x,y) is the order parameter as defined earlier.

The matrix $\boldsymbol{Q}$ is defined as below

$$\boldsymbol{Q} = s(2\mathbf{n} \otimes \mathbf{n} - I) \tag{2}$$

Unlike the Oseen Frank theory, the order parameter s in the $\boldsymbol{Q}$-tensor model varies across the modelling domain and, in particular, vanishes at the vertices as required.

REMARK:

I will be sticking to the Landau de Gennes theory for the further analysis and application. Presentation of results will be done using the strong anchoring method highlighted in the next section. A brief physical feel is given to the method. However the origin of the equations being used in the method have been assumed to be true.

The Strong Anchoring Method

In the strong anchoring case the director or, taking the LDG theory, the eigenvector is constrained to be strictly tangent to the edges of the rectangular domain. This information is encoded in $\boldsymbol{g}$ - the Dirichlet boundary conditions (Q_{11}, Q_{12}) = $\boldsymbol{g}$. For weak anchoring case this constraint is relaxed and the introduction of the surface anchoring energy has to be done, albeit the fact that the weak anchoring case is developed from the strong anchoring solution. Also it is important to keep in mind that the two methods are consistent and the weak anchoring case converges to the strong anchoring case as the anchoring strength tends to infinity. The energy of these states has to be minimised to get the multistable states. This energy is the total of the elastic energy, the bulk energy , the surface anchoring energy and the electrostatic energy.
The energy functional after making the original equation dimensionless is given by

$$\varepsilon[\boldsymbol{Q}] = \iint_\Omega |\nabla Q_{11}|^2 + |\nabla Q_{12}|^2 + \tfrac{1}{\varepsilon^2}({Q_{11}}^2 + {Q_{12}}^2 - 1)\, dA \tag{3}$$

accompanied with a Dirichlet boundary condition (Q_{11}, Q_{12}) = $\boldsymbol{g}$.

The equivalence of the above relation with the energy minimization formulation and the weak formulation is being assumed. The proof of this equivalence follows simply from the basic rules of minimizing functionals. It can easily be shown that the problem of minimizing the energy functional given by (3) is equivalent to solving the equations given below:

$$0 = \iint_\Omega \nabla Q_{11} \nabla v_{11} + \tfrac{2}{\varepsilon^2}({Q_{11}}^2 + {Q_{12}}^2 - 1) Q_{11} v_{11}\, dA \tag{4}$$

$$0 = \iint_\Omega \nabla Q_{12} \nabla v_{12} + \tfrac{2}{\varepsilon^2}({Q_{11}}^2 + {Q_{12}}^2 - 1) Q_{12} v_{12}\, dA \tag{5}$$

$\forall v_{11}, v_{12} \in {H_0}^1(\Omega)$

Note: v_{11} and v_{12} are test functions in the Sobolev space.

The above equations hold for any fixed $\boldsymbol{g}$. (Why should $\boldsymbol{g}$ be fixed? Because we are concerned

about the stable states of the multistable liquid crystal and not about the switching mechanism between the various stable states on the free energy diagram. In case of switching, as mentioned before the boundary conditions have to be varying. For a fixed boundary condition stable states occur. Their number? Depends on the anchoring strength provided by the substrate or the wells in which these liquid crystals are confined). Solving the equations (4) and (5) for (Q_{11}, Q_{12}) gives the minimum of (3) in accordance with the Lax- Milgram's theorems.

These solutions of eqns. (4) and (5) reflect the number of minima in the free energy diagram and hence the stable states of the system. These equations are solved numerically using the Newton-Galerkin method and the Finite Elements Method. This procedure is explained in the next section.

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Solving the equations

After encountering initial failures by approaching to solve the equations using FEM first and then discretizing it, we tried it the other way around. The problem with the initial approach was not due to logical inconsistencies but rather due to the increased complexity of actually solving it and hence giving rise to performance issues. Thus keeping in mind that the earlier method might be more accurate in giving the results, due to practical woes the second method was adopted ,thus easing calculations a lot more.

$$\mathrm{A}(\boldsymbol{Q},\boldsymbol{v})=\int\int_{\Omega} \nabla Q_{11}\nabla v_{11}+\nabla Q_{12}\nabla v_{12}\, dA \tag{6}$$

$$B(\boldsymbol{Q},\boldsymbol{v}) =\int\int_{\Omega} \tfrac{2}{\varepsilon^2}({Q_{11}}^2+{Q_{12}}^2-1)Q_{11}v_{11}\, dA+\int\int_{\Omega} \tfrac{2}{\varepsilon^2}({Q_{11}}^2+{Q_{12}}^2-1)Q_{12}v_{12}\, dA \tag{7}$$

Next using the approximation

$\boldsymbol{Q}=\boldsymbol{Q_0}+\delta\boldsymbol{Q}$

with $\boldsymbol{Q_0}$ as the initial condition. Using Taylor series approximation of the functionals (6) and

(7) upto the second term, we get the following two equations of linear order in $\delta\boldsymbol{Q}$to be solved on the Sobolev space $H_0{}^1(\Omega)$.

$$\delta\boldsymbol{Q} = (u_1, u_2) \qquad (v_{11}, v_{12}) \equiv (v_1, v_2) \qquad (\boldsymbol{Q}_{11}{}^{\mathrm{o}}, \boldsymbol{Q}_{12}{}^{\mathrm{o}}) \equiv (u_1{}^{\mathrm{o}}, u_2{}^{\mathrm{o}})$$
$$\iint_\Omega \nabla u_1 \nabla v_1 \, dA + \tfrac{2}{\varepsilon^2} \iint_\Omega [(3u_1{}^{\mathrm{o}})^2 + (u_2{}^{\mathrm{o}})^2 - 1) u_1 v_1 \, dA + \tfrac{2}{\varepsilon^2} \iint_\Omega 2u_1{}^{\mathrm{o}} u_2{}^{\mathrm{o}} u_2 v_1 \, dA =$$
$$- \iint_\Omega \nabla \, u_1{}^{\mathrm{o}} \nabla v_1 \, dA - \tfrac{2}{\varepsilon^2} \iint_\Omega [(u_1{}^{\mathrm{o}})^2 + (u_2{}^{\mathrm{o}})^2 - 1](u_1{}^{\mathrm{o}}) v_1 \, dA \tag{8}$$

$$\iint_\Omega \nabla u_2 \nabla v_2 \, dA + \tfrac{2}{\varepsilon^2} \iint_\Omega [(3u_2{}^{\mathrm{o}})^2 + (u_1{}^{\mathrm{o}})^2 - 1) u_2 v_2 \, dA + \tfrac{2}{\varepsilon^2} \iint_\Omega 2u_1{}^{\mathrm{o}} u_2{}^{\mathrm{o}} u_1 v_2 \, dA =$$
$$- \iint_\Omega \nabla \, u_2{}^{\mathrm{o}} \nabla v_2 \, dA - \tfrac{2}{\varepsilon^2} \iint_\Omega [(u_1{}^{\mathrm{o}})^2 + (u_2{}^{\mathrm{o}})^2 - 1](u_2{}^{\mathrm{o}}) v_2 \, dA \tag{9}$$

Thus using this approach gives two equations of linear order to be solved using FEM numerically which is an easier task than the FEM for a nonlinear problem. Further information on the initial condition $\boldsymbol{Q_0}$ will be given in the next section.

FEM and the Initial Conditions

In this section, some technical details on the initial conditions and how the equations were actually solved are given. The equations (8) and (9) are solved using the Finite Elements method for a linear problem. We partition the domain $\Omega = [0, 1]x[0, a_{\mathrm{r}}]$into a uniform triangular mesh. Here we take a_r to be 1 where a_r represents the dimension of the crystal well. We approximate $H^1(\Omega)$using piecewise linear finite elemnts. After discretization, the integral equations become a linear set of equations which can then be solved. We then use the Newton Galerkin approach by iterating the process, 50 times to get the solution. To check whether the solutions are consistent, error calculations are done and the L2 errors are found out for each component of $\boldsymbol{Q}$.

The six different initial conditions for Newton's method

Solution	x=0	x=1	y=0	y=1
D1	$\pi/2$	$\pi/2$	0	0
D2	$\pi/2$	$\pi/2$	π	π
R1	$\pi/2$	$\pi/2$	π	0
R2	$\pi/2$	$\pi/2$	0	π
R3	$3\pi/2$	$\pi/2$	π	π
R4	$\pi/2$	$3\pi/2$	π	π

For a given Dirichlet boundary condition $\boldsymbol{g}$, we construct the initial conditions for the strong anchoring problem as follows, taking the D1 solution as an example. We first solve the Laplace equation $\Delta\theta = 0$ on the uniform mesh using the finite elements method with discontinuous boundary condition $\theta(0,y) = \theta(1,y) = \pi/2$ and $\theta(x,0) = \theta(x,1) = 0$. Next, we construct (Q_{11},Q_{12})=s(cos(2θ),sin(2θ)), where s=1 at the interior nodes and s=($\boldsymbol{g}$) at he boundary nodes. Then we use the resulting (Q_{11},Q_{12}) as the initial condition for the strong anchoring D1 solution. In the above table we enumerate the boundary conditions for all six type of initial conditions. For a fixed parameter $d > 0$, we define the vector field $\boldsymbol{g}_d$ to be:

$\boldsymbol{g}_d$= $\begin{cases} [T_d(x,0)] & \text{on } y=0 \text{ and } y=1 \\ [-T_d(y,0)] & \text{on } x=0 \text{ and } x=1 \end{cases}$ where the trapezoidal shape function T_d:[0,1] $\rightarrow \mathbb{R}$ is given by :

$$T_d(t)= \begin{cases} t/\mathrm{d}, & 0 \leq t \leq d \\ 1 & d \leq t \leq 1-d \\ (1-t)/d & 1-d \leq t \leq 1 \end{cases}$$

The parameter $d \in (0,0.5]$. To obtain the optimal solutions, we use the strong anchoring solutions for $\boldsymbol{g}$=$\boldsymbol{g}_{3\varepsilon}$ as the initial conditions. Here ε is the parameter that appears in the energy functional (3).

Results

We solved for the solution with the initial condition given by the D1 case. The Newton's method iteration was carried out for 10 cycles and the L2 error of each cycle was calculated with ref-

erence to the final solution. The L2 errors were seen to decrease with each iteration. These results prove the consistency of the solution as compared to the ideal scenario. The errors are displayed in the table below. The typical vaue of ε is 0.02.

Iteration	L2 error in the first component	L2 error in the second component
1	0.135076406508173	0.053939861414237
2	0.114942113563651	0.045984762030206
3	0.097217023129397	0.040100911611079
4	0.081085624614373	0.034823057749011
5	0.066049092691687	0.029494040801338
6	0.051807086484499	0.023922771161118
7	0.038177215388866	0.018117922247467
8	0.025045359412808	0.012149176380488
9	0.012336811403933	0.006090083879400

Conclusion

We have mathematically modelled and analysed a planar bistable liquid crystal device with tangent boundary conditions. We have modelled the static equilibrium condition with just one initial Dirichlet boundary condition case, that of D1 state. We also found that the solutions we obtained were consistent with what was expected. This was inferred purely on the basis of an error analysis of the result. Positive results were achieved by obtaining a decreasing list of L2 errors, thereby confirming our assessment of the problem. The modelling has been done within the Landau-de Gennes theory for nematic liquid crystals. Only the Strong anchoring case has been discussed, however comments on the weak anchoring approach have been made in the respective section. Switching characteristics have not been discussed by us as that would involve varying boundary conditions adding to complexity. Even though in this case we have considered only one stable state for analysis, the code can be easily extended to the other cases. Also the analysis and the modelling can be extended in a robust manner to the case of 3D

crystal wells too using similar techniques. Due to the symmetric nature of the $\boldsymbol{Q}$ the number of variables to be considered are relatively less and the extension is fairly doable, albeit a few complexities.

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Link To the Code files

https://github.com/ameypg16/NPDE-Final-D1