Morphologies of Nano-Included Liquid Crystals in 2d Square Wells

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Plan of talk

I. Introduction

- Liquid Crystals (LCs) and Magnetism
- Nano-inclusion and stability problem

II. Methodology

- Coarse grained free energy models
- Variational method

III. Results

- Analysis in $d = 2$

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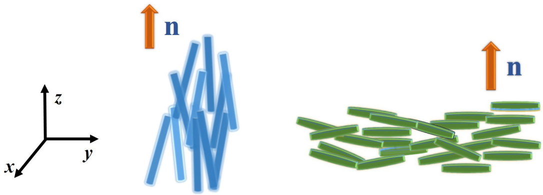
Liquid Crystals

- Liquid Crystals (LCs) are anisotropic systems which combine fluidity with long-range order.
- In the nematic phase, the long-range order is purely orientational.
- This order is described by a sign-invariant unit vector **n** known as the director.

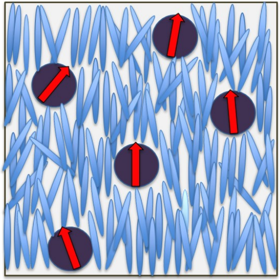


(a) Rod shaped LC molecules (b) Disc shaped LC molecules

- LCs are widely used in electro-optic devices such as optical switches and LCDs.

Ferro-Nematics with nano inclusion

- LCs are usually diamagnetic materials with small anisotropy of magnetic susceptibility $\sim 10^{-7}$.
- High Magnetic field ($H > 1$ kOe) is required to reorient directors.
- In 1970, Brochard and de Gennes published the theory of magnetic suspensions in LCs. **(Journal de Physique)**
- Rault et al. produced suspensions for the first time in 1970. **(Phys. Lett.)**
- Dipole moments of magnetic particles are aligned by a magnetic field, which in turn results in the reorientation of LCs due to the surface anchoring.
- Transfer of magnetic ordering to the underlying LC matrix and vice versa.



MNP-Nematic coupling

MNP-Nematic coupling depends on:

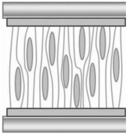
- volume fraction and dimension of particles.
- elastic constants of LC.

Strong Coupling

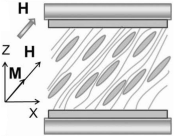
- Director follows the particles in a magnetic field.
- Reorientation of suspension is proportional to H for weak H and saturates for high H.

Weak Coupling

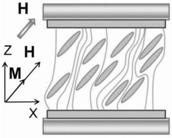
- There is a competition between restoring elastic force acting on director and aligning force due to MNP-nematic coupling.
- After reaching a maximum, reorientation angle decreases and director returns to intial state.



Initial Suspension



Strong Coupling

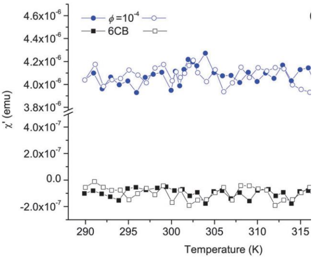


Weak Coupling

Reznikon et.al., Liquid Crystals with nano and microparticles.

Why nano-inclusion in LCs?

- Suspensions of magnetic nano particles (MNPs) in nematic LCs are of interest for both fundamental science and applications.
- Responses are enhanced and sensitised by nano-inclusion.
- MNPs in nematics can increase the magnetic susceptibility and generate new magnetic field-induced effects such as *Indirect Magneto-optic Effect* and *Converse Magnetoelectric Effect*.
- MNPs can change the hydrodynamic properties of nematics such as viscosity and diffusion.



Tomasocicova et. al., Soft Matter(2016)

Stability problem with nano-inclusion

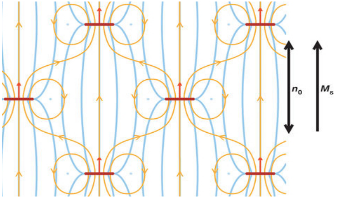
- MNPs usually aggregates, because of dipole-dipole interactions.
- The particles coagulated within tens of minutes.
- How to form stable nano included suspensions?
- Mertlej et al. (2013) reported the existence of ferromagnetic ordering in the stable suspension of magnetic platelets in NLC.
- Platelet shape and high magnetocrystalline anisotropy of MNPs were found to be crucial for realizing the ferromagnetic phase.

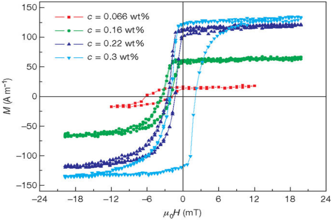
LCs: 5CB

MNPs: Barium hexaferrite

Thickness - 5 nm

Diameter - 70 $\pm$ 38 nm

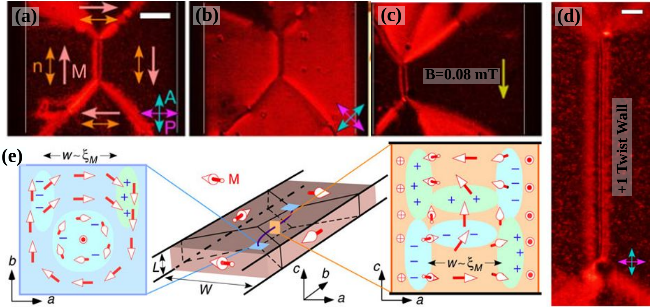




Mertelj et al., Nature (2013)

Experimental Morphologies of FN in Confinement

- Shuai et al. (2016) studied a fluid suspension of MNPs (BaHF) in NLCs (n-butanol) confined in a thin rectangular capillary.
- The equilibrium configuration in the absence of the external field is a loop of uniform magnetic domains separated by sharp walls.
- Applying external magnetic field induces domain wall movement.

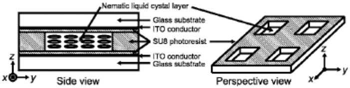


$L = 50\ \mu$m, $W = 1$ mm

Shuai et al., Nat. Commun. (2016)

Analysis in d = 2

- We study FN morphologies in a micron sized square well of size L^2 ($L \sim 80\ \mu$m) and having depth $d < L/2$.
- In this shallow geometry, the LC molecules and MNPs primarly lie in a plane.



(Tsakonas et al., Appl. Phys. Lett. (2007))

- The suspension is assumed to be diluted so that the MNPs are dispersed uniformly and there is no clustering.
- Self-assembled morphologies of suspension in the absence of external fields.
- We employ the phenomenological approach involving minimisation of free energy obtained by expansion in terms of mesoscopic order parameters.
- There are two order parameters in the system:
  - $\mathcal{Q}$ tensor $\Rightarrow$ directions and degree of nematic ordering.
  - Magnetization $\mathbf{M}$ $\Rightarrow$ spatially averaged magnetic moment of the suspended MNPs.

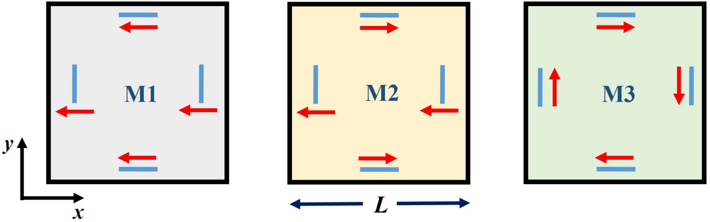
Boundary Conditions

Boundary Conditions for the LCs:

- For the purely nematic system, the minimum energy of bulk corresponds to $Q_{11}^2 + Q_{12}^2 = 1$.
- *Tangent boundary conditions*:
  $Q_{11} = -1,\ Q_{12} = 0$ at $y = 0,\ y = L$.
  $Q_{11} = 1,\ Q_{12} = 0$ at $x = 0,\ x = L$.

Boundary Conditions for **M**:

- M1: $\mathbf{M} = (-1, 0)$ at $x = 0, 1$ and $y = 0, 1$.
- M2: $\mathbf{M} = (1, 0)$ at $x = 0, 1$; $\mathbf{M} = (-1, 0)$ at $y = 0, 1$.
- M3: $\mathbf{M} = (0, 1)$ at $x = 0$; $\mathbf{M} = (0, -1)$ at $x = 1$; $\mathbf{M} = (-1, 0)$ at $y = 0$; $\mathbf{M} = (1, 0)$ at $y = 1$.

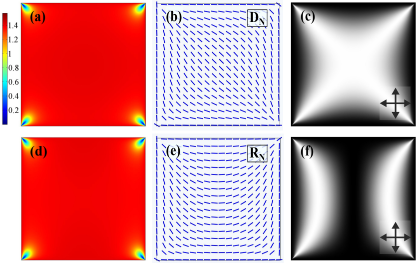


Morphologoies of Uncoupled NLC

- We reproduce the results for uncoupled systems with $c_1 = c_2 = 0$ and obtain the NLC equilibria in the well geometry.
- In all the following cases $\ell_1 = \ell_2 = 0.001$.
- There are two stable equilibria *diagonal D_N* and *rotated R_N*.

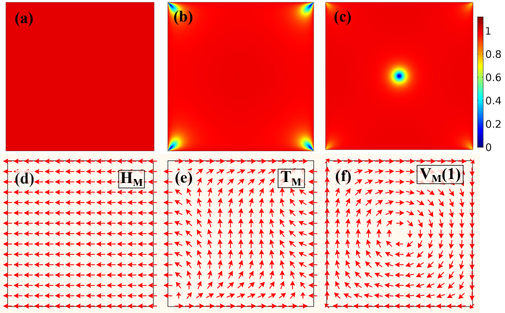
(Tsakonas et al., Appl. Phys. Lett. (2007), Luo et al., Phys. Rev. E (2012))

- Optical texutures are obtained by computing the transmission intensity $T \sim \sin^2 2\phi$, where ϕ is the angle made by $\mathbf{n}$ with the x-axis.



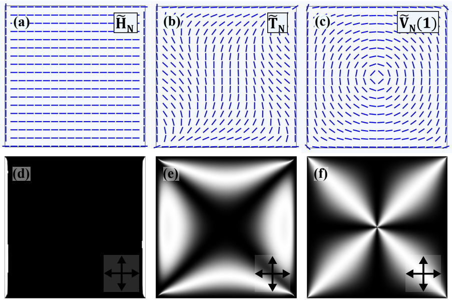
Morphologies of Uncoupled **M**

- Stable equilibrium solutions for $c_1 = c_2 = 0$ for BCs: M1, M2 and M3.
- M1 results in an aligned (homogeneous) magnetization state [in (a),(d)] which we refer to as H_M.
- M2 results in a twisted state T_M with defects in the corners [in (b), (e)].
- M3 results in a single vortex state $V_M(1)$ [in (c), (f)].



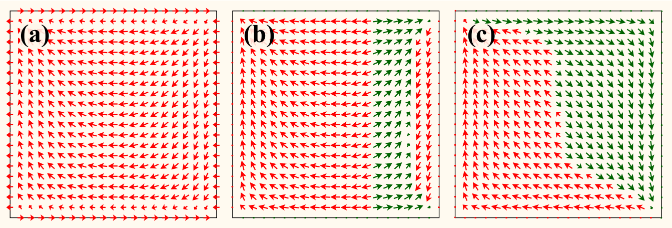
Case 1: $c_1 \neq 0$, $c_2 \simeq 0$

- In this case, the magnetic component affecting the nematic component but not vice-versa.
- (a) $c_1 = 1$ with BC M1 yield a homogeneous nematic morphology $\tilde{H}_N$.
- (b) $c_1 = 1$ with BC M2 yield a twisted nematic morphology $\tilde{T}_N$.
- (c) $c_1 = 10$ with BC M3 yield a morphology $\tilde{V}_N$ enclosing a defect with charge 1.



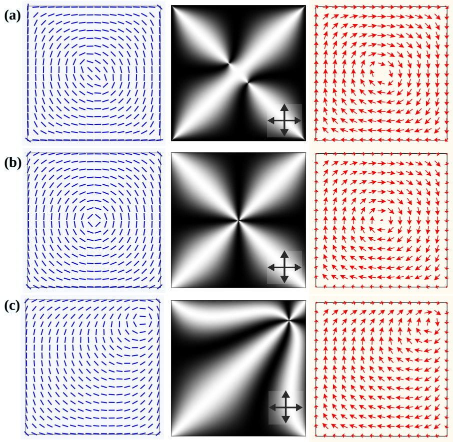
Case 2: $c_1 \simeq 0,\ c_2 \neq 0$

- It corresponds to the case when the nematic component influences the magnetic component but not vice-versa.
- Stable equilibrium configurations of $\mathbf{M}$ resulting from (a) M2 and $c_2 = 1$, (b) M2 and $c_2 = 50$, (c) M3 and $c_2 = 50$.
- The corresponding nematic patterns are R_N for (a), (b) and D_N for (c).



Case 3: $c_1 = c_2 = c$ with M3

- The **n** and **M** morphologies when coupling is equal.
- (a) $c = 1$, $\ell_1 = \ell_2 = 0.001$: The configuration exhibit two defects each with a charge of $1/2$.
- (b) $c = 10$, $\ell_1 = \ell_2 = 0.001$: The configuration have a single defect structure of charge $+1$ at the center.
- (c) $c = 10$, $\ell_2 = 0.001$, $\ell_1 = \ell_2/10$: The position of the defect changes with decrease in ℓ_1.



Summary

- We have used free energy formalism to obtain mophologies of nano-included LCs in 2d wells.
- We obtain a variety of morphologies by an interplay of model parameters c_1, c_2, ℓ_1 and ℓ_2 and construct the solution space.
- For $c_1 \neq 0$, $c_2 \simeq 0$, nematic director $\mathbf{n}$ align along the magnetic vector $\mathbf{M}$.
- For $c_1 \simeq 0$, $c_2 \neq 0$, there is emergence of magnetic domains with $\mathbf{M} \parallel \mathbf{n}$ and $-\mathbf{M} \parallel \mathbf{n}$.
- When $c_1 = c_2 = c$, we observe stable defects in nematic due to ferro-nematic coupling and confinement.
- How can we connect with experiments:
  - Feasible choices of c_1, c_2, ℓ_1, ℓ_2?
  - How can anchoring of the MNPs be achieved at the boundaries?

Thank You!