Sur les défauts du type “anneau de Saturne” des cristaux liquides nématiques

En l’honneur du 70ième anniversaire de John Ball

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Nematic Liquid Crystals

- Fluid of rod-like particles, partially ordered: particles prefer to order parallel to their neighbors
- Director $n(x)$, $|n(x)| = 1$ indicates local axis of preference: gives on average the direction of alignment.

- Oseen–Frank model: director should minimize elastic energy,

$$E(n) = \int_\Omega e(n, \nabla n)\, dx$$

$$e(n, \nabla n) = K_1(\nabla \cdot n)^2 + K_2[n \cdot (\nabla \times n)]^2 + K_3[n \times (\nabla \times n)]^2$$

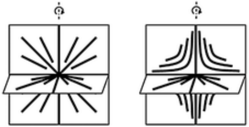
- Simple case: one-constant approximation $K_1 = K_2 = K_3 = 1$,

$$E(n) = \frac{1}{2}\int_\Omega |\nabla n|^2\, dx, \quad \text{the } \mathbb{S}^2 \text{ harmonic map energy.}$$

- n is not oriented, $-n \sim n$ gives same physical state.
  $\implies \quad n : \ \Omega \to \mathbb{R}P^2$.

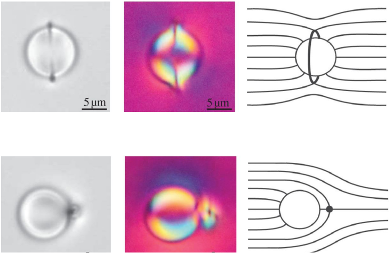
Harmonic Maps to $\mathbb{S}^2$ (or $\mathbb{R}P^2$)

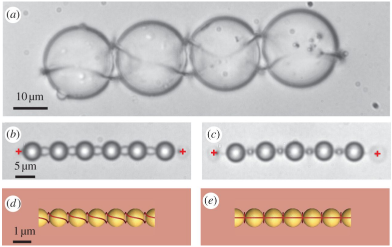
- Minimizers $n: \ \Omega \to \mathbb{S}^2$ of the Dirichlet energy $E(n) = \frac{1}{2}\int_\Omega |\nabla n|^2\, dx$ are harmonic maps.
- Minimizers solve a nonlinear elliptic system of PDE, $-\Delta n = |\nabla n|^2 n$
- Regularity theory for $\mathbb{S}^2$ or $\mathbb{R}P^2$-valued harmonic maps:
  - Schoen-Uhlenbeck (1982): $\mathbb{S}^2$-valued minimizers are Hölder continuous except for a discrete set of points.
  - Brezis-Coron-Lieb (1986): singularities have degree ± 1, $n \simeq \frac{Rx}{|x|}$, R orthogonal. ("hedgehog", "antihedgehog")



  - Hardt-Kinderlehrer-Lin (1986): for Oseen-Frank, min are real analytic except for a closed set Z, $\mathcal{H}^1(Z) = 0$.

Applications of colloidal suspensions in nematic liquid crystals: photonics, biomedical sensors, ...





I. Musevic, M. Skarabot and M. Ravnik, Phil Trans Roy Soc A, 2013

When small "colloid" particles are introduced in a nematic, we observe both point *and line* defects!

Model problem: Spherical colloid particle, nematic liquid crystal occupies the exterior domain $\Omega = \mathbb{R}^3 \setminus B_{r_0}(0)$.

Landau–de Gennes Model

A relaxation of the harmonic map energy.

- Introduce space of Q-tensors: $Q(x) \in \mathcal{Q}_3$, symmetric, traceless 3×3 matrix-valued maps. Q(x) models second moment of the orientational distribution of the rod-like molecules near x.
- Eigenvectors of $Q(x) =$ principal axes of the nematic alignment.
- Uniaxial Q-tensor: two equal eigenvalues; principal eigenvector defines a director $n \in \mathbb{S}^2$,

$$Q_n = s(n \otimes n - \tfrac{1}{3}\mathrm{Id}).$$

- $Q_n = Q_{-n}$; these represent $\mathbb{R}P^2$-valued maps.
- Biaxial Q-tensor: all eigenvalues are distinct. Strictly speaking, no director; but the principal eigenvector is an approximate director.
- Isotropic Q-tensor: all eigenvalues are equal, so $Q = 0$. No preferred direction, the liquid crystal has no alignment or ordering.

The LdG Energy

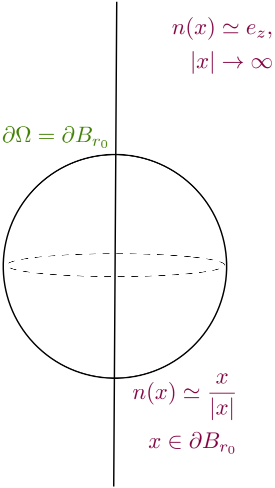
$$\mathcal{F}_L(Q) = \int_\Omega \left[\frac{L}{2} |\nabla Q|^2 + f(Q) \right] dx,$$

,

- Potential $f(Q) = -\frac{a}{2} \mathrm{tr}\,(Q^2) + \frac{b}{3} \mathrm{tr}\,(Q^3) + \frac{c}{4} (\mathrm{tr}\,(Q^2))^2 - d,$
- $a = a(T_{NI} - T)$, $b, c > 0$ constant, d chosen so $\min_Q f(Q) = 0$.
- $f(Q)$ depends only on the eigenvalues of Q.
- $f(Q) = 0 \iff Q = s_*(n \otimes n - \frac{1}{3} Id)$ with $n \in \mathbb{S}^2$ (uniaxial) and $s_* := (b + \sqrt{b^2 + 24ac})/4c > 0$
- Euler–Lagrange equations are semilinear,
  $$L\Delta Q = \nabla f(Q) = -aQ - b\left(Q^2 - \tfrac{1}{3}|Q|^2 I\right) + c|Q|^2 Q$$
- Uniaxial solutions are the exception; in most geometries expect biaxiality rules [Lamy, Contreras–Lamy]
- Analogy: Ginzburg–Landau model, a relaxation of the $\mathcal{S}^1$-harmonic map problem:
  $$\int_\Omega [\tfrac{\varepsilon^2}{2} |\nabla u|^2 + (|u|^2 - 1)^2], \ u: \ \Omega \to \mathbb{C}$$

The spherical colloid

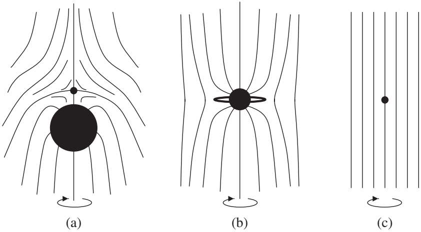
Consider a nematic in $\mathbb{R}^3$ surrounding a spherical particle $B_{r_0}(0)$.



- $\Omega = \mathbb{R}^3 \setminus B_{r_0}(0)$, exterior domain.
- Minimize LdG over $Q(x) \in H^1(\Omega; \mathcal{Q}_3)$.
- As $|x| \to \infty$, Q is uniaxial, with vertical director, $Q(x) \to s_* \left(e_z \otimes e_z - \frac{1}{3} I\right)$.
- On ∂B_{r_0}, homeotropic (normal) anchoring:
  - Strong (Dirichlet) with $n = e_r = \frac{x}{|x|}$,
    $Q(x)|_{\partial B_{r_0}} = Q_s := s_* \left(e_r \otimes e_r - \frac{1}{3} I\right)$.
  - Weak anchoring, via surface energy,
    $\frac{\hat{W}}{2} \int_{\partial B_{r_0}} |Q(x) - Q_s|^2 \, dS$
  - $\Longrightarrow \frac{L}{\hat{W}} \frac{\partial Q}{\partial \nu} = Q_s - Q$ on ∂B_{r_0}.

Part I: Size matters

Physicists observe that the character of the minimizers should depend on particle radius r_0 and anchoring strength $\mathcal{W}$.



Kleman & Lavrentovich, *Phil. Mag. 2006*.

(a) For large r_0, a "dipolar" configuration, with a detached (antihedghog) defect;

(b) For small r_0 with large $\mathcal{W}$, a "quadripolar" minimizer, with no point singularity but a "Saturn ring" disclination;

(c) For small r_0 and low $\mathcal{W}$, no singular structure at all.

Two scaling limits

Rescaling by particle radius r_0 and non-dimensionalizing with respect to reference energy, $a(T_{NI})$, we reduce to two parameters,

$$\tilde{\mathcal{F}}(Q) = \int_\Omega \left[\frac{1}{2}|\nabla Q|^2 + \frac{1}{\xi^2} f(Q) \right] dx + \frac{W}{2} \int_{\partial B_1} |Q_s - Q|^2 dA.$$

with coherence length $\xi^2 = \frac{\hat{L}}{r_0^2 a(T_{NI})}$, $W = \frac{\hat{W} r_0^2 a(T_{NI})}{L}$, anchoring strength.

- For fixed parameters ξ, W, there exists a minimizer in $\mathcal{H}_\infty$, $Q(x) \to Q_\infty$ uniformly as $|x| \to \infty$.
- We consider two limits:
  - Small particle limit. $\xi \to \infty$, with $W \to w \in (0, \infty]$.
  - Large particle limit. $\xi \to 0$, with Strong (Dirichlet) anchoring.

Size Theorem (Alama-B-Lamy, 2016)

Small particle limit:

When $\xi \to \infty$, $W \to w \in (0, \infty]$:

- Minimizers converge to a smooth limiting Q-tensor, which is biaxial a.e.; principal eigenvector is approximate nematic director.
- Defect is due to an eigenvalue crossing $\lambda_1 = \lambda_2$, eigenvectors exchange $\implies$ discontinuous director!
- Defect occurs along a circle, $U_w = (r_w, \theta, 0)$, with r_w root of:

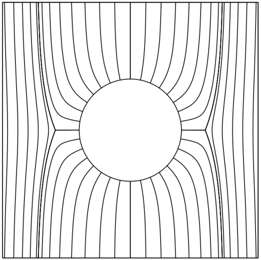
$$r^3 - \tfrac{w}{1+w} r^2 - \tfrac{w}{3+w} = 0.$$

Large particle limit:

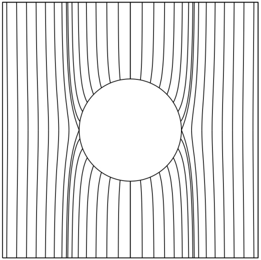
- Assume axial symmetry (consistent with physical intuition) and strong anchoring (Dirichlet BC).
- When $\xi \to 0$, converge to uniaxial Q-tensor, with oriented director $n(x)$, an $\mathbb{S}^2$-valued harmonic map.
- There is a unique point defect on the z-axis.

The Saturn Ring

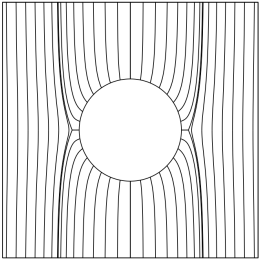
$w = \infty$



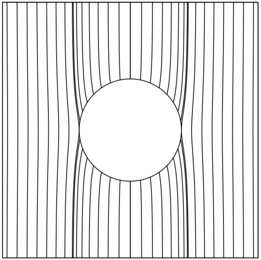
$w = 1.732 \approx \sqrt{3}.$



$w = 3.$

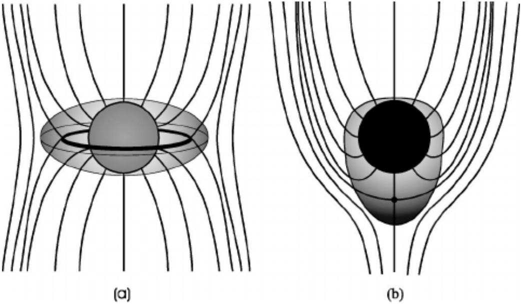


$w = 1.$



Part II: Confinement and magnetic fields

- In practice, ring defects are observed even for relatively large colloids.
- Role of confined geometries: colloid in a narrow channel prefers ring to point defect (Lavrentovich).



Narrower transition to vertical directors reduces energy of the ring.

- H. Stark (2002): a strong applied magnetic field plays the role of confinement, penalizing deviation from vertical director.

Adding a magnetic field term

We use the energy density (Fukuda-Yokohama)

$$e_{mag}(Q) = h^2\, g(Q) = h^2 \left[\sqrt{\tfrac{2}{3}} - \tfrac{Q_{33}}{|Q|}\right]$$

- For $Q = n \otimes n - \frac{1}{3} I$ uniaxial, $g(Q) = \sqrt{\frac{3}{2}}(1 - n_3^2)$ favors vertical alignment.
- The normalization $Q_{33}/|Q|$ prevents high h from influencing the norm of Q.
- Together with the bulk potential, the effective potential $f(Q) + hg(Q) \geq c(h)\, |Q - Q_\infty|^2$, $Q_\infty := e_3 \otimes e_3 - \frac{1}{3} I$.
- For large h, expect $Q \simeq Q_\infty$ except for a boundary layer around ∂B_1.
- Defect should live inside the boundary layer.

LdG with magnetic term

Two length scales:

- ξ=nematic coherence length: defect core size.
- $\eta = \xi/h$ magnetic correlation length: boundary layer thickness
- The LdG energy becomes:

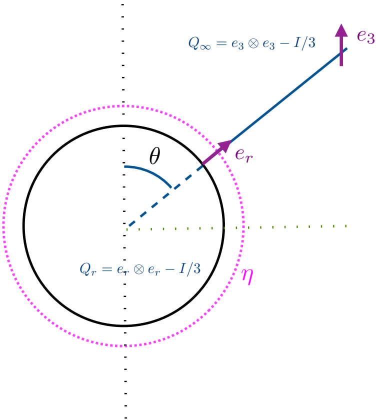
$$E_\eta(Q) = \underbrace{\int_\Omega \frac{1}{2}|\nabla Q|^2 + \frac{1}{\xi^2} f(Q)}_{E_{nem}} + \underbrace{\int_\Omega \frac{1}{\eta^2} g(Q) dx}_{E_{mag}},$$

$$f(Q) = -\frac{1}{2}|Q|^2 - \mathrm{tr}\,(Q^3) + \frac{3}{4}|Q|^4 + c, \quad g(Q) = \sqrt{\frac{2}{3}} - \frac{Q_{33}}{|Q|}.$$

- Heuristic (Stark):
  - Hedgehog: $E_{nem} \sim O(1)$ (point defect), $E_{mag} \sim O(\eta^{-1})$
  - Ring: $E_{nem} \sim O(|\ln \xi|)$ (line defect), $E_{mag} \sim O(1)$
- So ring should be preferred for high fields, $\eta < \eta_c \simeq \frac{1}{|\ln \xi|}$.
- Difficulty: we don't even know if solutions with ring or point defects exist!

Ansatz-free energy bounds

Idea: On each ray, Q connects from uniaxial Q_r on ∂B_1 to Q_∞ at infinity. The transition (of scale η) is like a vector-valued Allen-Cahn (Modica-Mortola; Sternberg)



$$E_\eta(Q_\eta) = \int_{\mathbb{S}^2} \underbrace{\int_1^\infty \left[\frac{1}{2}|\nabla Q_\eta(r,\omega)|^2 + \frac{1}{\xi^2} f(Q_\eta) + \frac{1}{\eta^2} g(Q_\eta)\right] r^2\, dr}_{=:\tilde{E}_\eta(Q_\eta(\cdot,\omega))} \, dS(\omega)$$

We bound $\tilde{E}_\eta(Q_\eta(\cdot,\omega))$ from below after a change of scale...

Ansatz-free bounds, II

- Fix a point $\omega \in \mathbb{S}^2$, and restrict a minimizer $Q = Q_\eta(r, \omega)$ to that ray:
- $\tilde{Q}_\omega(t) = Q_\eta(1 + \eta(t-1), \omega)$, $t \in [1, \infty)$ rescaled along ray,
- $\tilde{Q}_\omega(1) = e_r(\omega) \otimes e_r(\omega) - \frac{I}{3}$, $\tilde{Q}_\omega(\infty) = Q_\infty = e_z \otimes e_z - \frac{I}{3}$

$$\tilde{E}_\eta(Q_\eta(\cdot, \omega)) \geq \frac{1}{\eta} \int_1^\infty \left[\frac{1}{2} |\tilde{Q}'_\omega(t)|^2 + \frac{\eta^2}{\xi^2} f(\tilde{Q}_\omega) + g(\tilde{Q}_\omega) \right] dt$$

- We assume $\lambda = \lim_{\eta \to 0} \eta/\xi \in (0, \infty]$, and consider minimizers of a limiting energy along rays:
- If $\lambda < \infty$, $F_\lambda(\tilde{Q}_\omega) = \int_1^\infty \frac{1}{2} [|\tilde{Q}'_\omega(t)|^2 + \lambda f(\tilde{Q}_\omega) + g(\tilde{Q}_\omega)] \, dt$.
- When $\lambda = \infty$, we restrict Q to be uniaxial, and $F_\infty(\tilde{Q}_\omega) = \int_1^\infty \frac{1}{2} [|\tilde{Q}'_\omega(t)|^2 + g(\tilde{Q}_\omega)] \, dt$.
- In either case, the potential vanishes at a unique uniaxial Q-tensor $Q_\infty = e_z \otimes e_z - I/3$, its nondegenerate minimum.
- Call $D_\lambda(\omega)$ the minimum of F_λ over all $\tilde{Q}_\omega$ satisfying the BCs, so $\tilde{E}_\eta(Q_\eta(\cdot, \omega)) \geq \frac{1}{\eta} D_\lambda(\omega)$.

The lower bound on rays

$$D_\lambda(\omega) = \inf_{\substack{Q(1)=e_r(\omega)\otimes e_r(\omega)-I/3 \\ Q(\infty)=Q_\infty}} \int_1^\infty \frac{1}{2}[|Q'(t)|^2 + \lambda f(Q) + g(Q)]\,dt,$$

$$D_\infty(\omega) = \inf_{\substack{Q=n\otimes n-I/3 \\ n(1)=e_r(\omega),\,n(\infty)=\pm e_3}} \int_1^\infty \frac{1}{2}[|Q'(t)|^2 + g(Q)]\,dt$$

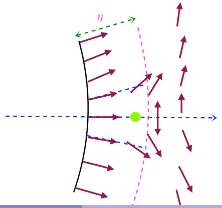
- As observed by Sternberg, $D_\lambda(\omega)$ is a geodesic distance in a degenerate weighted metric.
- Symmetry: for $\omega = (\theta, \phi)$ spherical coords, D_λ is independent of equatorial angle ϕ, and $D_\lambda(\omega(\pi - \theta, \phi)) = D_\lambda(\omega(\theta, \phi))$
- For $\lambda = \infty$, the minimizers trace geodesics on $\mathbb{S}^2$, to the North Pole if $0 < \theta < \frac{\pi}{2}$ and South Pole for $\frac{\pi}{2} < \theta < \pi$.
- Explicit calculation: $D_\infty(\omega(\theta, \phi)) = \sqrt[4]{24}(1 - |\cos\theta|)$
- At $\theta = \pi/2$ the minimizer is not unique (the defect!)

The defect

Constructing an upper bound to match the Modica-Mortola lower bound is like a recovery sequence in Γ-convergence:

- The minimizer $Q_\xi(r, \theta, \phi)$ is well-approximated by the minimizing heteroclinic along the ray at $(\theta, \phi) \in \mathbb{S}^2$.
- While the geodesic length $D_\lambda(\omega)$ is Lipschitz continous in $\omega \in \mathbb{S}^2$, the minimizing paths $\tilde{Q}_\omega$ may not be.
- For $\lambda = \infty$ (uniaxial case) this only occurs at $\theta = \pi/2$ ('cut locus') where geodesics are not unique. At $\theta = \pi/2$ there is a topological obstruction: this is our ring defect!
- For $\lambda < \infty$, we know less about the geodesics; we use the continuity of the energy via a Riemann sum approx.

- For $\lambda = \infty$:
- In a thin sector around the equator the degree is $-\frac{1}{2}$.
- The energy cost is $O(|\ln \xi|)$



Energy Asymptotics

For measurable $S \subset \mathbb{S}^2$, define the cone over S,
$\mathcal{C}_S = \{r\omega : \ \omega \in S, \ r > 1\}$.

Theorem (Alama-B-Lamy, '17)

Assume $\lambda = \lim_{\eta \to 0} \frac{\eta}{\xi} \in (0, \infty]$, *and* $\eta \ln \xi \to 0$. *Then, the minimizer* Q_η *has energy in* $\mathcal{C}_S$*:*

$$E_\eta(Q_\eta; \Omega \cap \mathcal{C}(S)) = \frac{1}{\eta} \int_{\omega \in S} D_\lambda(\omega)\, dS(\omega) + o\left(\frac{1}{\eta}\right)$$

- The energy calculation is local, over arbitrary sectors $\mathcal{C}_S$ over spherical domains. The main contribution is from a boundary layer of scale η around the sphere.
- To highest order in energy, Q_ξ has quadripolar symmetry *(axial rotation and equatorial reflection).*
  The Saturn Ring has quadripolar symmetry; a point defect would not.
- The defect itself has energy $O(|\ln \xi|) \ll \eta^{-1}$, so we cannot deduce the presence or absence of point or line defects.

Ring vs Hedgehog?

Can we verify Stark's heuristic comparison of ring vs point defect?

- Take $\lambda = \lim_{\eta \to 0} \frac{\eta}{\xi} = \infty$.
- Then the minimizing paths for $D_\infty(\theta)$ are uniaxial, associated to geodesics on $\mathbb{S}^2$,
$$D_\infty(\theta) = \sqrt[4]{24}(1 - |\cos\theta|).$$
- Assume uniaxial $Q_n(x) = n(x) \times n(x) - \frac{1}{3}I$, with orientable director field $n(x)$.
- For orientable n, the north and south poles are distinguished, so heteroclinics (geodesics) must connect to e_z, with energy $\sqrt[4]{24}(1 - \cos\theta)$.
- Thus, an orientable uniaxial tensor field Q_n must have much larger energy:
$$\eta E_\xi(Q_n) \geq 8\pi\sqrt[4]{24} \geq 4 \lim_{\xi \to 0} \left(\eta E_\xi(Q_\xi)\right).$$
- So Stark is right in principle, but wrong in the details: the energies of the ring and point defects are of the same scale, just a factor of 4 distinguishes them.

Félicitations!!

mulţumesc!