Qualitative properties of Landau-de Gennes energy minimizers

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joint work with Apala Majumdar

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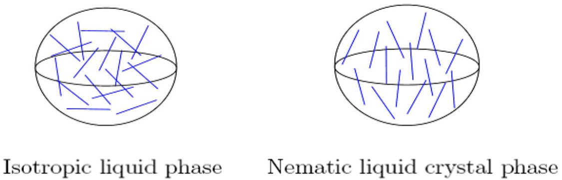
Liquid crystals: physics



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Landau-de Gennes Q-tensor reduction and earlier theories

- $$Q = \int_{\mathbb{S}^2} p \otimes p \, d\mu(p) - \frac{1}{3} Id$$
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Energy functionals in the three theories

- Landau-de Gennes:

$$\mathcal{F}_{LG}[Q] = \int_\Omega \frac{L}{2} Q_{ij,k}(x) Q_{ij,k}(x) + f_B(Q(x))\, dx$$

$$f_B(Q) = \frac{\alpha(T - T^*)}{2} \mathrm{tr}\left(Q^2\right) - \frac{b}{3} \mathrm{tr}\left(Q^3\right) + \frac{c}{4}\left(\mathrm{tr} Q^2\right)^2$$

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$$\mathcal{F}_E[s,n] = \int_\Omega s(x)^2 |\nabla n(x)|^2 + k|\nabla s(x)|^2 + W_0(s(x))\, dx$$

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Boundary conditions and the $W^{1,2}$ convergence

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$$Q_{min} = \{s_+ \left(n(x) \otimes n(x) - \frac{1}{3} Id \right), n \in \mathbb{S}^2\}$$

so that $\tilde{f}_B(Q) = 0 \Leftrightarrow Q \in Q_{min}$.

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$Q_b(x) = s_+ \left(n_b(x) \otimes n_b(x) - \frac{1}{3} Id \right), \; n_b(x) \in C^\infty(\partial\Omega, \mathbb{S}^2)$

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Heuristical bookkeeping: work with spectral quantitities

Examples

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Apriori L^∞ bounds

- $$L\Delta Q_{ij} = -a^2 Q_{ij} - b^2\left(Q_{ip}Q_{pj} - \frac{\delta_{ij}}{3}\mathrm{tr}Q^2\right) + c^2 Q_{ij}\left(\mathrm{tr}Q^2\right), i,j = 1,2,$$

- Multiply by Q_{ij} sum over repeated indices and obtain:

$$L\Delta(Q_{ij}Q_{ij}) - 2LQ_{ij,l}Q_{ij,l} = 2L\Delta Q_{ij}Q_{ij} \geq Lg(|Q|)$$

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The uniform convergence: obtaining uniform $W^{1,\infty}$ bounds-the general mechanism

- The energy inequality:

$$\frac{1}{r}\int_{B_r}\frac{|\nabla Q|^2}{2}+\frac{\tilde{f}_B(Q)}{L}dx\le\frac{1}{R}\int_{B_R}\frac{|\nabla Q|^2}{2}+\frac{\tilde{f}_B(Q)}{L}\,dx$$

for $r<R$

- Bochner-type inequality:

$$-\Delta e_L\le e_L^2$$

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- Cheap $W^{1,\infty}$ bound

$$|\nabla Q^{(L)}|_{L^\infty} \leq \frac{C}{\sqrt{L}}$$

- Combine with energy inequality and want to obtain that $\frac{1}{\rho}\int_{B_\rho(y)} \frac{|\nabla Q^{(L)}|^2}{2} + \frac{\tilde{f}_B(Q^{(L)})}{L}\,dx$ small enough (independently of L) for ρ small enough
- "Morally" the same with $\frac{1}{\rho}\int_{B_\rho(y)} \frac{|\nabla Q^{(0)}|^2}{2}\,dx$ where $Q^{(0)}$ is the limit (for which $f_B(Q^{(0)}) \equiv 0$)

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The uniform convergence of $\tilde{f}_B(Q)$ to 0 away from the singularities of the limiting harmonic map

- Cheap $W^{1,\infty}$ bound

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Two compatible quantities near the limit manifold $Q_{min} = \{s_+\left(n(x)\otimes n(x) - \frac{1}{3}Id\right), n\in\mathbb{S}^2\}$

- $$\frac{1}{\tilde{C}}\tilde{f}_B(Q) \le \Sigma_{i,j=1}^3\left(\frac{\partial \tilde{f}_B(Q)}{\partial Q_{ij}} + b^2\frac{\delta_{ij}}{3}\mathrm{tr}(Q^2)\right)^2 \le \tilde{C}\tilde{f}_B(Q)$$
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- where $\frac{\partial \tilde{f}_B(Q)}{\partial Q_{ij}} = -a^2Q_{ij} - b^2Q_{il}Q_{lj} + c^2Q_{ij}\mathrm{tr}(Q^2)$

Taylor expansion trick near the limit manifold

- For the matrix $Q(x)$ let us denote $n_1(x), n_2(x), n_3(x)$ its eigenvectors and $\lambda_1(x), \lambda_2(x)$, $\lambda_3(x) = -\lambda_1(x) - \lambda_2(x)$ the corresponding eigenvalues.
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The uniform convergence result

Proposition

Let $\Omega \subset \mathbb{R}^3$ be a simply-connected bounded open set with smooth boundary. Let $Q^{(L)}$ denote a global minimizer of the energy

$$\tilde{F}_{LG}[Q] = \int_\Omega \frac{L}{2} Q_{ij,k}(x) Q_{ij,k}(x) + \tilde{f}_B(Q(x))\, dx$$

with $Q \in W^{1,2}$ subject to boundary conditions $Q_b \in C^\infty(\partial\Omega)$, with $Q_b(x) = s_+ \left(n \otimes n - \frac{1}{3} Id\right), n \in \mathbb{S}^2$. Let $L_k \to 0$ be a sequence such that $Q^{(L_k)} \to Q^{(0)}$ in $W^{1,2}(\Omega)$.

Let $K \subset \Omega$ be a compact set which contains no singularity of $Q^{(0)}$. Then

$$\lim_{k\to\infty} Q^{(L_k)}(x) = Q^{(0)}(x), \text{ uniformly for } x \in K \tag{1}$$

Beyond the small L limit

- Heuristically: $Q^{(L)} \sim Q^{(0)} + LR^{(L)} + h.o.t$
- Beyond the first order term: biaxial $Q = s\left(n \otimes n - \frac{1}{3}Id\right) + r\left(m \otimes m - \frac{1}{3}Id\right)$

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Figure 1. Schematic representation of the biaxial core of a hedgehog. We show the section with a plane through the symmetry axis of the core. The ellipses suggest the molecular orientation on this section: the points where they degenerate in a disc are traversed by the uniaxial ring with negative scalar order parameter, which comes out of the page; accordingly, the broken circles show the trace of the torus with a maximum degree of biaxiality. Both the symmetry axis and the far director field are uniaxial with positive scalar order parameter.

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Biaxiality: high dimensional feature (i.e. no counterpart in Ginzburg-Landau)

- The space of Q-tensors $S_0 = \{M \in \mathbb{R}^{3\times 3}, \mathrm{tr}(M) = 0,\ M = M^t\}$ is $5D$.
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Landau-de Gennes minimizers
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- $\beta(Q) = 1 - \frac{6\left(\mathrm{tr}(Q^3)\right)^2}{\left(\mathrm{tr}(Q^2)\right)^3} \in [0,1]$ is a measure of biaxiality but is discontinuous. Use instead $\tilde{\beta}(Q) = \left(\mathrm{tr}(Q)^2\right)^3 - 6\left(\mathrm{tr}(Q^3)\right)^2$ which is analytic.
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Upper bounds size of 'defects' zone and biaxiality

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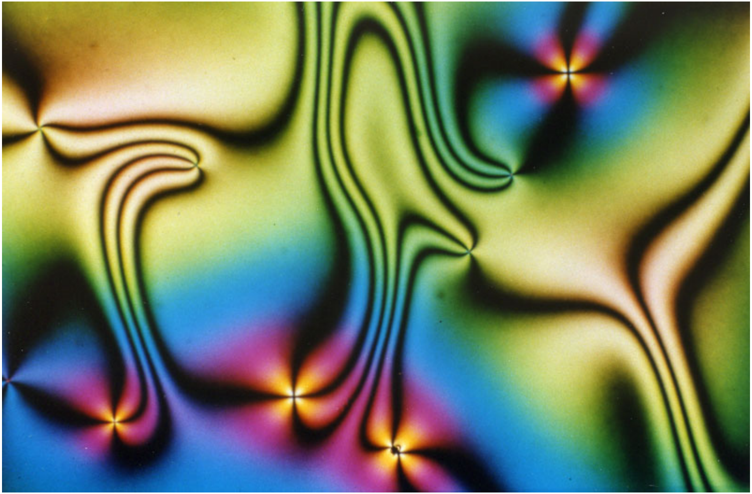
A physical experiment



A new (?) possible interpretation of defects in Landau-de Gennes theory

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The regularity of eigenvectors in our case

Proposition

(i) Let $Q^{(L)}$ be a global minimizer of $\tilde{F}_{LG}[Q]$. Then there exists a set of measure zero, possibly empty, Ω_0 in Ω such that the eigenvectors of $Q^{(L)}$ are smooth at all points $x \in \Omega \setminus \Omega_0$. The uniaxial-biaxial , isotropic-uniaxial or isotropic-biaxial interfaces are contained in Ω_0.

(ii) Let $K \subset \Omega$ be a compact subset of Ω that does not contain singularities of the limiting map $Q^{(0)}$. Let $n^{(L)}$ denote the leading eigenvector of $Q^{(L)}$ Then, for L small enough (depending on K), the leading eigendirection $n^{(L)} \otimes n^{(L)} \in C^\infty\left(K; M^{3\times 3}\right)$.

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- Better biaxiality bounds

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