Liquid crystal modeling

The constrained de Gennes' theory (with JM Ball)

Analogy with Ginzburg-Landau

The uniform convergence (with A. Majumdar)

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Coarsening and statistical dynamics (with E. Kirr and M. Wilkinson)

Q-tensors+NSE (with M. Paicu)

Mathematical problems of the Q-tensor theory of nematic liquid crystals

Arghir Dani Zarnescu

Carnegie Mellon
22 March 2011

Collaborators:

Q-tensor theory

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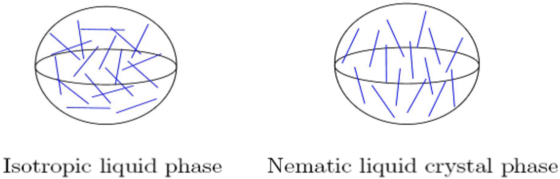
- M. Atiyah (Edinburgh), J. Ball (Oxford), E. Feireisl (Prague),
- R. Ignat(Paris), E. Kirr(Urbana-Champaign), A. Majumdar(Oxford),
- L. Nguyen(Princeton), M. Paicu(Bordeaux), J. Robbins (Bristol),
- G. Schimperna (Pavia), V. Slastikov (Bristol), M. Wilkinson (Oxford)

Liquid crystals: physics



- A measure μ such that $0 \leq \mu(A) \leq 1 \; \forall A \subset \mathbb{S}^2$
- The probability that the molecules are pointing in a direction contained in the surface $A \subset \mathbb{S}^2$ is $\mu(A)$

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Isotropic liquid phase   Nematic liquid crystal phase

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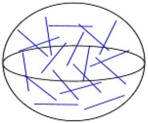

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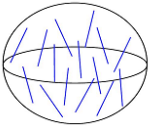

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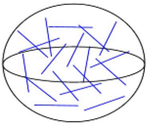

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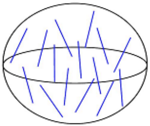

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Landau-de Gennes Q-tensor reduction and earlier theories

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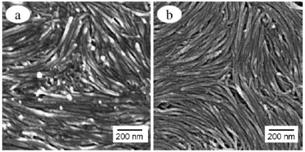
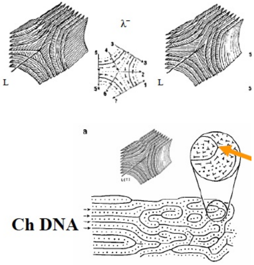
Q-tensors: beyond liquid crystals

- Carbon nanotubes:



- LC states of DNA:



- Active LC: cytoskeletal filaments and motor proteins

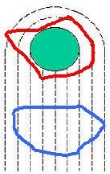
The big picture

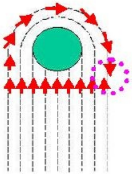
Increasing complexity of equations

- Full system-weak solutions (work in progress) with G. Schimperna (Pavia) and E. Fereisl (Prague)
- Coupled Navier-Stokes Q-tensor system(weak solutions and regularity in $2D$) (submitted) with M. Paicu (Bordeaux)
- Dynamics for the Q-tensor system only-statistical dynamics (work in progress) with Ph.D. student M. Wilkinson (Oxford) and E. Kirr (Urbana-Champaign)
- Stationary elliptic system
  - singular perturbation problem(published) with A. Majumdar(Oxford) and refinement (submitted) with L. Nguyen (Princeton)
  - existence and energetic stability(work in progress) index $\frac{1}{2}$-defects (with V. Slastikov (Bristol) and J. Robbins (Bristol)
  - existence and energetic stability(work in progress) radial hegehog (with R. Ignat (Paris), L. Nguyen and V. Slastikov)
- Q-harmonic maps: topological issues (submitted and in progress) with M. Atiyah, J. Ball (Oxford)

Topological aspects: line fields (constrained Q-tensors)

Use functions $Q:\Omega\to\{s_+\left(n\otimes n-\frac{1}{3}Id\right)\}$ with $s_+=s_+(\alpha,T,b,c)$ and $n\in\mathbb{S}^2$.

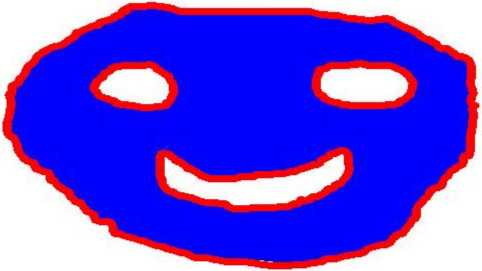




Theorem

(JM Ball-AZ) In a simply connected domain a line field in $W^{1,p}$ is orientable if $p\geq 2$. For $p<2$ there exist line fields that are not orientable.

A complex topology



Theorem (JM Ball, AZ) Let G be a domain with holes in the plane. A line field in $W^{1,p}$ for $p \geq 2$ is orientable if and only if its restriction to the boundary is orientable.

A domain with holes and partial boundary conditions

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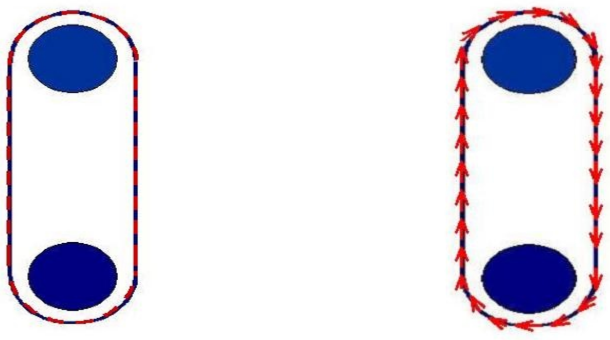
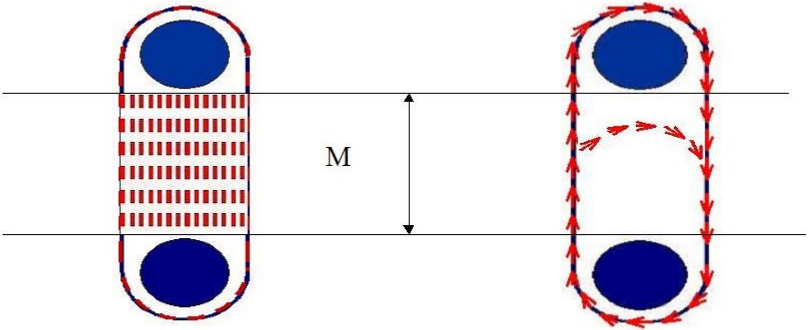


Comparison between line fields and vector fields global energy minimizers



For M large enough the **line field** perspective has lower energy

Beyond constrained Q-tensors

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Energy functionals in the three theories:

- Landau-de Gennes:

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

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

with $Q(x) : \Omega \to \{M \in \mathbb{R}^3, M = M^t, \mathrm{tr}M = 0\}$ a Q-tensor

- Ericksen's theory:

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

with $(s,n) \in \mathbb{R} \times \mathbb{S}^2$

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

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

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$Q_b(x) = s_+\left(n_b(x)\otimes n_b(x) - \frac{1}{3}Id\right),\ n_b(x) \in C^\infty(\partial\Omega, \mathbb{S}^2)$
- Recall: $\tilde{F}_{LG} = \int_\Omega \frac{|\nabla Q|^2}{2} + \frac{\tilde{f}_B(Q)}{L}\,dx$
- $Q^{(L)} \to Q^{(0)}$ in $W^{1,2}$ on a subsequence, as $L \to 0$.
- $Q^{(0)}$ a global energy minimizer of $\int_\Omega \frac{|\nabla Q|^2}{2}$ in the space $W^{1,2}(\Omega, Q_{min})$
- $Q^{(0)} = s_+\left(n^{(0)}\otimes n^{(0)} - \frac{1}{3}Id\right)$ and $\int_\Omega \frac{|\nabla Q^{(0)}|^2}{2}\,dx = 2s_+^2\int_\Omega \frac{|\nabla n^{(0)}|^2}{2}dx$ with $n^{(0)}$ a global minimizer of $\mathcal{F}_{OF}[n] = \int_\Omega |\nabla n|^2\,dx$ in $W^{1,2}(\Omega, \mathbb{S}^2)$

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

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- We denote

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

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

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

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

- The energy inequality:

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

for $r < R$

- Bochner-type inequality:

$$-\Delta e_L \leq e_L^2$$

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

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Heuristical bookkeeping: work with spectral quantitities

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Examples

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Heuristical bookkeeping: work with spectral quantitities

Examples

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Apriori L^∞ bounds

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

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

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

$$g(|Q|) \stackrel{def}{=} -a^2|Q|^2 - \frac{b^2}{\sqrt{6}}|Q|^3 + c^2|Q|^4$$

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- Hence $L\Delta\left(|Q|^2\right)(x) > 0$ for all interior points $x \in \Omega$, where $|Q(x)| > \sqrt{\frac{2}{3}}s_+$.

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The uniform convergence result

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Proposition

(A. Majumdar, AZ) 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

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

Beyond the small L limit

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- $\beta(Q) = 1 - \frac{6\left(\mathrm{tr}(Q^3)\right)^2}{\left(\mathrm{tr}(Q^2)\right)^3}$-biaxiality parameter
- *S. Kralj, E.G. Virga, J. Phys. A (2001)*

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.

Beyond the small L limit

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Defects:A physical experiment

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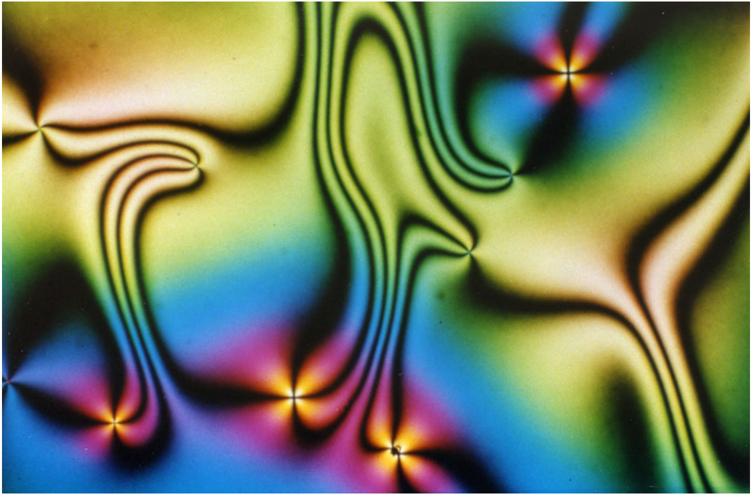

A possible interpretation of defects in Landau-de Gennes theory

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- A matrix depending smoothly on a parameter can have discontinuous eigenvectors
- Example: A real analytic matrix

$$Q^{(L)}(x,y,z) = \underbrace{\begin{pmatrix} 1 & y & 0 \\ y & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}}_{\stackrel{def}{=} Q^{(0)}} + \underbrace{\begin{pmatrix} Lx & 0 & 0 \\ 0 & -Lx & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\stackrel{def}{=} LR^{(1)}}$$

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- Consistent with the interpretation of PG De Gennes (Comptes Rendus Hebdomadaires des Seances de l'Academie des sciences, Serie B, 275(9) 1972)
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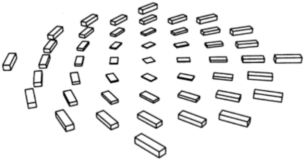

FIG. 1. Core of an $s=1/2$ disclination. The center is uniaxial with negative Maier-Saupe order parameter (planar uniaxial). It transforms via a biaxial ring into a uniaxial form with a positive S.

A possible interpretation of defects in Landau-de Gennes theory

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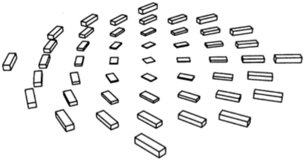

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The regularity of eigenvectors in our case

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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 $n^{(L)} \otimes n^{(L)} \in C^\infty\left(K; M^{3\times 3}\right)$.

The geometry of the Q-tensor (I)

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Coarsening and statistical dynamics (with E. Kirr and M. Wilkinson)

Q-tensors+NSE (with M. Paicu)

- Recall $\Delta Q^{(L)} = \frac{1}{L}\left[-a^2 Q - b^2\left(Q^2 - \frac{\mathrm{tr}(Q^2)}{3} Id\right) + c^2 Q\mathrm{tr}(Q^2)\right]$
- Heuristically: $Q^{(L)} \sim Q^{(0)} + LR^{(1)} + h.o.t$
- The limit $Q^{(0)} = s_+\left(n \otimes n - \frac{1}{3} Id\right)$ and $Q^{(0)}\Delta Q^{(0)} = \Delta Q^{(0)} Q^{(0)}$

The geometry of the Q-tensor (I)

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- After some geometry... $\Delta Q^{(0)} = -\frac{4}{s_+^2}(Q^{(0)} - \frac{1}{6} Id)\sum_{\alpha=1}^{3}(\nabla_\alpha Q^{(0)})^2$
- Equivalently the initial equation is $\Delta Q_{L_{k'}} = -\frac{4}{s_+^2}(Q_{L_{k'}} - \frac{1}{6} Id)\sum_{\alpha=1}^{3}(\nabla_\alpha Q_{L_{k'}})^2 + L_{k'} R_{L_{k'}}$
- We want to determine $R^{(1)} \stackrel{def}{=} \lim_{L\to 0} \frac{1}{L}(Q^{(L)} - Q^{(0)})$

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The geometry of the Q-tensor (II)

Lemma

For a point $Q \in S_*$, the tangent and normal spaces to S_* at Q are

$$T_Q S_* = \{\dot{Q} \in M^{sym}_{3\times 3} : \frac{1}{3} s_+ \dot{Q} = \dot{Q}\, Q + Q\, \dot{Q}\}, \tag{2}$$

$$(T_Q S_*)^\perp = \{Q^\perp \in M^{sym}_{3\times 3} : Q^\perp Q = Q\, Q^\perp\}. \tag{3}$$

Lemma

Let Q be a point in S_*. For X, Y in $T_Q S_*$ and Z, W in $(T_Q S_*)^\perp$, we have $XY + YX$, $ZW + WZ \in (T_Q S_*)^\perp$ and $XZ + ZX \in T_Q S_*$.

The equation for the next term in the asymptotic expansion

Proposition

(L. Nguyen, AZ) Assume that $Q_{L_k} \in C^2(\Omega, S_0)$ is a critical point of I_{L_k}, and that as $L_k \to 0$, Q_{L_k} converges on compact subsets of Ω in C^2-norm to $Q_* \in C^2(\Omega, S_*)$ which is a critical point of I_* and $\frac{1}{L_k}(Q_{L_k} - Q_*)$ converges in C^2-norm to some $Q_\bullet \in C^2(\Omega, S_0)$. If we write $Q_\bullet = Q_\bullet^{\|} + Q_\bullet^{\perp}$ with $Q_\bullet^{\|} \in T_{Q_*}S_*$ and $Q_\bullet^{\perp} \in (T_{Q_*}S_*)^{\perp}$, then

(i) *$Q_\bullet^{\perp}$ is given by*

$$Q_\bullet^{\perp} = -\frac{2}{b^2 s_+^2}\left[\frac{6}{6a^2 + b^2 s_+}|\nabla Q_*|^2\Big(c^2 Q_* + \frac{1}{3}b^2 Id\Big)\Big(Q_* - \frac{1}{6}s_+ Id\Big) - \sum_{\alpha=1}^{3}(\nabla_\alpha Q_*)^2\right], \tag{4}$$

(ii) *and $Q_\bullet^{\|}$ satisfies in Ω the equations*

$$\Delta Q_\bullet^{\|} = \Big[-b^2(Q_\bullet^{\|} Q_\bullet^{\perp} + Q_\bullet^{\perp} Q_\bullet^{\|}) - \frac{6c^2}{6a^2 + b^2 s_+}|\nabla Q_*|^2 Q_\bullet^{\|}\Big] - \frac{4}{s_+^2}\Big[\big(\nabla Q_\bullet^{\|}\big)^{\|}\nabla Q_* + \nabla Q_*\big(\nabla Q_\bullet^{\|}\big)^{\|}\Big]\Big(Q_* - \frac{1}{6}s_+ Id\Big) - \big(\Delta Q_\bullet^{\perp}\big)^{\|}, \tag{5}$$

where $\big(\nabla Q_\bullet^{\|}\big)^{\|}$ and $\big(\Delta Q_\bullet^{\perp}\big)^{\|}$ are the tangential components of $\nabla Q_\bullet^{\|}$ and $\Delta Q_\bullet^{\perp}$, respectively.

Dynamical issues: statistical aspects of coarsening

- The quenching from the isotropic into the nematic occurs through the creation of nematically ordered islands into the ambient isotropic fluid.
- A scaling phenomenon: the pattern of domains at a later time looks statistically similar to that at an earlier time, up to a time-dependent change of scale.
- $$C(r,t) = \frac{\langle Tr\,[Q(x+r,t)Q(x,t)]\rangle}{\langle Tr\,[Q(x,t)Q(x,t)]\rangle} \tag{6}$$

  where the brackets $\langle , \rangle$ denote an average over $x \in \mathbb{R}^d$ and **over the initial conditions**.
- The statistical scaling hypothesis states that for late enough times the correlation function $C(r,t)$ will assume a scaling form:

  $$C(r,t) \sim f\left(\frac{r}{L(t)}\right) \tag{7}$$

  where $L(t)$ is the time-dependent length scale of the nematic domains.

Statistical solutions and the correlation function

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- The simplest gradient flow of the energy $\int_{\mathbb{R}^d} \frac{L}{2}|\nabla Q|^2 + \frac{a}{2}\mathrm{tr}(Q^2) - \frac{b}{3}\mathrm{tr}(Q^3) + \frac{c}{4}\mathrm{tr}^2(Q^2)\, dx$

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

- Consider an averaging measure μ_0 on the infinite-dimensional functional space of initial datas, let us call it H. If Probability that $Q_0 \in A = \mu_0(A)$, for a Borel set $A \subset H$ then one can rigorously define the time-dependent family of measures $\mu_t(A) \overset{def}{=} \mu_0(\{S(t, Q_0) \in A\}) = \mu_0(S(t)^{-1}A)$(where $S(t, Q_0)$ is the solution with initial data Q_0 at time t) and study the evolution of these measures.
- We define then $C(r, t)$:

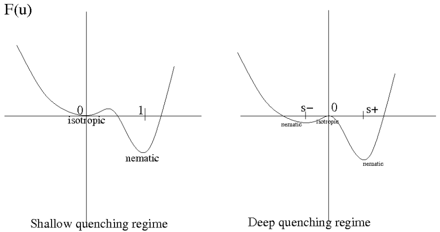
$$C(r,t) \overset{def}{=} \frac{\int_H \left(\int_{\mathbb{R}^3} \mathrm{Tr}\left[Q(x+r)Q(x)\right]\, dx\right) d\mu_t(Q)}{\int_H \left(\int_{\mathbb{R}^3} \mathrm{Tr}\left[Q(x)Q(x)\right]\, dx\right) d\mu_t(Q)}$$

The evolutionary equation: just a bistable gradient system

- High dimensional (in the domain and target space) version of:

$$\partial_t u = u_{xx} - F'(u), \;\; u(t,x) : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$$

- Choosing a suitable initial data, our system reduces to the scalar equation above.



- The equation is: $u_t = u_{xx} - au + bu^2 - c^2u^3$ with $a > 0$ in the shallow quenching and $a < 0$ in the deep quenching
- We continue referring just to the shallow quenching regime!

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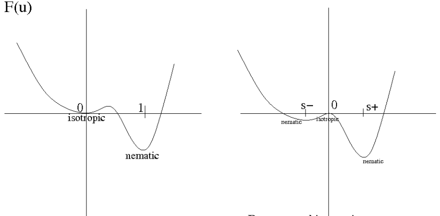

Shallow quenching regime Deep quenching regime

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Statistical solutions as averages of individual solutions and the individual behaviour I

- (A. Zlatos, JAMS, 19 (2006)) For initial data $u(0,x)=\chi_{[-L,L]}$ we have that there exists $L_0>0$ so that
  - If $L<L_0$ $u(t,x)\to 0$ uniformly on compacts
  - If $L=L_0$ $u(t,x)\to U$ uniformly on compacts, with U a stationary solution
  - If $L>L_0$ $u(t,x)\to 1$ uniformly on compacts
- $$C_n(r,t)=\frac{\Sigma_{j=1}^{J(n)}\theta_j^{(n)}\int_H\left(\int_{\mathbb{R}^3}\mathrm{Tr}\left[Q(x+r)Q(x)\right]\,dx\right)\,d\delta_{Q_j^{(n)}}}{\int_H\left(\int_{\mathbb{R}^3}\mathrm{Tr}\left[Q(x)Q(x)\right]\,dx\right)\,d\sigma\,d\delta_{Q_j^{(n)}}}\to C(r,t)\quad(8)$$

  where $\Sigma_{j=1}^{J(n)}\theta_j^{(n)}=1$.
- Understanding the behaviour of individual solution helps to understand the statistical solutions. But it might not be necessary...

Statistical solutions as averages of individual solutions and the individual behaviour II

- For small enough initial data we have a representation

$$Q_{ij}(t,x) = A_{ij}(Q)\frac{e^{-\frac{|x|^2}{4(t+1)}}}{e^{a^2 t}\left(4\pi(t+1)\right)^{3/2}} + w_{ij}(t,x)$$

where w_{ij} decays faster than the first term.

- Let $C_\delta(r,t) \stackrel{def}{=} \frac{\int_H \left(\int_{\mathbb{R}^3} \mathrm{Tr}[Q(x+r)Q(x)]\,dx\right) d\delta_{Q(t)}(Q)}{\int_H \left(\int_{\mathbb{R}^3} \mathrm{Tr}[Q(x)Q(x)]\,dx\right) d\delta_{Q(t)}(Q)}$. Then $\|C_\delta(r,t) - e^{-\frac{|r|^2}{8(t+1)}}\|_{L^\infty(dr)} = o(1)$ as $t \to \infty$.

- Thus for small initial data, $L(t) \sim t^{\frac{1}{2}}$, but this scaling only captures the underlying brownian motion.

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Statistical solutions as averages of individual solutions and the individual behaviour III

- If $u_0(x)$ is spherically symmetric $u_0(x) = \chi_{B(0,R)}$ for R large enough we have $u(t,x) \sim \chi_{B(0,\bar{c}t)}$ and $C_\delta(r,t) \sim P(\frac{r}{t})$ as $t \to \infty$ (where P is a third order polynomial).
- Thus for some large enough initial data $L(t) \sim t$ as $t \to \infty$

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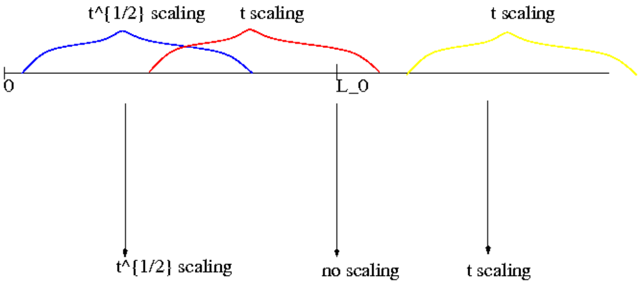

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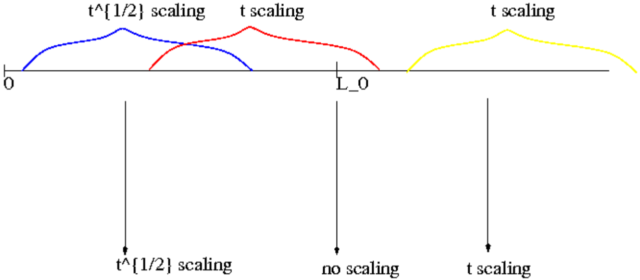

The Q-tensors+NSE system of equations

Q-tensor theory

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The flow equations:

- $$\begin{cases} \partial_t u + u\nabla u = \nu\Delta u + \nabla p + \nabla\cdot\tau + \nabla\cdot\sigma \\ \nabla\cdot u = 0 \end{cases}$$

  where we have the symmetric part of the additional stress tensor:

  $$\tau = -\xi\left(Q + \frac{1}{3}Id\right)H - \xi H\left(Q + \frac{1}{3}Id\right)$$

  $$+2\xi(Q + \frac{1}{3}Id)QH - L\left(\nabla Q\odot\nabla Q + \frac{\mathrm{tr}(Q^2)}{3}Id\right)$$

  and an antisymmetric part $\sigma = QH - HQ$ where

  $$H = L\Delta Q - aQ + b[Q^2 - \frac{\mathrm{tr}(Q^2)}{3}Id] - cQ\mathrm{tr}(Q^2)$$

- The equation for the liquid crystal molecules, represented by functions with values in the space of Q-tensors (i.e. symmetric and traceless $d\times d$ matrices):

  $$(\partial_t + u\cdot\nabla)Q - S(\nabla u, Q) = \Gamma H$$

  with

  $$S(\nabla u, Q) \stackrel{def}{=} (\xi D + \Omega)(Q + \frac{1}{3}Id) + (Q + \frac{1}{3}Id)(\xi D - \Omega) - 2\xi(Q + \frac{1}{3}Id)\mathrm{tr}(Q\nabla u)$$

Energy dissipation and weak solutions-apriori bounds

- $$E(t) \stackrel{\text{def}}{=} \underbrace{\int_{\mathbb{R}^d} \frac{L}{2}|\nabla Q|^2 + \frac{a}{2}\mathrm{tr}(Q^2) - \frac{b}{3}\mathrm{tr}(Q^3) + \frac{c}{4}\mathrm{tr}^2(Q^2)\,dx}_{\text{free energy of the liquid crystal molecules}} + \underbrace{\frac{1}{2}\int_{\mathbb{R}^d} |u|^2(t,x)\,dx}_{\text{kinetic energy of the flow}}$$

  is decreasing $\frac{d}{dt}E(t) \leq 0$.
- Note that this does not readily provide L^p norm estimates.

Proposition

For $d = 2, 3$ there exists a weak solution (Q, u) of the coupled system, with restrictions $c > 0$ and $|\xi| < \xi_0 s$, subject to initial conditions

$$Q(0,x) = \bar{Q}(x) \in H^1(\mathbb{R}^d),\ u(0,x) = \bar{u}(x) \in L^2(\mathbb{R}^d), \nabla \cdot \bar{u} = 0 \ \ in\ \mathcal{D}'(\mathbb{R}^d) \qquad (9)$$

The solution (Q, u) is such that $Q \in L^\infty_{loc}(\mathbb{R}_+; H^1) \cap L^2_{loc}(\mathbb{R}_+; H^2)$ and $u \in L^\infty_{loc}(\mathbb{R}_+; L^2) \cap L^2_{loc}(\mathbb{R}_+; H^1)$.

Regularity difficulties: the maximal derivatives and “the co-rotational parameter”

- Recall the system:

$$\begin{cases} (\partial_t + u\cdot\nabla)Q - \big(\xi D(u) + \Omega(u)\big)(Q + \frac{1}{3}Id) + (Q + \frac{1}{3}Id)\big(\xi D(u) - \Omega(u)\big) \\ -2\xi(Q + \frac{1}{3}Id)\mathrm{tr}(Q\nabla u) = \Gamma H \\ \\ \partial_t u + u\nabla u = \nu\Delta u_\alpha + \nabla p + \nabla\cdot\Big(QH - HQ\Big) \\ -\nabla\cdot\Big(\xi\Big(Q + \frac{1}{3}Id\Big)H + \xi H\Big(Q + \frac{1}{3}Id\Big)\Big) \\ +2\xi\nabla\cdot\Big((Q + \frac{1}{3})QH\Big) - L\nabla\cdot\big(\nabla Q \odot \nabla Q + \frac{1}{3}\mathrm{tr}(Q^2)\big) \\ \nabla\cdot u = 0 \end{cases}$$

with $H = L\Delta Q - aQ + b[Q^2 - \frac{\mathrm{tr}(Q^2)}{3}Id] - cQ\mathrm{tr}(Q^2)$.

- Worse than Navier-Stokes
- Where's the difficulty?
- If $\xi = 0$ maximal derivatives only

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The regularity result, in *2D*

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Theorem

Let $s>0$ and $(\bar{Q},\bar{u})\in H^{s+1}(\mathbb{R}^2)\times H^s(\mathbb{R}^2)$. There exists a global a solution $(Q(t,x),u(t,x))$ of the coupled system, with restrictions $c>0$ and $|\xi|<\xi_0$, subject to initial conditions

$$Q(0,x)=\bar{Q}(x),\ u(0,x)=\bar{u}(x)$$

and $Q\in L^2_{loc}(\mathbb{R}_+;H^{s+2}(\mathbb{R}^2))\cap L^\infty_{loc}(\mathbb{R}_+;H^{s+1}(\mathbb{R}^2))$,
$u\in L^2_{loc}(\mathbb{R}_+;H^{s+1}(\mathbb{R}^2)\cap L^\infty_{loc}(\mathbb{R}_+;H^s)$. Moreover, we have:

$$L\|\nabla Q(t,\cdot)\|^2_{H^s(\mathbb{R}^2)}+\|u(t,\cdot)\|^2_{H^s(\mathbb{R}^2)}\le C\Big(e+\|\bar{Q}\|_{H^{s+1}(\mathbb{R}^2)}+\|\bar{u}\|_{H^s(\mathbb{R}^2)}\Big)^{e^{e^{e^{Ct}}}} \tag{10}$$

where the constant C depends only on $\bar{Q},\bar{u}$, a,b,c,Γ and L. If $\xi=0$ the increase in time of the norms above can be made to be only doubly exponential.

The full system (in progress with E. Feireisl and G. Schimperna)

Q-LC molecules, u-fluid velocity, θ-temperature

$$(\partial_t + u\cdot\nabla)Q - \left[(\xi+1)\nabla u + (\xi-1)\nabla u^t\right]\left(\frac{Q}{2} + \frac{1}{2d}Id\right) - \left(\frac{Q}{2} + \frac{1}{2d}Id\right)\left[(\xi+1)\nabla u + (\xi-1)\nabla u^t\right]$$
$$+2\xi\left(Q + \frac{1}{d}Id\right)\mathrm{tr}(Q\nabla u) = \Gamma \underbrace{\left(L\Delta Q - \frac{\partial\psi(Q)}{\partial Q} + \frac{1}{d}\mathrm{tr}\left(\frac{\partial\psi}{\partial Q}\right)Id\right)}_{\stackrel{\mathrm{def}}{=} H}$$

$$\partial_t u + \nabla\cdot(u\otimes u) - \nabla\cdot\underbrace{\left(\lambda(\theta)[QH - HQ] - pId - \frac{\mu(\theta)}{2}(\nabla u + \nabla u^t)\right)}_{\stackrel{\mathrm{def}}{=}\mathbb{T}_1}$$

$$= \nabla\cdot\underbrace{\left(\lambda(\theta)\left[-\xi\left(Q+\frac{1}{d}Id\right)H - \xi H\left(Q+\frac{1}{d}Id\right) + 2\xi\left(Q+\frac{1}{d}\right)QH - L\nabla Q\odot\nabla Q\right]\right)}_{\stackrel{\mathrm{def}}{=}\mathbb{T}_2} + f$$

$$\nabla\cdot u = 0$$

$$\partial_t\theta + \nabla\cdot(\theta u) + \nabla\cdot(J(Q,\theta)\nabla\theta)) = \left(\mathbb{T}_1 + \mathbb{T}_2\right) : \nabla u$$

Q-tensor theory

Arghir Dani Zarnescu

Liquid crystal modeling

The constrained de Gennes' theory (with JM Ball)

Analogy with Ginzburg-Landau

The uniform convergence (with A. Majumdar)

Refined description of minimizers (with Luc Nguyen)

Coarsening and statistical dynamics (with E. Kirr and M. Wilkinson)

Q-tensors+NSE (with M. Paicu)

THANK YOU!