Defects in Landau-de Gennes Theory

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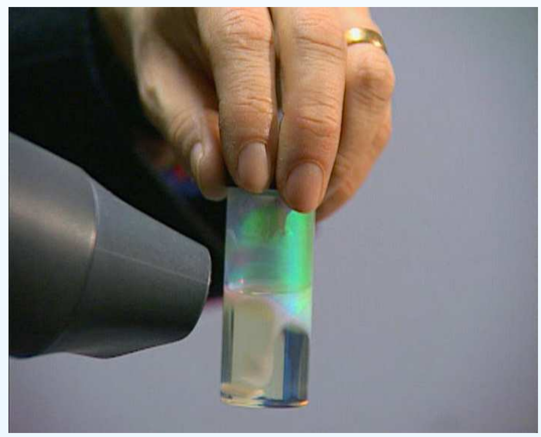
Complex materials; Mathematical models and numerical methods
Oslo University

(and parallel work by R Ignat, L Nguyen, V Slastikov, A Zarnescu)

June 10, 2015

Liquid crystals - Phenomena

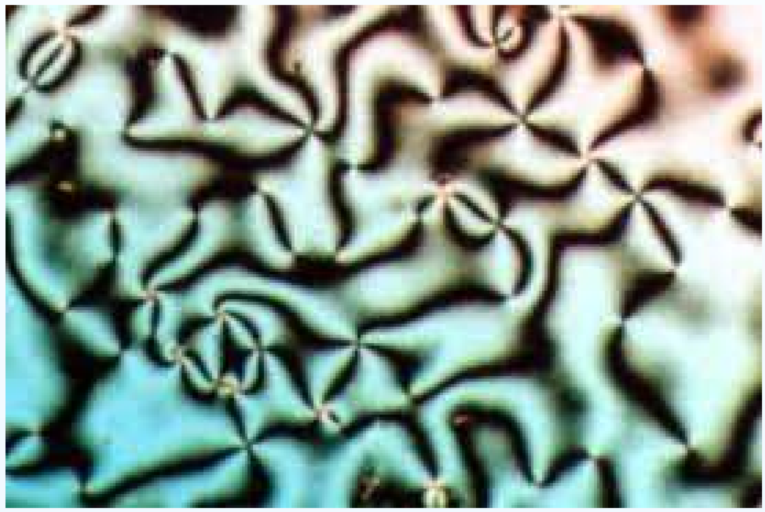
Clearing transition



Nematic phase, $T < T_*$

Isotropic phase, $T > T_*$

Liquid crystals - Phenomena



Viewed through crossed polarisers

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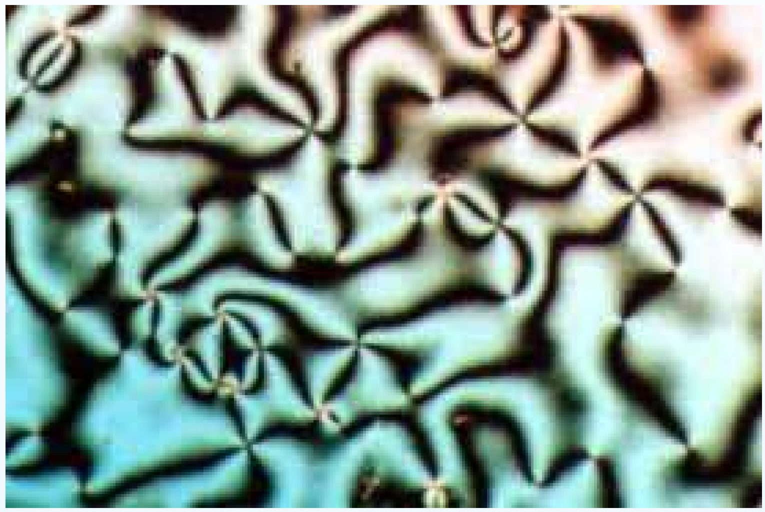
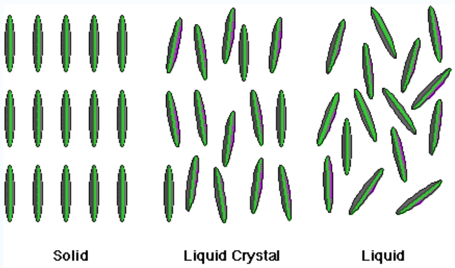


Viewed through crossed polarisers

Spatially varying anisotropy, $n(r)$

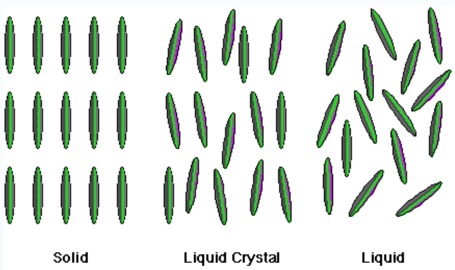
$n(r)$ has singularities, or defects

Oseen-Frank theory



$n(r)$, local orientation

Oseen-Frank theory



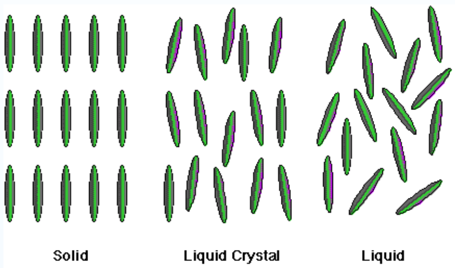
$n(r)$, local orientation

Oseen-Frank energy,

$$\mathcal{E}[n] = \int_\Omega \frac{K_1}{2}(\nabla\cdot n)^2 + \frac{K_2}{2}(n\cdot(\nabla\times n))^2 + \frac{K_3}{2}(n\times(\nabla\times n))^2,$$

invariant under rotations, $n \to -n$

Oseen-Frank theory



$n(r)$, local orientation

One-constant approximation,

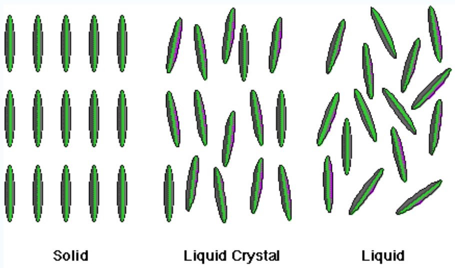
$$\mathcal{E}[n] = \int_\Omega \frac{L}{2}(\nabla n)^2, \qquad (\nabla n)^2 = \sum_{i,j=1}^{3} (\partial_i n_j)^2.$$

Euler-Lagrange equation,

$$\Delta n = -(\nabla n)^2 n,$$

solutions are S^2-valued harmonic maps

Oseen-Frank theory



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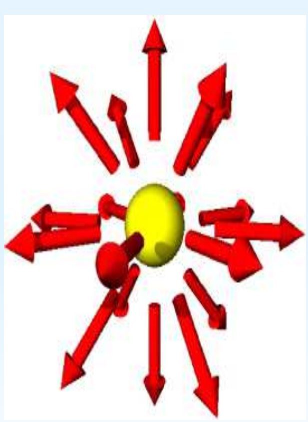
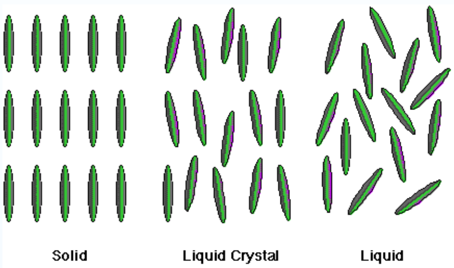


Okay for 3d point defects

Oseen-Frank theory



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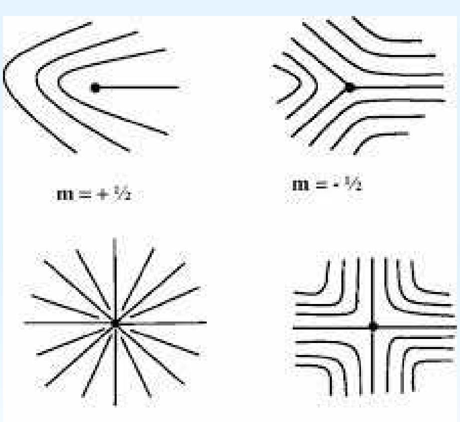
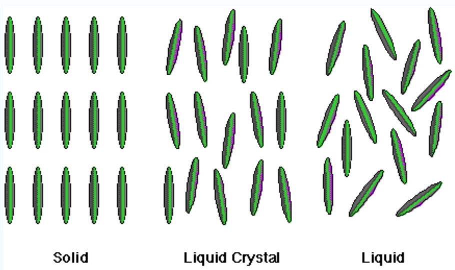


Problematic for 2d point defects

Oseen-Frank theory



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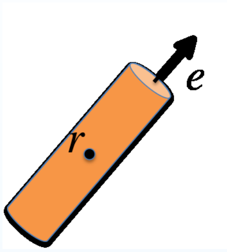
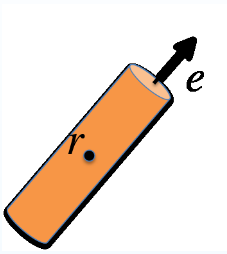
Would like to resolve the structure of defects. . .

Landau-de Gennes I – Q-tensors



N-particle distribution $\rho_N(r_j, e_j) \to$
$\rho(r, e)$, 1-particle distribution

Landau-de Gennes I – Q-tensors



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$$\rho(r, e) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c_{lm}(r) Y_{lm}(e)$$

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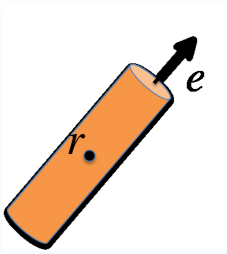

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Assume uniform density,

$$\int_{S^2} \rho(r,e)\, d^2e = 1 \implies c_{00}(r) = 1.$$

Assume nematic (not polar),

$$\rho(r,e) = \rho(r,-e) \implies c_{lm} = 0, \quad l \text{ odd}$$

Lowest-order nontrivial terms,

$$c_{2,m}(r) = \int_S^2 \rho(r,e) Y^*_{2m}(e)\, d^2e, \;\; m = -2, \ldots, 2$$

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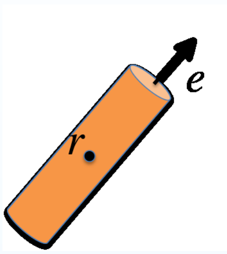

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Same information is contained in

$$Q_{jk}(r) = \int_{S^2} \rho(r,e) e_j e_k\, d^2e - \frac{1}{3}\delta_{jk}$$

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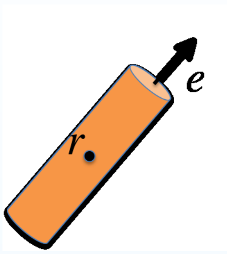

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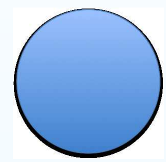
The Q-tensor $Q(r)$ is a real 3×3 symmetric traceless matrix-valued function.

Landau-de Gennes II – Symmetry characterisation of Q-tensors

$$Q \mapsto \mathcal{R} Q \mathcal{R}^T$$



Isotropic $\lambda_1 = \lambda_2 = \lambda_3$

$$Q = 0$$

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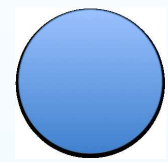

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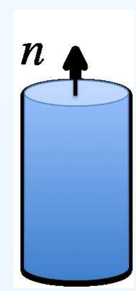

Prolate uniaxial $\lambda_1 > \lambda_2 = \lambda_3$

$Q = s(n \otimes n - \frac{1}{3} I), s > 0$

Connection to Frank theory. . .

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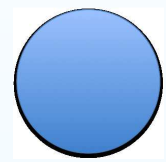

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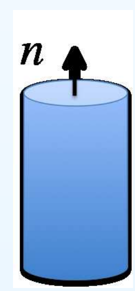

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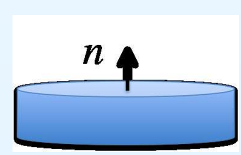
Connection to Frank theory...

Oblate uniaxial $\lambda_1 = \lambda_2 > \lambda_3$



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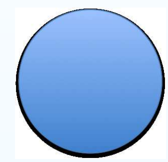

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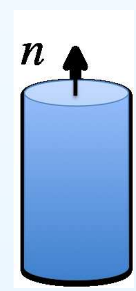

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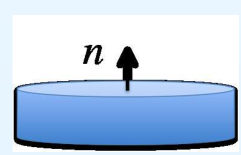

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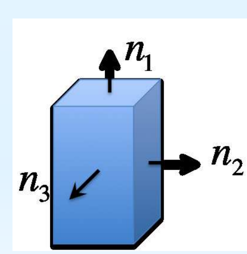
<u>Biaxial</u> $\lambda_1 > \lambda_2 > \lambda_3$



$Q = \lambda_1 n_1 \otimes n_1 + \lambda_2 n_2 \otimes n_2 + \lambda_3 n_3 \otimes n_3,$
$\lambda_1 + \lambda_2 + \lambda_3 = 0$

Landau-de Gennes III – Potential energy

Want $f(Q)$, rotationally invariant.

$$f(Q) = \frac{A}{2} \operatorname{Tr} Q^2 + \frac{B}{3} \operatorname{Tr} Q^3 + \frac{C}{4} (\operatorname{Tr} Q^2)^2,$$

bulk energy. $\quad C > 0$

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A, B, $C \sim 10^3 J/m^3$

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A, B, $C \sim 10^3 J/m^3$

We take

$$A = -a^2, \quad B = -b^2, \quad C = c^2.$$

In this regime, minimisers of f are prolate uniaxial of the form

$$Q = s_+(n \otimes n - \frac{1}{3}I),$$
$$s_+ = \frac{b^2 + (b^2 + 24a^2c^2)^{1/2}}{4c^2}$$

Landau-de Gennes IV – Full energy

$$\boxed{\mathcal{E}[Q] = \int_\Omega \frac{1}{2}\,\mathsf{Tr}\,(\nabla Q)^2 + \frac{1}{L} f(Q),}$$

$\mathsf{Tr}\,(\nabla Q)^2 = \sum_{ijk} (\partial_i Q_{jk})^2$, one-constant elastic energy
L, elastic constant

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Relation to Oseen-Frank theory (Majumdar + Zarnescu).

For $\Omega \subset \mathbb{R}^3$, fix $n_*(r)$ smooth on $\partial\Omega$. Let n denote the minimiser of the one-constant Oseen-Frank energy with $n = n_*$ on $\partial\Omega$. Let $Q_* := s_+(n_* \otimes n_* - \frac{1}{3}I)$ on $\partial\Omega$. Let Q_L denote global minimizer of LdG energy with $Q = Q_*$ on $\partial\Omega$. If r_0 is not a singularity of n, then as $L \to 0$,

$$Q_L(r_0) \to s_+(n(r_0) \otimes n(r_0) - \frac{1}{3}I).$$

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Current research is directed at the fine structure of defects in the Landau-de Gennes model. Cf vortices in the Ginzburg-Landau model, where the order parameter is a complex scalar (in place of Q-tensor).

Universal features of defects play a role in mesoscopic descriptions.

Full problem

$D_R \subset \mathbb{R}^2$, 2-d disk about 0 of radius R

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We consider Q-tensors on D_R satisfying ”defect boundary conditions”

$$Q(R, \phi) = Q_k(\phi),$$

where

$$Q_k(\phi) = s_+ \left(n_k \otimes n_k - \frac{1}{3} I \right),$$

$$n_k = (\cos(\tfrac{k}{2}\phi), \sin(\tfrac{k}{2}\phi), 0).$$

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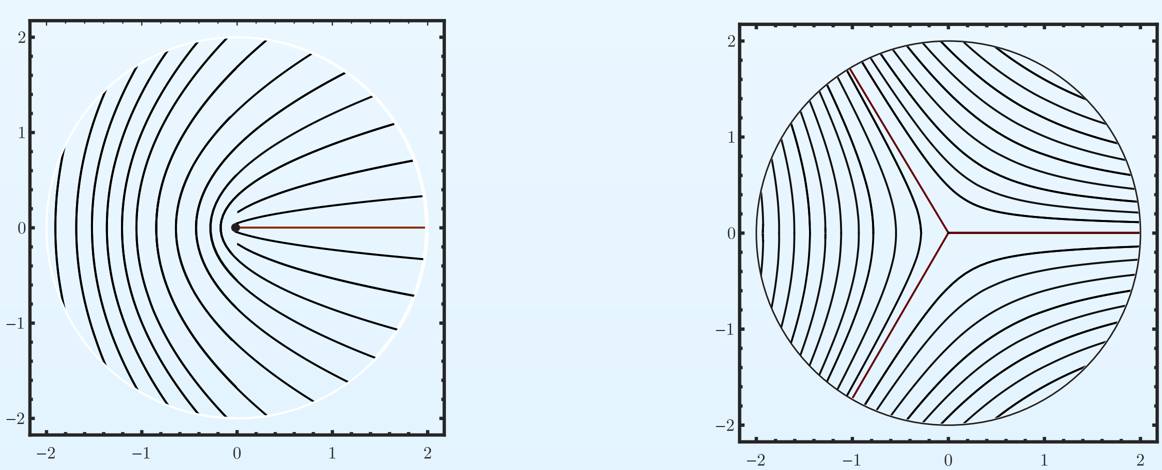

Defects of index $\frac{1}{2}$ (left) and $-\frac{1}{2}$ (right)

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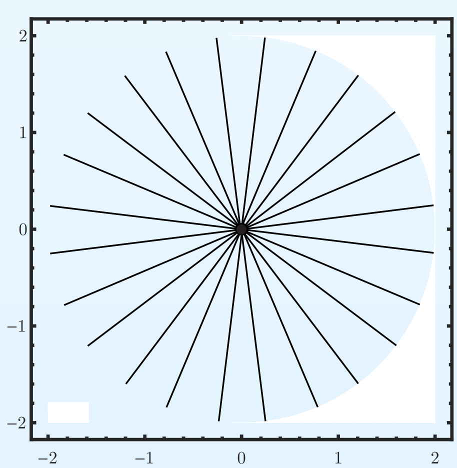

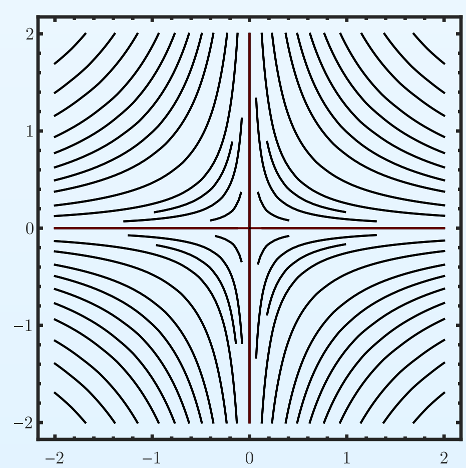

Defects of index 1 (left) and -1 (right)

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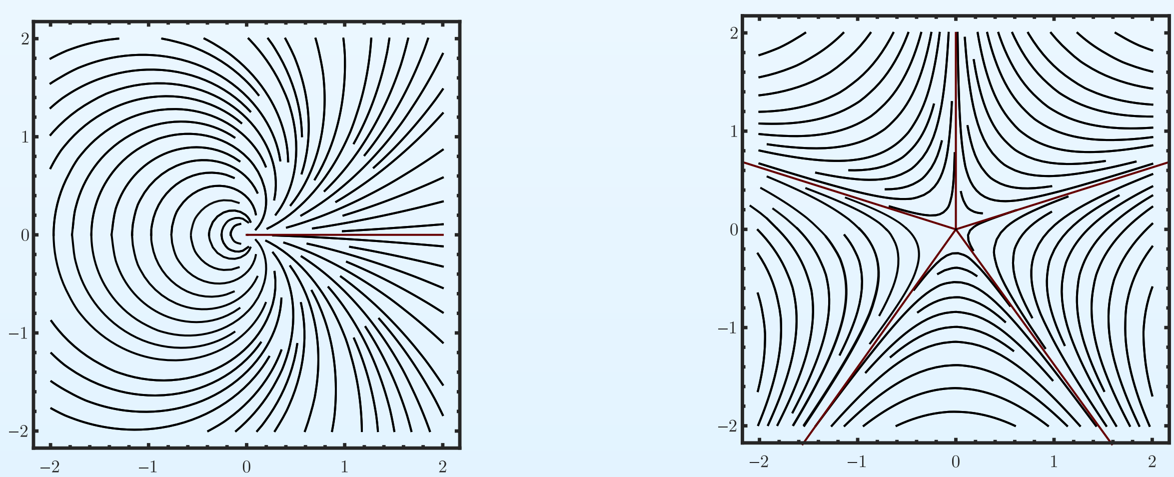

Defects of index $3/2$ (left) and $-3/2$ (right)

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$\mathcal{A} = \left\{Q \in H^1(D_R), \quad Q(R,\phi) = Q_k(\phi)\right\}$, admissible space

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Full problem (FP): Minimise $\mathcal{E}[Q]$ for $Q \in \mathcal{A}$.

Euler-Lagrange equation,

$$L \Delta Q = -a^2 Q - b^2 \operatorname{Tr} (Q^2 - \frac{1}{3} \operatorname{Tr} Q^2 \, I) + c^2 \operatorname{Tr} (Q^2) Q.$$

Candidates for solutions

- Uniaxial

  $$\tilde{Y}(r,\phi) = f(r)Q_k(\phi) = f(r)\left(n_k(\phi)\otimes n_k(\phi) - \frac{1}{3}\right),$$

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- Biaxial (with a principal axis along e_3)

  $$Y(r) = u(r)F_k(\phi) + v(r)F_3(\phi),$$

  where

  $$F_k(\phi) = \sqrt{2}\left(n_k(\phi)\otimes n_k(\phi) - \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right),$$

  $$F_3 = \sqrt{\frac{3}{2}}\left(e_3\otimes e_3 - \frac{1}{3}I\right).$$

  Then

  $$Q_k = s_+\left(\frac{1}{\sqrt{2}}F_k - \frac{1}{\sqrt{6}}F_3\right).$$

  Substituting Y into the Euler-Lagrange equations leads to 2 coupled ODE's for u and v ...

Restricted problem

Consider $Y(r) = u(r)F_k(\phi) + v(r)F_3(\phi)$.
Restricted energy,

$$\mathcal{E}_R[u,v] = \int_0^R \left[\tfrac{1}{2}(u'^2 + v'^2 + \frac{k^2}{r^2}u^2 + \frac{1}{L}g(u,v)\right] r\,dr,$$

where $g(u,v) = f(Y)$.

Admissible space,

$$\mathcal{A}_R = \Big\{(u,v) \mid \sqrt{r}u', \sqrt{r}v', \frac{u}{\sqrt{r}}, \sqrt{r}v \in L^2(0,R), \\ u(R) = \frac{s_+}{\sqrt{2}}, v(R) = -\frac{s_+}{\sqrt{6}}\Big\}.$$

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Restricted problem (RP): Minimise $\mathcal{E}_R[u,v]$ for $(u,v) \in \mathcal{A}_R$.

Euler-Lagrange equation,

$$\frac{1}{r}(ru')' - \frac{k^2 u}{r^2} = \frac{u}{L}\left[-a^2 + \sqrt{\frac{2}{3}} b^2 v + c^2\left(u^2 + v^2\right) \right],$$

$$\frac{1}{r}(ru')' = \frac{v}{L}\left[-a^2 - \frac{1}{\sqrt{6}} b^2 v + c^2\left(u^2 + v^2\right) \right] \\ + \frac{1}{\sqrt{6}L} b^2 u^2.$$

Result for Restricted Problem

Theorem 1. *There exists a global minimiser (u, v) of the restricted problem (RP), and u and v satisfy its Euler-Lagrange equations.*

$u \in C^\infty(0, R) \cap C^0[0, R]$, and $u(0) = 0$.

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In fact, the global minimiser (u, v) of the restricted problem satisfies the Euler-Lagrange equation for the full problem.

But it needn't be a global or even a local minimiser of the full problem (in fact, for $|k| > 1$, it isn't – Bauman, Park, Phillips (2012))...

Special case: $b^2 = 0$

Bulk potential,

$$f(Q) = -\frac{a^2}{2}\,\mathrm{Tr}\,(Q^2) - \frac{b^2}{3}\,\mathrm{Tr}\,(Q^3) + \frac{c^2}{4}(\,\mathrm{Tr}\,(Q^2))^2$$

For $b^2 = 0$,

$$f_0(Q) = \frac{c^2}{4}\left(\mathrm{Tr}\,Q^2 - \frac{a^2}{c^2}\right)^2 + \text{const.}$$

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Minimisers of the bulk energy:

For $b^2 = 0$, minimisers are characterised by

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For $b^2 \neq 0$, minimisers are characterised by

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and prolate uniaxiality,

$$-\lambda_1 = -\lambda_2 = \tfrac{1}{2}\lambda_3 > 0,$$

and may be identified with RP^2.

For $b^2 = 0$, biaxiality is no longer penalised. . .

Special problem

Special energy,

$$\mathcal{E}_{S0}[Q] = \int_{D_R} \tfrac{1}{2}\,\mathrm{Tr}\,(\nabla Q)^2 + \frac{1}{L} f_0(Q)$$

where

$$f_0(Q) = \frac{c^2}{4}\left(\mathrm{Tr}\,Q^2 - \frac{a^2}{c^2}\right)^2 .$$

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Special problem (SP): Minimise $\mathcal{E}_{S0}[Q]$ for $Q \in \mathcal{A}_S$.

Euler-Lagrange equation,

$$L\Delta Q = (c^2 Q^2 - a^2)Q.$$

The global minimiser of the restricted problem remains a candidate. . .

Lemma. *Let* $Y = uF_k + vF_3$ *be a global minimiser of the restricted energy with* $b^2 = 0$*. Then* $u \geq 0$ *and* $v < 0$ *on* $[0, R]$*.*

Lemma. *Let $Y = uF_k + vF_3$ be a global minimiser of the restricted energy with $b^2 = 0$. Then $u \geq 0$ and $v < 0$ on $[0, R]$.*

Proof: For $b^2 = 0$, the restricted energy density

$$\left[\tfrac{1}{2}(u'^2 + v'^2 + \frac{k^2}{r^2}u^2 + \frac{c^2}{4L}\left(u^2 + v^2 - \frac{a^2}{c^2}\right)^2 \right]$$

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Suppose $\tilde{u}(r_0) = 0$. Then $\tilde{u}'(r_0) = 0$. Then EL would imply that $\tilde{u} = 0$, contradicting the boundary condition $\tilde{u}(R) = u(R) > 0$. So $\tilde{u} \neq 0$ on $(0, R)$, so that $u \geq 0$ on $[0, R]$.

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A similar argument shows that $v < 0$ on $[0, R]$.

Result for special problem

Theorem 2. *Let $Y = uF_k + vF_3$ be a global minimiser of the restricted energy with $b^2 = 0$. Then Y is the unique global minimiser of the full problem (FP) with $b^2 = 0$.*

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$$\mathcal{E}_0(Q) - \mathcal{E}_0(Y) = I(Q - Y) + \int_{D_R} \frac{c^2}{4} (\operatorname{Tr} Q^2)^2, \text{ where}$$

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Hardy trick: Suppose $\Psi \in H^2(\Omega)$ is a nonvanishing null eigenfunction of $L = -\Delta + V$. Then for $f \in H_0^2(\Omega)$,

$$I(f) = \int_\Omega \Psi^2 \left(\nabla \frac{f}{\Psi}\right)^2 \geq C||f||_{L^2}.$$

In the present case, $Lv = 0$, from the Euler-Lagrange equation, and $v < 0$ from Lemma. Hence:

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But what do the solutions look like. . .

The small-L regime

$$\mathcal{E}_0[Q] = \int_{D_R} \tfrac{1}{2}\,\mathrm{Tr}\,(\nabla Q)^2 + \frac{c^2}{4L}\left(\mathrm{Tr}\,Q^2 - \frac{a^2}{c^2}\right)^2.$$

For $L \to 0$, the bulk potential term acts as a constraint,

$$\mathrm{Tr}\,Q^2 = \frac{a^2}{c^2}.$$

This motivates the following:

$$\mathcal{E}_{L0} = \int_{D_R} \tfrac{1}{2}\,\mathrm{Tr}\,(\nabla Q)^2$$

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Limit problem (LP0): Minimise $\mathcal{E}_{L0}[Q]$ for $Q \in \mathcal{A}_{S0}$.
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Solutions of EL are S^4-valued harmonic maps.

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Three explicit solutions to the limit problem are available. . .

Results for limit problem

- Two biaxial solutions

$$Y_\pm(r,\phi) = \frac{a^2}{c^2}\left(\cos\psi_\pm(r)F_k(\phi) - \sin\psi_\pm(r)F_3\right),$$
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Y_- is the unique global minimiser of $\mathcal{E}_{L0}$.

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- For k even, a uniaxial solution ('escape to the third dimension' – Cladis-Kléman).

$$U(r,\phi) = \sqrt{\frac{3}{2}}\frac{a^2}{c^2}\left(m\otimes m - \frac{1}{3}I\right),$$
$$m(x,y) = \frac{\left(2\mathrm{Re}\, f, 2\mathrm{Im}\, f, 1-|f|^2\right)}{1+|f|^2},$$
$$f(x,y) = \left(\frac{x+iy}{R}\right)^{k/2},$$

  m is a harmonic map from D_R to S^2. In general, if $m: D_R \to S^2$ is harmonic, then $U: D_R \to S^4$ is not harmonic. However, if m is conformal, then U is harmonic.

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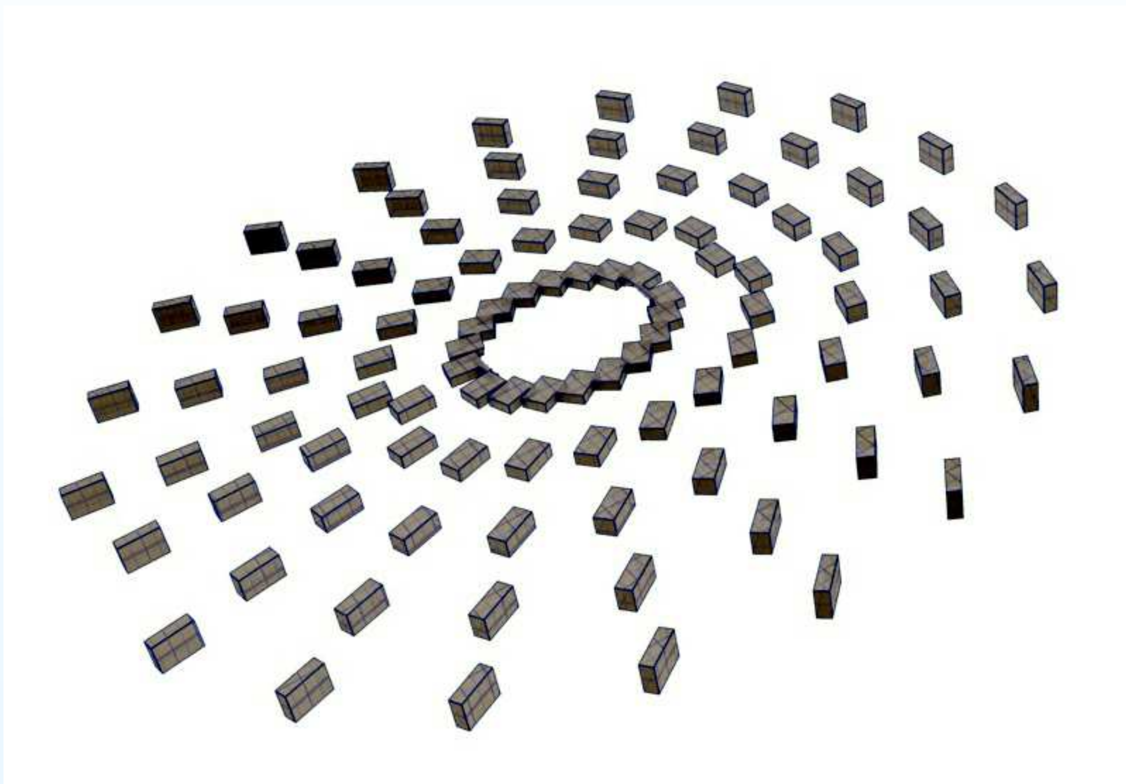
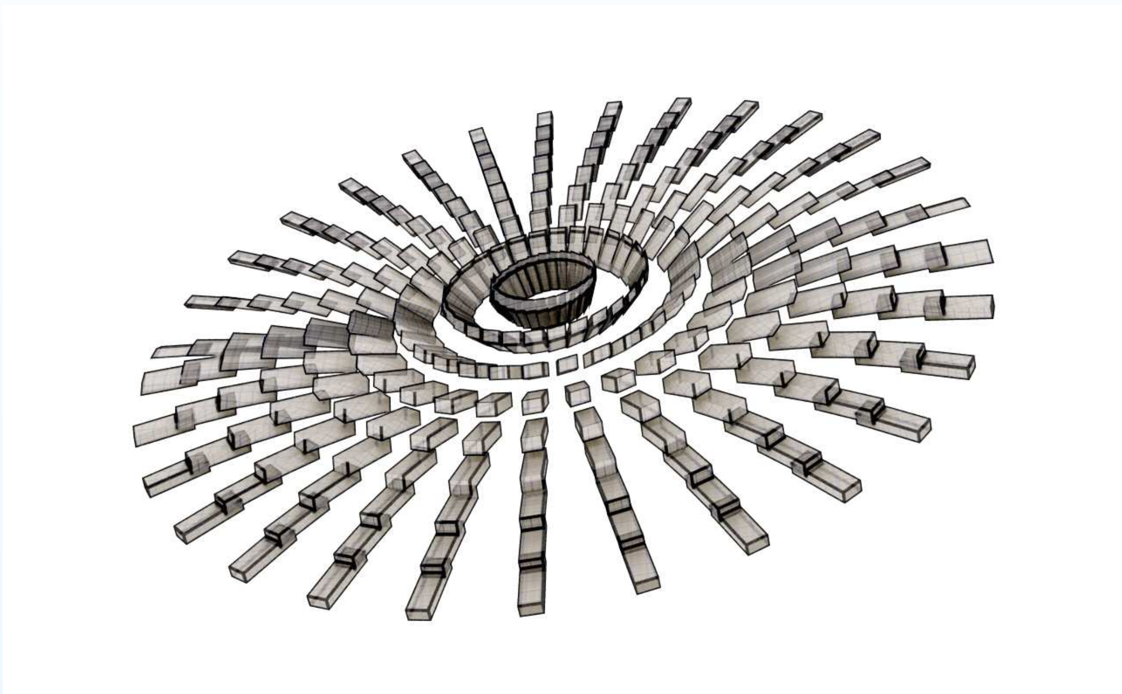
$$\mathcal{E}_{L0}(Y_-) = |k|\pi\frac{a^2}{c^2}, \quad \mathcal{E}_{L0}(Y_+) = \mathcal{E}_{L0}(U) = 3|k|\pi\frac{a^2}{c^2}.$$



$Y_-, k = 1$

$$Y_-, k = -1$$



$$U, k = 2$$

Special vs full problem

$$\mathcal{E}[Q] = \int_{D_R} \tfrac{1}{2}\,\mathrm{Tr}\,(\nabla Q)^2 + \frac{1}{L} f(Q).$$

For $b^2 \neq 0$, expect $U(r,\phi) \sim s_+ Q_k(\phi)$ outside a core of radius d, where

$$d \sim \frac{\sqrt{L}}{c} \sim 1 \text{ micron}, \quad \text{core radius.}$$

For $b^2 = 0$, the “core” is the whole domain.

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Crossover: “biaxial penalty” = “core energy”

$$b^2 \sim \frac{L}{R^2}.$$

For $b^2 \neq 0$ and R large, Y is unstable for $|k| \neq 1$ (Ignat, Nguyen, Slastikov, Zarnescu, in preparation). In line with expectation that n defects of index $\pm 1/2$ have less energy that one defect of strength n (energy $\sim$ (index)^2).

They have also established the stability of the Y profile for $|k| = 1$ (in preparation).