Recent advances in the variational aspects of the Landau-de Gennes theory of liquid crystals

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joint work with Radu Ignat, Luc Nguyen and Valeriy Slastikov

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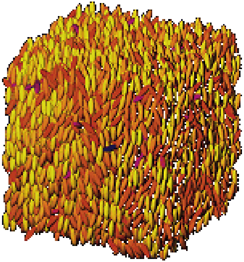
Liquid crystals modelling: physics

 [1]

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[1] Simulation by C. Zannoni group

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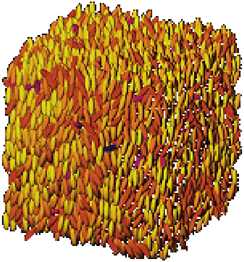 [1]

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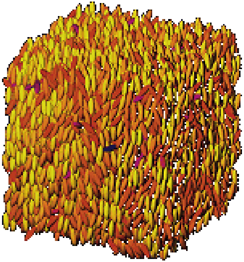
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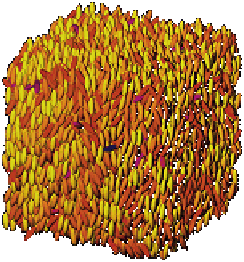

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Landau-de Gennes Q-tensor and other simpler theories

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- **Ericksen's theory (1991)** for uniaxial Q-tensors which can be written as

$$Q(x) = s(x)\left(n(x) \otimes n(x) - \frac{1}{3} Id\right), \quad s \in \mathbb{R}, n \in \mathbb{S}^2$$

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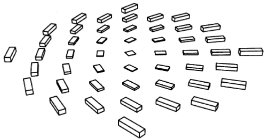
- **Oseen-Frank theory (1958)** take s in the uniaxial representation to be a fixed constant s_+

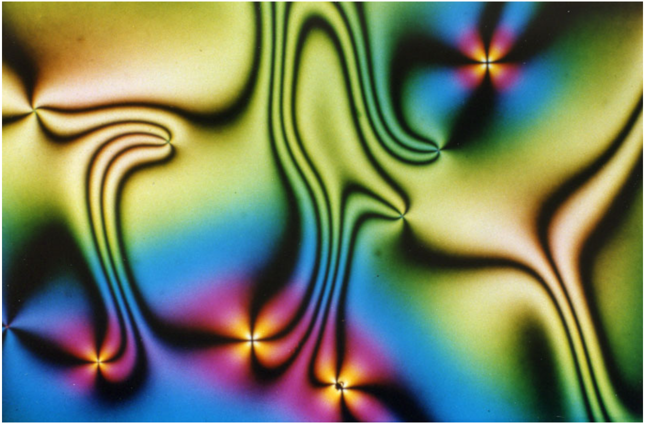
Q-tensors: visualisation

- One can visualise a Q-tensor as either a:
  - *parallelepiped* whose axis are parallel with the eigenvectors of Q and whose lengths are proportional to the eigenvalues of Q
    or an
  - *ellipsoid* whose axis are parallel with the eigenvectors of Q and whose radii are proportional to the eigenvalues of Q
- Some Q-tensor fields in the two representations:



Index 1/2 defect (parallelepipeds) Index 1/2 defect
(ellipsoids)

Defects



Stationary states and energy minimization

- Energy functional:

$$\mathcal{F}_{LG}[Q] = \int_\Omega \frac{L}{2} \sum_{i,j,k=1}^{3} \frac{\partial Q_{ij}}{\partial x_k}(x) \frac{\partial Q_{ij}}{\partial x_k}(x) + f_B(Q(x))\,dx$$

  with bulk term

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

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

- The set Q_{min} where f_B attains its minimums is:
  - For $b \neq 0$: A **2D** manifold $\{s_+\left(n(x)\otimes n(x) - \frac{1}{3}Id\right), n \in \mathbb{S}^2\}$ homemorphic to $\mathbb{R}P^2$
  - For $b = 0$: (and $a > 0$): A **4D** manifold $\{\sum_{i,j=1}^{3} Q_{ij}Q_{ij} = \frac{a}{c}\}$ homeomorphic to $\mathbb{S}^4$.

Scalings and the role of b

Euler-Lagrange system of equations:

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

- Scalings $Q_{\lambda,\mu} = \lambda Q(\frac{x}{\mu})$ give:

$$L\Delta Q_{\lambda,\mu} = -\frac{a}{\mu^2}Q_{\lambda,\mu} - \frac{b}{\mu^2\lambda}[Q^2 - \frac{1}{3}|Q|^2 Id] + \frac{c}{\mu^2\lambda^2}Q_{\lambda,\mu}|Q_{\lambda,\mu}|^2$$

just two independent variables, say L and b OR L and a.

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- One can consider a non-dimensionalisation suited for studying defect cores (Mkadddem and Gartland, Virga and Kralj) in which a has the significance of a reduced temperature.

Boundary conditions and Q-tensor versus director theory

- If we take boundary conditions $Q_b(x), x \in \partial\Omega$ taking values in the minimisation set of the bulk, Q_{min} potential then we can consider the minimisation problem:

$$\min_{\substack{Q \in W^{1,2}(\Omega; Q_{min}) \\ Q(x) = Q_b(x), x \in \partial\Omega}} \int_\Omega |\nabla Q|^2(x)\, dx$$

For $Q_{min} = \{s_+ \left(n(x) \otimes n(x) - \frac{1}{3} Id\right), n \in \mathbb{S}^2\}$ we have $|\nabla Q|^2 = 2s_+^2 |\nabla n|^2$ so this problem becomes

$$\min_{\substack{n \in W^{1,2}(\Omega; \mathbb{S}^2) \\ n(x) = n_b(x), x \in \partial\Omega}} 2s_+^2 \int_\Omega |\nabla n|^2(x)\, dx$$

is really just about the director theory (but written using matrices!) and we can compare the predictions of the director and the tensor theories.

Prototypical Point Defects in 2D

Half-integer defects in 2D domains: director representation (∞ energy!)

The index counts how many 2π-times the director rotates as one goes along a full-circle.

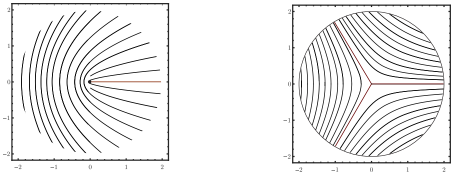
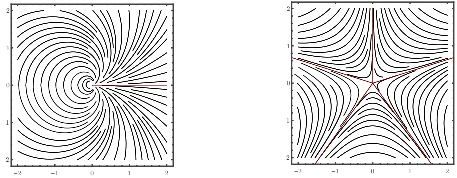


Figure: Defects of index $\frac{1}{2}$ (left) and $-\frac{1}{2}$ (right)



Half-integer defects in $2D$ domains: Q-tensor representation(finite energy!)

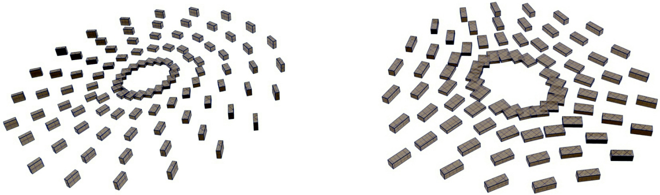


Figure: Q-tensor defect of index $\frac{1}{2}$ (left) and $-\frac{1}{2}$ (right)

Thus the index one-half defects in the Q-tensor theory permit to "mollify" the infinite energy core.

Half-integer defects in 2D domains: Q-tensor representation allows for multiple solutions

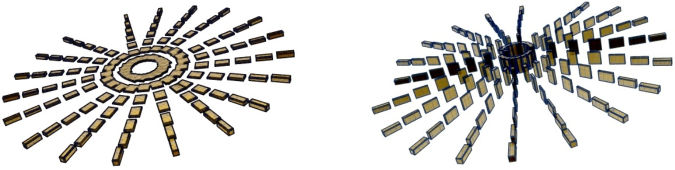


Figure: Y_- (left) and Y_+ (right) defects for of strength 1

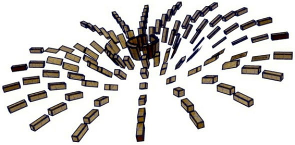


Figure: Uniaxial defect of strength 1

Ansatz and the reduction to an ODE system

- Ansatz :

$$Y = u(r)\,\sqrt{2}\left(n(\varphi)\otimes n(\varphi) - \frac{1}{2}I_2\right) + v(r)\,\sqrt{\frac{3}{2}}\left(e_3\otimes e_3 - \frac{1}{3}I\right),$$

where $n(\varphi) = (\cos(k\frac{\varphi}{2}), \sin(k\frac{\varphi}{2}), 0)$.

- Then the PDE system reduces to an ODE system, that is easier (though highly nontrivial!) to analyse qualitatively:

$$\begin{cases} u'' + \frac{u'}{r} - \frac{k^2 u}{r^2} &= \frac{u}{L}\left[-a^2 + \sqrt{\frac{2}{3}}b^2 v + c^2\left(u^2+v^2\right)\right], \\ v'' + \frac{v'}{r} &= \frac{v}{L}\left[-a^2 - \frac{1}{\sqrt{6}}b^2 v + c^2\left(u^2+v^2\right)\right] + \frac{1}{\sqrt{6}_L}b^2 u^2, \quad r\in(0,R). \end{cases}$$

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- The dependence on k, the index of the solution is very weak.
- The term b makes a significant difference: makes the system more coupled (for $b\neq 0$ as opposed to $b=0$) and changes the shape of the solutions.

The shape of solutions

The shape of the solutions depends strongly on the size of b with respect to the other coefficients:

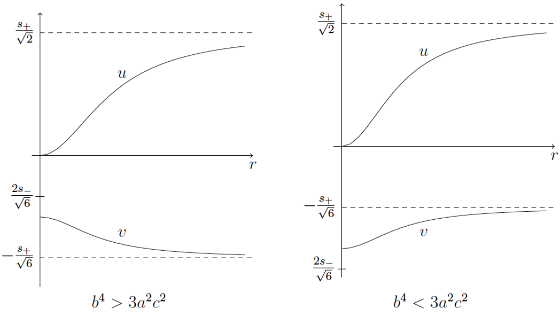


Figure 1: Schematic graphs of u and v in different regimes of a^2, b^2 and c^2.

- For the critical regime $b^2 = 3a^2c^2$ we have that v is a constant and the system reduces to a single ODE for u.
- For $b^2 > 0$ there exists a solution in the whole space but not for $b^2 = 0$!

The main question: stability

Given Y a symmetric solution as before, is the second variation non-negative? This is physically important and also its failure often signals a symmetry breaking....

$$\mathcal{L}[Y](P) = \frac{1}{2}\frac{d^2}{dt^2}|_{t=0}\int_{\mathbb{R}^2}\left\{\frac{1}{2}|\nabla(Y+tP)|^2 + f_{bulk}(Y+tP) - \frac{1}{2}|\nabla Y|^2 - f_{bulk}(Y)\right\}dx$$
$$= \int_{\mathbb{R}^2}\left\{\frac{1}{2}|\nabla P|^2 - \frac{a^2}{2}|P|^2 - b^2\mathrm{tr}(P^2Y) + \frac{c^2}{2}\left(|Y|^2|P|^2 + 2|\mathrm{tr}(YP)|^2\right)\right\}dx. \tag{1}$$

where $P \in C_c^\infty(B_R(0), \mathcal{S}_0)$.

Note that P has five degrees of freedom so one needs to find ways to carefully "peel them out"

The stability story, the easy case: $b^2 = 0$

Theorem (G. Di Fratta, J. Robbins, V. Slastikov, AZ, 2014)

Let $b^2 = 0$, and let Y be given by

$$Y = u(r)\,\sqrt{2}\left(n(\varphi)\otimes n(\varphi) - \frac{1}{2}I_2\right) + v(r)\,\sqrt{\frac{3}{2}}\left(e_3\otimes e_3 - \frac{1}{3}I\right),$$

with (u, v) the unique global minimiser of the reduced energy

$$\mathcal{E}(u,v) = \int_0^R \left[\frac{1}{2}\left((u')^2 + (v')^2 + \frac{k^2}{r^2}u^2\right) - \frac{a^2}{2L}(u^2+v^2) + \frac{c^2}{4L}\left(u^2+v^2\right)^2\right] rdr$$
$$- \frac{b^2}{3L\,\sqrt{6}}\int_0^R v(v^2 - 3u^2)\, rdr.$$

Then for any index k and for any $R \in (0,\infty)$ the symmetric solution Y is the unique global minimiser of the full Landau-de Gennes energy in $H^1(B_R;\mathcal{S}_0)$.

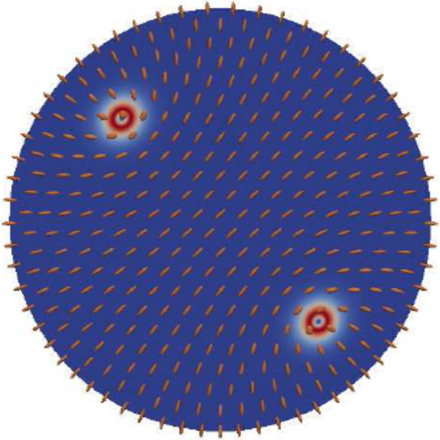
The stability story, the trickier case: $b^2 \neq 0$

Theorem (R. Ignat, L. Nguyen, V.Slastikov, AZ, 2015, 2016)

Let $a^2, b^2, c^2 > 0$ be any fixed constants and $k \in \mathbb{Z} \setminus \{0, \pm 1\}$. Any k-radially symmetric critical point Y in the whole space is locally unstable, i.e. there is a perturbation $P \in C_c^\infty(\mathbb{R}^2, \mathcal{S}_0)$, supported in a bounded disk B_R, such that the second variation $\mathcal{L}[Y](P) < 0$.

If $k = \pm 1$ then there exist a solution (u, v) of the ODE system such that k-radially symmetric Q-tensor Y is locally stable, i.e. the second variation $\mathcal{L}[Y](P) \geq 0$ for all $P \in H^1(\mathbb{R}^2, \mathcal{S}_0)$. Moreover, $\mathcal{L}[Y](P) = 0$ if and only if $P \in \{\partial_{x_i} Y\}_{i=1}^2$, i.e. the kernel of the second variation coincides with translations of Y.

Beyond stability: symmetry breaking



The global minimiser for hedgehog boundary conditions (in 2D), numerics:

Y. Hu, Y.Qu and P. Zhang *On the disinclination lines of nematic liquid crystals*

Two technical tools: I the suitable basis decomposition

Let $\{e_i\}_{i=1}^3$ be the standard basis in $\mathbb{R}^3$ and denote, for $\varphi \in [0, 2\pi)$,

$$n = n(\varphi) = \left(\cos(\tfrac{k}{2}\varphi), \sin(\tfrac{k}{2}\varphi), 0\right), \; m = m(\varphi) = \left(-\sin(\tfrac{k}{2}\varphi), \cos(\tfrac{k}{2}\varphi), 0\right).$$

We endow the space $\mathcal{S}_0$ of Q-tensors with the scalar product $Q \cdot \tilde{Q} = \mathrm{tr}(Q\tilde{Q})$ and for any $\varphi \in [0, 2\pi)$, we define the following orthonormal basis in $\mathcal{S}_0$:

$$E_0 = \sqrt{\frac{3}{2}}\left(e_3 \otimes e_3 - \frac{1}{3} I_3\right),$$

$$E_1 = E_1(\varphi) = \sqrt{2}\left(n \otimes n - \frac{1}{2} I_2\right), \; E_2 = E_2(\varphi) = \frac{1}{\sqrt{2}}\left(n \otimes m + m \otimes n\right),$$

$$E_3 = \frac{1}{\sqrt{2}}(e_1 \otimes e_3 + e_3 \otimes e_1), \; E_4 = \frac{1}{\sqrt{2}}\left(e_2 \otimes e_3 + e_3 \otimes e_2\right).$$

Let

$$P(x) = \sum_{i=0}^{4} w_i(x) E_i, \quad x \in \mathbb{R}^2,$$

Then the second variation decomposes into two independent parts:
$\mathcal{L}_1[Y](P) = \mathcal{L}_1[Y](w_0, w_1, w_2) + \mathcal{L}_2[Y](w_3, w_4)$

Two technical tools: Ibis the suitable basis decomposition

$$\mathcal{L}_1[Y](w_0, w_1, w_2) = \int_0^\infty \int_0^{2\pi} \left\{ \sum_{i=0}^{2} |\partial_r w_i|^2 + \frac{1}{r^2} \left(|\partial_\varphi w_0|^2 + |\partial_\varphi w_1 - k w_2|^2 + |\partial_\varphi w_2 + k w_1|^2 \right) \right.$$
$$+ \left(-a^2 + c^2(u^2 + v^2)\right) \sum_{i=0}^{2} |w_i|^2 + 2c^2 \left(v w_0 + u w_1\right)^2$$
$$\left. - \frac{2b^2}{\sqrt{6}} \left(v(w_0^2 - w_1^2 - w_2^2) - 2u w_0 w_1 \right) \right\} r dr\, d\varphi$$

$$\mathcal{L}[Y](w_3, w_4) = \int_0^\infty \int_0^{2\pi} \left\{ \sum_{i=3}^{4} \left[|\partial_r w_i|^2 + \frac{1}{r^2} |\partial_\varphi w_i|^2 + \left(-a^2 - \frac{b^2}{\sqrt{6}} v + c^2(u^2 + v^2) \right) |w_i|^2 \right] \right.$$
$$\left. - \frac{b^2 u}{\sqrt{2}} \left((w_3^2 - w_4^2) \cos(k\varphi) + 2u w_3 w_4 \sin(k\varphi) \right) \right\} r dr d\varphi.$$

The “inhomogeneity” in u and v are dealt with using the Hardy trick.

Two technical tools: II the Hardy trick

(Idea for the $b^2 = 0$ case)

$$\mathcal{F}(Y+P) - \mathcal{F}(Y) \quad = \quad \mathcal{I}[Y](P,P) + \tfrac{1}{L}\int_{B_R} \tfrac{c^2}{4}(|P|^2 + 2\,\mathrm{tr}(YP))^2,$$

where

$$\mathcal{I}[Y](P,P) = \frac{1}{2}\int_{B_R} |\nabla P|^2 + \frac{1}{2L}\int_{B_R} |P|^2\left(-a^2 + c^2|Y|^2\right) \qquad (2)$$

To investigate (2) we use a Hardy trick:

We have that $v < 0$ on $[0,R]$. Then, any $P \in H_0^1(B_R, \mathcal{S}_0)$ can be written $P(x) = v(r)U(x)$, where $U \in H_0^1(B_R, \mathcal{S}_0)$. Equation for v gives

$$v\Delta v = \frac{v^2}{L}\left(-a^2 + c^2|Y|^2\right)$$

and therefore

$$\mathcal{I}[Y](P,P) = \frac{1}{2}\sum_{i,j}\int_{B_R} |\nabla v(|x|)U_{ij}(x) + v(|x|)\nabla U_{ij}(x)|^2 + \Delta v(|x|)v(|x|)U_{ij}^2(x).$$

Integrating by parts in the second term above, we obtain

$$\sum_{i,j}\int_{B_R} \Delta v\, v\, U_{ij}^2 = -\sum_{i,j}\int_{B_R} |\nabla v|^2 U_{ij}^2 + 2\nabla v\cdot\nabla U_{ij}\, v\, U_{ij}.$$

It follows that

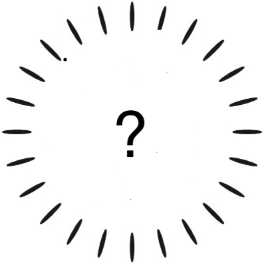
$$\mathcal{I}[Y](P,P) = \frac{1}{2}\int_{B_R} v^2\,|\nabla U|^2.$$

Using the fact that $0 < c_1 \leq v^2 \leq c_2$ and the Poincaré inequality we obtain

$$\mathcal{I}[Y](P,P) \geq C\int_{B_R} |P|^2.$$

II: Point Defects in 3D

Universal(?) boundary conditions near point singularities of the limiting (approximating) harmonic map and the possible solutions



S.Mkaddem, E.C. Gartland, Phys. Rev. E, 62, no. 5, (2000), p. 6694

The stability diagram

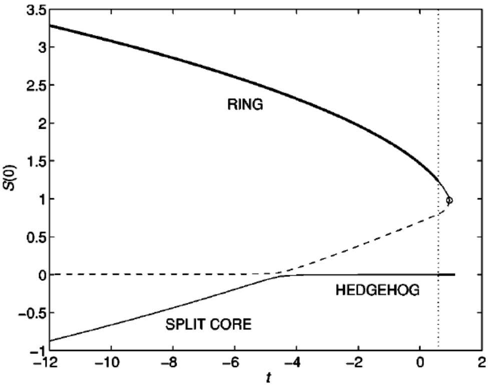


FIG. 7. Bifurcation diagram of discretized model for radial hedgehog, ring-disclination, and split-core solutions. Scalar order parameter at the origin $[S(0)]$ vs reduced temperature (t). Bold line indicates stable equilibrium (minimum free energy); solid line indicates metastable (locally stable); dashed line indicates not metastable (not locally stable). Parameters: $\eta=0$, $R=25$. Transition value: $t=0.583$. Ring limit/turning point: $t\simeq0.947$.

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A prototypical 3D profile: the melting hedgehog

A map $Q \in H^1(\mathbb{R}^3, \mathcal{S}_0)$ is radially-symmetric if

$$Q(\mathcal{R}x) = \mathcal{R}\, Q(x)\, \mathcal{R}^t \text{ for any } \mathcal{R} \in SO(3) \text{ and a.e. } x \in \mathbb{R}^3. \tag{3}$$

In fact, such a map $Q(x)$ has only one degree of freedom , namely, there exists a continuous radial scalar profile $s : (0, +\infty) \to \mathbb{R}$ such that $Q(x) = u(|x|)\,\overline{\mathrm{H}}(x)$ for a.e. $x \in \mathbb{R}^3$, where $\overline{\mathrm{H}}$ is called *hedgehog*

$$\overline{\mathrm{H}}(x) = \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} Id.$$

If Q is a critical point of the EL equations then u is a solution of the ODE:

$$u''(r) + \frac{2}{r}\, u'(r) - \frac{6}{r^2}\, u(r) = -a^2\, u(r) - \frac{b^2}{3}\, u(r)^2 + \frac{2c^2}{3}\, u(r)^3, \tag{4}$$

$$u(0) = 0, \quad \lim_{r \to \infty} u(r) = s_+. \tag{5}$$

Here, $s_+ := \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}$.

The local stability problem for the melting hedgehog

The second variation of the energy $\mathcal{F}$ at the point H in the direction $V \in H^1(\mathbb{R}^3; \mathcal{S}_0)$ is defined as [2]

$$Q(V) = \frac{1}{2}\frac{d^2}{dt^2}\Big|_{t=0}\int_{\mathbb{R}^3}\left[\frac{1}{2}|\nabla(H+tV)|^2 + f_{bulk}(H+tV) - \frac{1}{2}|\nabla H|^2 - f_{bulk}(H)\right]dx$$
$$= \int_{\mathbb{R}^3}\left[\frac{1}{2}|\nabla V|^2 + g(x,V)\right]dx \tag{6}$$

where

$$g(x,V) := \Big(-\frac{a^2}{2} + \frac{c^2u^2}{3}\Big)|V|^2 - b^2\, u\, \mathrm{tr}(\bar{H}V^2) + c^2 u^2\, \mathrm{tr}^2(\bar{H}V). \tag{7}$$

Theorem (R.Ignat, L. Nguyen, V. Slastikov, AZ)

Let b^2 and c^2 be fixed positive constants. Then there exists $a_0^2 > 0$ (depending on b^2 and c^2) such that for all $a^2 < a_0^2$ the radially symmetric solution H is locally stable in $H^1(\mathbb{R}^3; \mathcal{S}_0)$, meaning that $Q(V) \geq 0$ for all $V \in H^1(\mathbb{R}^3; \mathcal{S}_0)$. Moreover $Q(V) = 0$ if and only if $V \in \{\partial_{x_i}H\}_{i=1}^3$, i.e. the kernel of the second variation coincides with translations of $H(x)$.
Also, there exists $a_1^2 > 0$ (depending on b^2 and c^2) so that for any $a^2 > a_1^2$ there exists $V_* \in C_c^\infty(\mathbb{R}^3; \mathcal{S}_0)$ such that $Q(V_*) < 0$. Moreover, any such V_* cannot be purely uniaxial (i.e., $V_*(x)$ has three different eigenvalues for some point $x \in \mathbb{R}^3$).

[2] Equivalently, for every $V \in C_c^\infty(\mathbb{R}^3; \mathcal{S}_0)$, one defines $Q(V) = \frac{d^2}{dt^2}\Big|_{t=0}\mathcal{F}[H + tV; \Omega]$ where the domain Ω is any bounded open set containing the support of V.

Some ideas: a special basis, adapted to the hedgehog

$$\begin{aligned} n &= (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) = \tfrac{x}{|x|}, \\ m &= (\cos\theta\cos\varphi, \cos\theta\sin\varphi, -\sin\theta), \\ p &= (\sin\varphi, -\cos\varphi, 0). \end{aligned}$$

Using this basis, we can also define an orthogonal frame in $\mathcal{S}_0$ as

$$E_0 = \bar{H} = n\otimes n - \frac{1}{3}\mathrm{Id},\ E_1 = n\otimes p + p\otimes n,\ E_2 = n\otimes m + m\otimes n,$$
$$E_3 = m\otimes p + p\otimes m,\ E_4 = m\otimes m - p\otimes p.$$

Then:

$$V(x) = \sum_{i=0}^{4} w_i(r,\theta,\varphi)E_i(\theta,\varphi), \quad x \neq 0,$$

hence

$$g(x, V(x)) = \frac{1}{3}w_0^2\hat{f}(u(r)) + (w_1^2 + w_2^2)f(u(r)) + (w_3^2 + w_4^2)\tilde{f}(u(r)), \quad x \neq 0,$$

where

$$f(u(r)) = \frac{F(u(r))}{u(r)} = -a^2 - \frac{b^2u(r)}{3} + \frac{2c^2u(r)^2}{3},$$
$$\hat{f}(u(r)) = F'(u(r)) = -a^2 - \frac{2b^2u(r)}{3} + 2c^2u(r)^2,$$
$$\tilde{f}(u(r)) = -a^2 + \frac{2b^2u(r)}{3} + \frac{2c^2u(r)^2}{3}.$$

The second variation now:

$$
\begin{aligned}
Q(V) = \int_0^\infty \int_0^{2\pi} \int_0^\pi \Big\{ & \frac{1}{3}|\partial_r w_0|^2 + |\partial_r w_1|^2 + |\partial_r w_2|^2 + |\partial_r w_3|^2 + |\partial_r w_4|^2 \\
& + \frac{1}{r^2}\Big[\frac{1}{3}(\partial_\theta w_0 - 3w_2)^2 + (\partial_\theta w_1 - w_3)^2 + (\partial_\theta w_2 + w_0 - w_4)^2 \\
& \quad + (\partial_\theta w_3 + w_1)^2 + (\partial_\theta w_4 + w_2)^2\Big] \\
& + \frac{1}{r^2 \sin^2\theta}\Big[\frac{1}{3}(\partial_\varphi w_0 + 3\sin\theta\, w_1)^2 + (\partial_\varphi w_1 - \sin\theta\, w_0 - \cos\theta\, w_2 - \sin\theta\, w_4)^2 \\
& \quad + (\partial_\varphi w_2 + \cos\theta\, w_1 + \sin\theta\, w_3)^2 + (\partial_\varphi w_3 - \sin\theta\, w_2 - 2\cos\theta\, w_4)^2 \\
& \quad + (\partial_\varphi w_4 + \sin\theta\, w_1 + 2\cos\theta\, w_3)^2\Big] \\
& + \frac{1}{3}\hat{f}(u)\, w_0^2 + f(u)\left(w_1^2 + w_2^2\right) + \tilde{f}(u)\left(w_3^2 + w_4^2\right)\Big\}\, r^2 \sin\theta\, d\theta\, d\varphi\, dr.
\end{aligned}
$$

Peeling off the variables: the easy one-Fourier decomposition

We start by the representation of V as $V = \sum_{i=0}^{4} w_i(r,\theta,\varphi)E_i$. Let us expand w_i using Fourier series in the φ-variable

$$w_i(r,\theta,\varphi) = \sum_{k=0}^{\infty}(\mu_k^{(i)}(r,\theta)\cos k\varphi + \nu_k^{(i)}(r,\theta)\sin k\varphi).$$

Then $V(r,\theta,\varphi) = \sum_{k=0}^{\infty} V_k(r,\theta,\varphi) = \sum_{k=0}^{\infty}(M_k(r,\theta,\varphi)\cos k\varphi + N_k(r,\theta,\varphi)\sin k\varphi)$, hence

$$\mathcal{Q}(V) = \sum_{k=0}^{\infty}\mathcal{Q}(V_k).$$

After some more work:

We eliminate the φ component, play a bit with some symmetries of the system and are left to deal with:

$$\begin{aligned}\Phi_k(\upsilon_0,\upsilon_2,\upsilon_4) = \int_0^\infty \int_0^\pi \Big\{ & \frac{|\partial_r \upsilon_0|^2}{3} + |\partial_r \upsilon_2|^2 + |\partial_r \upsilon_4|^2 + \frac{1}{r^2}\Big[\frac{|\partial_\theta \upsilon_0|^2}{3} + |\partial_\theta \upsilon_2|^2 + |\partial_\theta \upsilon_4|^2\Big] \\ & + \frac{1}{r^2}\Big[(2 + \frac{1}{3}k^2 \csc^2\theta)|\upsilon_0|^2 + (5 + (\cot\theta + k\ \csc\theta)^2)|\upsilon_2|^2 \\ & \quad + (2 + (2\cot\theta + k\ \csc\theta)^2)|\upsilon_4|^2\Big] \\ & + \frac{4}{r^2}\Big[-\upsilon_0\left(\partial_\theta \upsilon_2 + \cot\theta \upsilon_2 + k\ \csc\theta\, \upsilon_2\right) \\ & \quad + (-\partial_\theta \upsilon_2 + \cot\theta\, \upsilon_2 + k\ \csc\theta\, \upsilon_2)\, \upsilon_4\Big] \\ & + \frac{1}{3}\hat{f}(u)\,|\upsilon_0|^2 + f(u)|\upsilon_2|^2 + \tilde{f}(u)|\upsilon_4|^2\Big\}\, r^2 \sin\theta\, d\theta\, dr.\end{aligned}$$

Separating r and θ variables: heuristics

We analyze of the sign of $\Phi_k(\upsilon_0, \upsilon_2, \upsilon_4)$ ($k = 0, 1, 2$) where the functions $\upsilon_0, \upsilon_2, \upsilon_4$ are φ-independent. The idea is to separate variables in $\upsilon_m(r, \theta)$, $m = 0, 2, 4$. The natural thing to do is for each $k = 0, 1, 2$ represent υ_m, $m = 0, 2, 4$ as a series

$$\upsilon_m(r, \theta) = \sum_i w_{k,i}^{(m)}(r) u_{k,i}^{(m)}(\theta)$$

and then **hope** that there will be the following separation in Φ_k

$$\Phi_k(\upsilon_0, \upsilon_2, \upsilon_4) = \pi \sum_i \Phi_{k,i}(w_{k,i}^{(0)}, w_{k,i}^{(2)}, w_{k,i}^{(4)}), \quad k = 0, 1, 2$$

It's not clear why it will work since there is a mixing between υ_0, υ_2, and υ_4.

Separating r and θ variables-the basis I

Therefore we need a special basis in $L^2((0,\pi), \sin\theta\, d\theta)$ in order to have this separation. We will construct this basis. Let's formally consider eigenvalue problems for υ_m, take an anzatz $\upsilon_m = \frac{1}{r^{\alpha_m}} u_m(\theta)$ and look at the behavior near ∞:

$$-\frac{1}{3r^2}\partial_r(r^2\,\partial_r\upsilon_0) - \frac{1}{3r^2\sin\theta}\partial_\theta(\sin\theta\partial_\theta\upsilon_0) + \frac{1}{r^2}(2+\frac{1}{3}k^2\csc^2\theta)\upsilon_0$$
$$-\frac{2}{r^2}(\partial_\theta\upsilon_2 + \cot\theta\upsilon_2 + k\csc\theta\upsilon_2) + \frac{1}{3}\hat{f}(u)\,\upsilon_0 = \lambda\upsilon_0.$$

When $r \to \infty$ we should have $\alpha_0 = \alpha_2 + 2$ and

$$u_0 \sim \partial_\theta u_2 + \cot\theta u_2 + k\ \csc\theta\, u_2.$$

Separating r and θ variables-the basis II

$$
\begin{aligned}
&-\frac{1}{r^2}\partial_r(r^2\,\partial_r\upsilon_2)-\frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\partial_\theta\upsilon_2)+\frac{1}{r^2}[5+(\cot\theta+k\csc\theta)^2]\upsilon_2\\
&\quad+\frac{2}{r^2\sin\theta}[\partial_\theta(\sin\theta\upsilon_0)+\partial_\theta(\sin\theta\upsilon_4)+(\cos\theta+k)(-\upsilon_0+\upsilon_4)]\\
&\quad+f(u)\,\upsilon_2=\frac{\lambda}{r^2}\,\upsilon_2.
\end{aligned}
$$

When $r\to\infty$ we should have

$$
u_2\sim-\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta u_2)+(\cot\theta+k\csc\theta)^2u_2.
$$

$$
\begin{aligned}
&-\frac{1}{r^2}\partial_r(r^2\,\partial_r\upsilon_4)-\frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\partial_\theta\upsilon_4)\\
&\quad+\frac{1}{r^2}[2+(2\cot\theta+k\csc\theta)^2]\upsilon_4+\frac{2}{r^2}(-\partial_\theta\upsilon_2+\cot\theta\upsilon_2+k\csc\theta\upsilon_2)\\
&\quad+\tilde f(u)\,\upsilon_4=\lambda\upsilon_4.
\end{aligned}
$$

When $r\to\infty$ we should have $\alpha_4=\alpha_2+2$ and

$$
u_4\sim-\partial_\theta u_2+\cot\theta u_2+k\ \csc\theta\,u_2.
$$

Separating r and θ-the basis III

These heuristic calculations give us

$$u_0 \sim \partial_\theta u_2 + \cot\theta u_2 + k\ \csc\theta\, u_2.$$

$$u_2 \sim -\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta u_2) + (\cot\theta + k\csc\theta)^2 u_2.$$

$$u_4 \sim -\partial_\theta u_2 + \cot\theta u_2 + k\ \csc\theta\, u_2.$$

Notice that with these relations mixed terms in spectral problems are absorbed by the right hand side. Therefore, for each $k = 0, 1, 2$, we focus on the spectral problem associated to the operator

$$T_k^{(2)} \equiv -\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta) + [1 + (\cot\theta + k\csc\theta)^2], \tag{8}$$

more precisely, on the couples (eigenfunction, eigenvalue)$= (u_{k,i}^{(2)}, \lambda_{k,i})$

$$T_k^{(2)} u_{k,i}^{(2)} = \lambda_{k,i} u_{k,i}^{(2)}, \quad i \geq 1.$$

For each $k = 0, 1, 2$, these eigenfunctions $\{u_{k,i}^{(2)}\}_{i\geq 1}$ will form a basis in $L^2((0,\pi); \sin\theta\, d\theta)$ and therefore we have the following expansion for υ_2

$$\upsilon_2(r,\theta) = \sum_i w_{k,i}^{(2)}(r) u_{k,i}^{(2)}(\theta).$$

Separating r and θ variables -the basis IV

The key observation is the following: for every $k = 0, 1, 2$, if $(u^{(2)}_{k,i}, \lambda_{k,i})$ is an eigenpair of the operator $T^{(2)}_k$, following the above ansatz, we set

$$u^{(0)}_{k,i} := \partial_\theta u^{(2)}_{k,i} + \cot\theta u^{(2)}_{k,i} + k\ \csc\theta\, u^{(2)}_{k,i}, \tag{9}$$

$$u^{(4)}_{k,i} = -\partial_\theta u^{(2)}_{k,i} + \cot\theta u^{(2)}_{k,i} + k\ \csc\theta\, u^{(2)}_{k,i}. \tag{10}$$

Then $u^{(0)}_{k,i}$ and $u^{(4)}_{k,i}$ are eigenfunctions of the following operators

$$T^{(0)}_k \equiv -\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta) + k^2\csc^2\theta, \tag{11}$$

$$T^{(4)}_k \equiv -\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta) + [4 + (2\cot\theta + k\csc\theta)^2], \tag{12}$$

and satisfy

$$T^{(0)}_k u^{(0)}_{k,i} = \lambda_{k,i} u^{(0)}_{k,i}, \quad T^{(4)}_k u^{(4)}_{k,i} = \lambda_{k,i} u^{(4)}_{k,i}. \tag{13}$$

The functions $\{u^{(0)}_{k,i}\}$ and $\{u^{(4)}_{k,i}\}$ also form bases of $L^2((0,\pi); \sin\theta\, d\theta)$ and therefore one can separate variables. In particular, we can represent υ_m as

$$\upsilon_m(r,\theta) = \sum_i w^{(m)}_{k,i}(r)\, u^{(m)}_{k,i}(\theta), \quad m = 0, 4$$

and we observe that we will reduce Φ_k to the sum of functionals depending only on r-variable:

$$\Phi_k(\upsilon_0, \upsilon_2, \upsilon_4) = \pi \sum_i \Phi_{k,i}(w^{(0)}_{k,i}, w^{(2)}_{k,i}, w^{(4)}_{k,i}), \quad k = 0, 1, 2.$$

An important simplification to notice is that only $\Phi_{0,i}$ enter into Φ_k and therefore it is enough to study the sign of one functional.

After some seriously hard work...

Eventually left with studying:

$$\Phi_{0,2}(w_0, w_2, w_4) = \int_0^\infty \Big\{ 2|\partial_r w_0|^2 + |\partial_r w_2|^2 + 4|\partial_r w_4|^2 + \frac{1}{r^2}\Big[24|w_0|^2 + 10|w_2|^2 + 16|w_4|^2 - 24 w_0 w_2 + 16 w_2 w_4 \Big] + 2\hat{f}(u)|w_0|^2 + f(u)|w_2|^2 + 4\tilde{f}(u)|w_4|^2 \Big\} r^2 \, dr.$$

Dealt with using a few Hardy tricks and very, very (very!) detailed study of the ODE for u.

THANK YOU!