Stability of the melting hedgehog in a Landau-de Gennes model

Radu IGNAT
Université Paul-Sabatier - Toulouse III
Institut de Mathématiques de Toulouse

joint work with
Luc Nguyen (University of Oxford),
Valeriy Slastikov (University of Bristol),
Arghir Zarnescu (University of Sussex)

Landau-de Gennes Model

We consider the following (non-dimensional) Landau-de Gennes energy functional

$$\mathscr{F}[Q;\Omega] := \int_\Omega \left(\frac{1}{2}|\nabla Q|^2 + f_{bulk}(Q) \right) dx, \quad Q \in H^1(\Omega, \mathscr{S}_0), \ \Omega \subset \mathbb{R}^3,$$

where $\mathscr{S}_0 := \{Q \in \mathbb{R}^{3\times 3}, Q = Q^t, \operatorname{tr}(Q) = 0\}$. The bulk energy density f_{bulk} accounts for the bulk effects and has the following form :

$$f_{bulk}(Q) := -\frac{a^2}{2}|Q|^2 - \frac{b^2}{3}\operatorname{tr}(Q^3) + \frac{c^2}{4}|Q|^4,$$

where a^2, b^2 and c^2 are positive constants and $|Q|^2 := \operatorname{tr}(Q^2)$.

Melting Hedgehog Solution

Let $\Omega = B_R(0)$ be a ball with $R \in (0, \infty]$. The melting hedgehog is defined as:

$$H(x) = \underbrace{u(|x|)\bar{H}(x)}_{melting\ hedgehog} \quad \text{with} \quad \bar{H}(x) = \underbrace{\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}Id}_{\text{"}singular\text{" } hedgehog}$$

where $u : [0, R) \to \mathbb{R}$ is a solution of the following ODE in $r = |x|$:

$$u''(r) + \frac{2}{r}u'(r) - \frac{6}{r^2}u(r) = F(u(r)),\ u(0) = 0,\ u(R) = s_+\ ,$$

$$\text{with} \quad F(u(r)) = -a^2 u(r) - \frac{b^2}{3}u(r)^2 + \frac{2c^2}{3}u(r)^3, \quad s_+ := \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}.$$

One checks that $H(x)$ satisfies the Euler-Lagrange equations for $\mathscr{F}[Q; B_R(0)]$, i.e.,

$$\Delta Q = -a^2 Q - b^2[Q^2 - \frac{1}{3}|Q|^2 Id] + c^2 |Q|^2 Q \quad \text{in} \quad B_R(0), \tag{1}$$

with the following boundary conditions

$$Q(x) = s_+ \bar{H}(x) \text{ for } x \in \partial B_R(0) \,.$$

Therefore, $H(x)$ is a critical point of the energy $\mathscr{F}[Q; B_R(0)]$.

Remark 1: If $R = \infty$, i.e., $\Omega = \mathbb{R}^3$, then $\mathscr{F}[H; \mathbb{R}^3] = \infty$! However,

$$\frac{d}{dt}\bigg|_{t=0} \mathscr{F}[H + tV; \mathbb{R}^3] = 0 \quad \text{for every} \quad V \in C_c^\infty(\mathbb{R}^3, \mathscr{S}_0).$$

Remark 2: After rescaling $Q_{\lambda,\mu}(x) := \lambda Q(\frac{x}{\mu})$, we can assume that (1) depends only on one parameter. We choose this parameter to be a^2.

Formulation of the problem

Main question: Is melting hedgehog a stable critical point of $\mathscr{F}[\cdot;\Omega]$?

Let $\Omega = \mathbb{R}^3$ and vary a^2 (as b^2 and c^2 are fixed). We investigate the sign of the second variation $\mathscr{Q}(V)$ of energy $\mathscr{F}$ at the melting hedgehog H in the direction V:

$$\mathscr{Q}(V) = \frac{d^2}{dt^2}\Big|_{t=0} \mathscr{F}[H + t\,V; \mathbb{R}^3]$$
$$= \int_{\mathbb{R}^3} \Big[\frac{1}{2}|\nabla V|^2 + \underbrace{\big(-\frac{a^2}{2} + \frac{c^2u^2}{3}\big)|V|^2 - b^2\, u\, \mathrm{tr}(\bar{H}\, V^2) + c^2\, u^2\, \mathrm{tr}^2(\bar{H}\, V)}_{\text{quadratic form in } V}\Big]\, dx,$$

where $V \in C_c^\infty(\mathbb{R}^3; \mathscr{S}_0)$.

Recall that $H(x) = u(|x|)\bar{H}(x)$ with $\bar{H}$ =singular hedgehog.

Previous analysis

- Rosso, Virga (1996): local stability in a restricted class of perturbations;
- If $\Omega = B_R(0)$ with R and a^2 sufficiently large, then $H(x)$ is unstable see Gartland, Mkaddem (1999); Henao, Majumdar (2012)

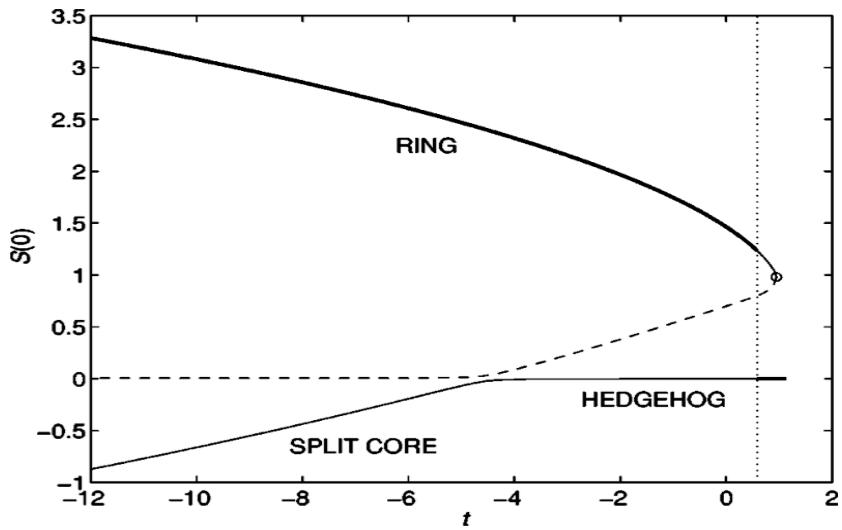


Figure 1: *Stability diagram (bold line - globally stable, solid line - locally stable, dashed line - unstable) (Gartland, Mkaddem (1999)).*

Relation to Ginzburg-Landau model

The deep nematic regime: $a^2 = \infty$ ($\Leftrightarrow b^2 = 0$). The potential energy becomes

$$f_{bulk}(Q) = \frac{1}{4}(|Q|^2 - 1)^2.$$

Minimizers of $f_{bulk}(Q)$ satisfy $|Q|^2 = 1$ ($4D$ manifold in $5D$ space).

- potential is similar to Ginzburg-Landau but problem has more degrees of freedom;
- second variation in biaxial direction is negative $\Rightarrow$ instability.

existence, uniqueness, basic properties of profile: Gartland, Mkaddem (1999); Majumdar (2010); Lamy (2013)

stability and instability in Ginzburg-Landau : Mironescu (1995), Gustafson (1997)

Our prototypical regime: $\Omega = \mathbb{R}^3$ and $a^2 = 0$; here, the bulk potential writes as

$$f_{bulk}(Q) = -\frac{b^2}{3}\mathrm{tr}(Q^3) + \frac{c^2}{4}|Q|^4.$$

Minimizers of $f_{bulk}(Q)$ satisfy $Q = s_+ \left(n \otimes n - \frac{1}{3}Id\right)$ with $s_+ = \frac{b^2}{2c^2}$ and $n \in \mathbb{S}^2$ ($2D$ manifold in $5D$ space).

- numerics suggest stability $\Rightarrow$ no "shooting" for negative direction;
- analysis "a la" Mironescu (1995) is not easily transferrable:
  - target space is $5D$, not $2D$;
  - base space Ω is $\mathbb{R}^3$, not $\mathbb{R}^2$, hence no simple decomposition.

Main results

- **Stability** of the melting hedgehog $H(x) = u(r)\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}Id\right)$ for **small** a^2.

- Existence, uniqueness or non-uniqueness and properties of solution for the following general ODE (no imposed sign on u):

$$u''(r) + \frac{p}{r}u'(r) - \frac{q}{r^2}u(r) = F(u(r)),\ u(0) = 0,\ u(R) = s_+\ (R \leq \infty). \quad (2)$$

$$p,\ q \in \mathbb{R},\ \text{and}\ q > 0$$

Recall that for our model, $p = 2$ and $q = 6$.

ODE results

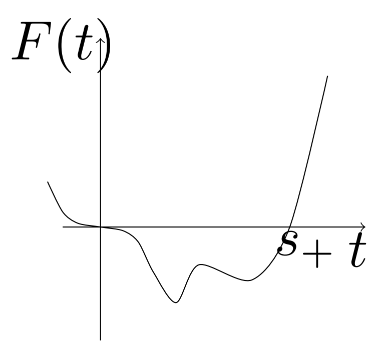
Theorem. Assume that $p, q \in \mathbb{R}$, $q > 0$ and $F : \mathbb{R} \to \mathbb{R}$ is a C^1 function satisfying

$$\begin{cases} F(0) = F(s_+) = 0, \ F'(s_+) > 0, \\ F(t) < 0 \ \text{ if } \ t \in (0, s_+), \quad F(t) \geq 0 \ \text{ if } \ t \in (s_+, +\infty). \end{cases} \tag{3}$$

Then there exists a non-negative solution u of

$$u''(r) + \frac{p}{r} u'(r) - \frac{q}{r^2} u(r) = F(u(r)), \ u(0) = 0, \ u(R) = s_+ \ (R \leq \infty)$$

which is unique in the class of non-negative solutions. Moreover, this solution is strictly increasing.

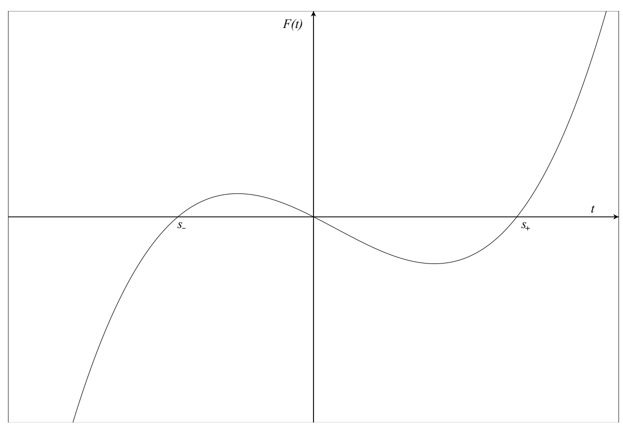


Theorem. Assume that $p \geq 0, q > 0$ and $F : \mathbb{R} \to \mathbb{R}$ is a C^1 function satisfying (3). Assume in addition that there exists $s_- \in [-s_+, 0)$ such that:

$$\begin{cases} F(t) \leq 0 \text{ if } t \in (-\infty, s_-), F(t) \geq 0 \text{ if } t \in (s_-, 0), \\ \dfrac{F(t_1)}{t_1} \leq \dfrac{F(-t_2)}{-t_2} \text{ if } 0 < t_1 \leq t_2 \leq |s_-|. \end{cases} \tag{4}$$

Then there exists a unique nodal solution u of the boundary value problem (2) .

- if $p < 0$ **or** nonlinearity $F(t)$ is "bad" $\Rightarrow$ uniqueness fails



Stability result for small a^2

Theorem. There exists $a_0^2 > 0$ such that for all $a^2 < a_0^2$ the melting hedgehog $H(x) = u(r)\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}Id\right)$, where u satisfies the following BVP

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

$$u(0) = 0, \; u(\infty) = s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}.$$

is locally stable in $H^1(\mathbb{R}^3; \mathscr{S}_0)$, meaning that the second variation at the point H in the V direction, $\mathscr{Q}(V) \geq 0$ for all $V \in C_c^\infty(\mathbb{R}^3; \mathscr{S}_0)$. Moreover $\mathscr{Q}(V) = 0$ if and only if $V \in \{\partial_{x_i} H\}_{i=1}^3$, i.e. kernel of the second variation coincides with translations of $H(x)$.

Ideas of the proofs for ODE

- Existence: variational approach on $(0, R)$ and take limit $R \to \infty$.
- Uniqueness: maximum principle and asymptotic behavior near 0 and ∞.
- Non-uniqueness: mountain pass lemma.
- Qualitative properties: maximum and comparison principle

Ideas of the proofs for stability

1. Define an orthogonal frame in the set of traceless symmetric matrices $\mathscr{S}_0$

$$E_0 = \bar{H} = n \otimes n - \frac{1}{3}\mathrm{Id},\ E_1 = n \otimes p + p \otimes n,\ E_2 = n \otimes m + m \otimes n,$$
$$E_3 = m \otimes p + p \otimes m,\ E_4 = m \otimes m - p \otimes p, \tag{5}$$

where we used spherical coordinates:

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

with $\theta \in [0, \pi]$ the inclination angle and $\varphi \in [0, 2\pi)$ the azimuthal angle.

Note that $E_i \cdot E_j = \mathrm{tr}(E_i E_j^t) = 0$ for $i \neq j$ and $|E_0|^2 = \frac{2}{3},\ |E_i|^2 = 2$ for $i = 1 \ldots 4$.

Any Q-tensor order parameter V can be represented as a linear combination of

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

with $w_i : \mathbb{R}^3 \to \mathbb{R}$ scalar functions, $i = 0, \ldots, 4$.

This decomposition separates uniaxial and biaxial perturbations into two subspaces $\{E_0, E_1, E_2\}$ and $\{E_3, E_4\}$.

Recall that $\mathscr{Q}(V) = \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla V|^2 + g(x,V)\right] dx$ with

$$\begin{aligned} g(x,V) &= \Big(-\frac{a^2}{2} + \frac{c^2u^2}{3}\Big)|V|^2 - b^2\, u\, \mathrm{tr}(\bar{H}\, V^2) + c^2\, u^2\, \mathrm{tr}^2(\bar{H}\, V) \\ &= \frac{1}{3} w_0^2 \hat{f}(u) + (w_1^2 + w_2^2) f(u) + (w_3^2 + w_4^2) \tilde{f}(u), \end{aligned}$$

where

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

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

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

Here u is the unique solution of the ODE for the optimal profile

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

with $u(0) = 0$, $u(\infty) = s_+$.

2. For $V(r,\theta,\varphi) = \sum_{i=0}^{4} w_i(r,\theta,\varphi) E_i(\theta,\varphi)$, expand $\{w_i\}_{i=0\ldots 4}$ in Fourier series to reduce the φ-dependence:

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

$$M_k(r,\theta,\varphi) = \sum_{i=0}^{4} \mu_k^{(i)}(r,\theta)\, E_i(\theta,\varphi) \quad \text{and} \quad N_k(r,\theta,\varphi) = \sum_{i=0}^{4} \nu_k^{(i)}(r,\theta)\, E_i(\theta,\varphi).$$

This gives decomposition of V and the second variation

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

Using definition of the second variation we have that $\mathscr{Q}(V) = \sum_{k=0}^{\infty} \mathscr{Q}(V_k)$.

Using basic algebraic inequalities we can show that:

if $\mathscr{Q}(V_k) \geq 0$ for $k = 0, 1, 2$ **then** $\mathscr{Q}(V_k) \geq 0$ for $k \geq 3$.

3. Non-negativity of $\mathscr{Q}(V_k)$ for $k = 0, 1, 2$ is equivalent to non-negativity of some functionals $\Phi_k(v_0, v_2, v_4)$, $k = 0, 1, 2$ depending only on 3 functions $v_m(r, \theta)$, $m = 0, 2, 4$ (instead of the 10 components of V_k) .

The idea is to separate variables in $v_m(r, \theta)$, $m = 0, 2, 4$.

The natural thing to do is for each $k = 0, 1, 2$ use some basis and represent v_m, $m = 0, 2, 4$ as a series

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

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

$$\Phi_k(v_0, v_2, v_4) = \sum_i \Phi_{k,i}(w_{k,i}^{(0)}, w_{k,i}^{(2)}, w_{k,i}^{(4)}), \quad k = 0, 1, 2$$

It's not clear why it will work since there is a mixing between v_0, v_2, and v_4.

4. At the end we obtain that everything relies on the sign of

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

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

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

5. Use Hardy-type trick and some analysis to show positivity of $\Phi_{0,2}$.

Let's illustrate it in the case where $w_0 = w_4 = 0$:

$$\Phi_{0,2}(w_0, w_2, w_4) \geq \mathscr{Q}_1(w_2) = \int_0^\infty \Big[|\partial_r w|^2 + \big(\frac{6}{r^2} + f(u)\big)|w|^2\Big]\, r^2\, dr$$

Using representation $w(r,\theta) = u(r)\mathring{w}(r,\theta)$, where u satisfies ODE for optimal profile and $\mathring{w} \in C_c(0,\infty)$ we obtain

$$\begin{aligned}\mathscr{Q}_1(w) &= \int_0^\infty \Big[|u'\,\mathring{w} + u\,\partial_r \mathring{w}|^2 + \frac{6}{r^2}\, u^2\, \mathring{w}^2 + f(u)\, u^2\, \mathring{w}^2\Big]\, r^2\, dr \\ &= \int_0^\infty u^2\, |\partial_r \mathring{w}|^2\, r^2\, dr > 0.\end{aligned}$$

Some observations related to the above proposition

- $\tilde{f}(u)$ is the most difficult term to deal with.
- Mixing terms are extremely important in making life difficult.
- Hardy trick works but it's not easy to find the splitting.
- Need fine properties of the solution of the ODE, in particular, "nice" relations between u, u', and u''.
- Numerics help a lot in understanding what to shoot for.

It yields local stability of the melting hedgehog for small a^2.

Thank you for your attention!