

Stability of the vortex defect in Landau - de Gennes theory of nematic liquid crystals

Radu Ignat ^a, Luc Nguyen ^b Valeriy Slastikov ^c Arghir Zarnescu ^d

^aLaboratoire de Mathématiques, Université Paris-Sud 11, bât. 425, 91405 Orsay, France

^bMathematics Department, Princeton University, Fine Hall, Washington Road, Princeton, NJ 08544, USA

^cSchool of Mathematics, University of Bristol, Bristol, BS8 1TW, United Kingdom

^dUniversity of Sussex, Department of Mathematics, Pevensey 2, Falmer, BN1 9QH, United Kingdom

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Abstract

We analyze the radially symmetric solution corresponding to the vortex defect (the so called *melting hedgehog*) in Landau - de Gennes theory for nematic liquid crystals. We prove existence, uniqueness and stability results of the melting hedgehog. *To cite this article: A. Name1, A. Name2, C. R. Acad. Sci. Paris, Ser. I 340 (2005).*

Résumé

Stabilité du défaut vortex dans la théorie Landau - de Gennes pour les cristaux liquides. Nous étudions la solution à symétrie radiale associée au défaut de type vortex dans la théorie Landau - de Gennes pour les cristaux liquides. Nous montrons des résultats d'existence, unicité et stabilité de cette solution. *Pour citer cet article : A. Name1, A. Name2, C. R. Acad. Sci. Paris, Ser. I 340 (2005).*

Version française abrégée

Dans cette note, nous étudions la fonctionnelle de Landau - de Gennes (LdG) pour les cristaux liquides dont le paramètre d'ordre $Q(x)$ est défini en tout point $x \in \mathbb{R}^3$ et à valeurs dans l'espace \mathcal{S}_0 des Q -tenseurs de dimension 5, i.e., les matrices symétriques 3×3 à trace nulle. L'énergie LdG est constituée de deux termes : l'énergie élastique et l'énergie potentielle dont la densité est donnée par un polynôme $f_B(Q)$ de degré 4 en Q (voir (1.1)) qui atteint sa valeur minimale sur une sous-variété de \mathcal{S}_0 de dimension 2. Notre but consiste à analyser le point critique de cette fonctionnelle qui a une symétrie radiale et satisfait des conditions limites correspondant au défaut vortex. Cette solution s'appelle "melting hedgehog" et s'écrit sous la forme $H(x) = u(|x|)\bar{H}(x)$ (voir (1.3)) où le profil radial u satisfait une EDO semilinéaire d'ordre deux (voir (1.4)) avec des conditions limites à l'origine 0 et à l'infini. En effet, $\bar{H}(x)$ représente le Q -tenseur associé au champ de vortex singulier $x/|x|$ dans la théorie Ginzburg-Landau en $3D$ et la fonction scalaire $u(|x|)$ correspond au profil (scalaire) régulier du vortex qui s'annule à l'origine.

D'abord, nous montrons l'existence et l'unicité du profil radial positif u . La preuve de l'existence du profil u repose sur une approche variationnelle, tandis que l'unicité est basée sur un principe de

Email addresses: Radu Ignat@math.u-psud.fr (Radu Ignat), llnghuyen@math.princeton.edu (Luc Nguyen), Valeriy.Slastikov@bristol.ac.uk (Valeriy Slastikov), A.Zarnescu@sussex.ac.uk (Arghir Zarnescu).

comparaison pour les sur/sous-solutions de l'EDO (1.4) et une analyse du comportement asymptotique de la solution en 0 et à l'infini.

Ensuite, nous présentons le résultat principal de cette note sur la stabilité / instabilité de la solution H selon le paramètre a^2 du système. Premièrement, nous montrons l'instabilité de H dans le régime où a^2 est grand (correspondant physiquement à une basse température réduite). Ceci repose sur la construction d'une perturbation autour de la solution H qui rend négative la variation seconde de l'énergie. Deuxièmement, nous prouvons la stabilité de H dans le régime où le paramètre a^2 est petit. En effet, nous montrons la positivité de la variation seconde $\mathcal{Q}(V)$ pour toute perturbation V autour de H : nous utilisons d'abord une décomposition de V en une base bien choisie dans \mathcal{S}_0 et ensuite, la méthode de la séparation de variable pour réduire d'abord le problème au contexte à symétrie axiale et ensuite, au contexte radial. La conclusion suit par un argument de type Hardy qui rend compte de la nonlinéarité $f_B(Q)$ du système.

1. Introduction

We consider the following Landau-de Gennes energy functional:

$$\mathcal{F}(Q) = \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla Q|^2 + f_B(Q) \right] dx, \quad Q \in H^1(\mathbb{R}^3, \mathcal{S}_0),$$

where

$$\mathcal{S}_0 \stackrel{\text{def}}{=} \{Q \in \mathbb{R}^{3 \times 3}, Q = Q^t, \text{tr}(Q) = 0\}$$

denotes the set of Q -tensors (i.e., traceless symmetric matrices in $\mathbb{R}^{3 \times 3}$, see [1] for their physical interpretation). The bulk energy density f_B accounts for the bulk effects and has the following form

$$f_B(Q) = -\frac{a^2}{2} |Q|^2 - \frac{b^2}{3} \text{tr}(Q^3) + \frac{c^2}{4} |Q|^4, \quad (1.1)$$

where $a^2, c^2 > 0$ and $b^2 \geq 0$ are constants and $|Q|^2 \stackrel{\text{def}}{=} \text{tr}(Q^2)$. A critical point of the functional \mathcal{F} satisfies the Euler-Lagrange equation

$$\Delta Q = -a^2 Q - b^2 [Q^2 - \frac{1}{3} |Q|^2 Id] + c^2 |Q|^2 Q, \quad (1.2)$$

where the term $\frac{1}{3} b^2 |Q|^2 Id$ is a Lagrange multiplier that accounts for the tracelessness constraint. It is well known that solutions of (1.2) are smooth (see for instance [8]).

Remark 1 We should point out now that although the equation (1.2) seems to depend on three parameters a^2, b^2 and c^2 , there is only one independent parameter in the problem which can be chosen to be a^2 for fixed b^2 and c^2 (after a suitable rescaling $Q \mapsto \lambda Q(x/\mu)$ for two parameters $\lambda, \mu > 0$).

We are interested in studying the *radially-symmetric* solution of (1.2). For that, a measurable \mathcal{S}_0 -valued map $Q : \mathbb{R}^3 \rightarrow \mathcal{S}_0$ is called radially-symmetric if

$$Q(Rx) = RQ(x)R^t \text{ for any rotation } R \in SO(3) \text{ and a.e. } x \in \mathbb{R}^3.$$

In fact, such a map $Q(x)$ has only one degree of freedom: there exists a measurable radial scalar function $u : (0, +\infty) \rightarrow \mathbb{R}$ such that $Q(x) = u(|x|) \bar{H}(x)$ for a.e. $x \in \mathbb{R}^3$, where \bar{H} is the so called *hedgehog*:

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

and the radial scalar profile u of Q is given by $u(|x|) = \frac{3}{2} \text{tr}(Q(x) \bar{H}(x))$ for a.e. $x \in \mathbb{R}^3$.

We will focus on the stability and properties of the profile of the following radially symmetric solution of (1.2), called *melting hedgehog* :

$$H(x) = u(|x|)\bar{H}(x) \quad (1.3)$$

where the radial scalar profile u is the unique *positive* solution of the following semilinear ODE:

$$u''(r) + \frac{2}{r}u'(r) - \frac{6}{r^2}u(r) = F(u(r)) \quad \text{for } r > 0 \quad (1.4)$$

subject to boundary conditions $u(0) = 0$ and $\lim_{r \rightarrow \infty} u(r) = s_+$ where

$$F(u) = -a^2 u - \frac{b^2}{3}u^2 + \frac{2c^2}{3}u^3 \quad (1.5)$$

and $s_+ \stackrel{\text{def}}{=} \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}$ is the positive zero of F .

Our main result concerns the local stability of the melting hedgehog (see [6]). We highlight that H is a critical point of (1.2), but has infinite energy \mathcal{F} , i.e., $\mathcal{F}(H) = \infty$. Therefore, the stability issue is carried out by analyzing the following second variation of the modified functional \mathcal{F} at the point H in the direction $V \in C_c^\infty(\mathbb{R}^3; \mathcal{S}_0)$, denoted by $\mathcal{Q}(V)$:

$$\begin{aligned} \mathcal{Q}(V) &= \frac{1}{2} \frac{d^2}{dt^2} \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla(H + tV)|^2 + f_B(H + tV) - \frac{1}{2} |\nabla H|^2 - f_B(H) \right] dx \\ &= \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla V|^2 + \left(-\frac{a^2}{2} + \frac{c^2 u^2}{3} \right) |V|^2 - b^2 u \operatorname{tr}(\bar{H} V^2) + c^2 u^2 \operatorname{tr}^2(\bar{H} V) \right] dx. \end{aligned} \quad (1.6)$$

Theorem 1.1 *There exists $a_0^2 > 0$ such that for all $a^2 < a_0^2$ the melting hedgehog H defined at (1.3) is a locally stable critical point of (1.2), i.e., $\mathcal{Q}(V) \geq 0$ for all $V \in C_c^\infty(\mathbb{R}^3; \mathcal{S}_0)$. Moreover $\mathcal{Q}(V) = 0$ if and only if $V \in \operatorname{span}\{\partial_{x_i} H\}_{i=1}^3$, i.e., the kernel of the second variation is generated by translations of $H(x)$.*

There exists $a_1^2 > 0$ so that for any $a^2 > a_1^2$ there exists $V_ \in C_c^\infty(\mathbb{R}^3; \mathcal{S}_0)$ such that $\mathcal{Q}(V_*) < 0$. Any such V_* cannot be purely uniaxial (i.e., $V_*(x)$ has three different eigenvalues for some point $x \in \mathbb{R}^3$).*

2. Comparison with the Ginzburg-Landau model

Let us compare Landau-de Gennes (LdG) model with 2D and 3D Ginzburg-Landau (GL) systems [2,10,9]. Both LdG and GL energies consist of two terms: a Dirichlet energy and a well potential energy. The N -dimensional GL energy is defined for N -dimensional vector fields (here, $N = 2, 3$) and the minima of the well potential is a co-dimension one manifold, e.g., the unit sphere $S^{N-1} \subset \mathbb{R}^N$. However, our 3D LdG energy is defined for maps with values into the five-dimensional space \mathcal{S}_0 of Q -tensors and the global minimizing Q -tensors of the bulk potential f_B , as defined in (1.1), form a 2D manifold $\mathcal{M} \subset \mathcal{S}_0$ (the limit target manifold), homeomorphic to the projective plane $\mathbb{R}\mathbb{P}^2 \subset \mathbb{R}^3$:

$$\mathcal{M} = \left\{ Q \in \mathcal{S}_0 : Q = s_+ \left(n \otimes n - \frac{1}{3} Id \right), n \in S^2 \right\}. \quad (2.1)$$

Thus, one might expect similar stability behavior between the melting hedgehog for the LdG and the vortex defect for the 3D GL (as maps defined from \mathbb{R}^3 into a 2D manifold), see [4]; nevertheless, there is still a significant difference to 3D GL since variations in LdG are allowed in 5D and the target limit manifolds ($\mathbb{R}\mathbb{P}^2$ for LdG and S^2 for 3D GL) have different fundamental groups. We highlight that the situation would be rather different if $b^2 = 0$ in the expression of f_B of the LdG model: in that case, the global minimizing Q -tensors form a 4D sphere $\{Q \in \mathcal{S}_0 : \operatorname{tr}(Q^2) = a^2/c^2\}$ hence we expect instability of the melting hedgehog as a map from \mathbb{R}^3 with values into a 4D manifold. It was proved in [3] that this behavior holds true if b^2 is small (corresponding to a^2 large after the rescaling in Remark 1). Our major

contribution is to develop a systematic approach (going beyond the Ginzburg-Landau type of methods) that is capable of dealing not only with the regime $a^2 \rightarrow \infty$ but also with the much more challenging case when a^2 is small.

3. Existence and uniqueness of the radial scalar profile

We present now an existence and uniqueness result of the positive solution for a special type of semilinear ODE that generalizes (1.4). For that, let $F : \mathbb{R}_+ \rightarrow \mathbb{R}$ be a C^1 function satisfying the following conditions:

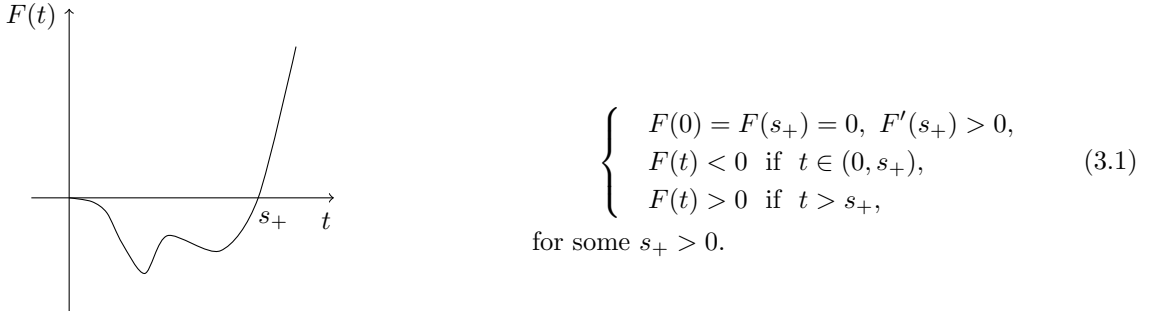


Figure 1. A schematic graph of F on \mathbb{R}_+ .

We will focus on the following semilinear ODE:

$$u''(r) + \frac{p}{r} u'(r) - \frac{q}{r^2} u(r) = F(u(r)) \quad \text{on } (0, R) \quad (3.2)$$

where we assume

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

We will present the result for the case of finite domains (i.e., $(0, R)$ with $R \in (0, +\infty)$) and the infinite domain $(0, +\infty)$ (i.e. $R = +\infty$) under the limit conditions

$$u(0) = 0, \quad u(R) = s_+, \quad (3.3)$$

with the standard convention $u(\infty) = \lim_{r \rightarrow \infty} u(r) = s_+$ if $R = +\infty$.

Theorem 3.1 *Under the assumption (3.1), there exists a unique non-negative solution u of (3.2) with boundary conditions (3.3). Moreover, this solution is strictly increasing.*

The existence result is proved by constructing positive energy minimizing solutions on finite intervals $(0, R)$ satisfying (3.3). In the case of $R = +\infty$, we prove that those minimizers converge to a non-negative solution of (3.2) on the entire \mathbb{R}_+ ; the limit conditions (3.3) are satisfied due to the local minimizing behavior of the constructed solution that ensures non-flatness at $+\infty$. The trickiest part consists in proving the uniqueness. In fact, the argument is based on a comparison principle for sub/super-solutions of the semilinear ODE (3.2) and a detailed understanding of the asymptotic behavior of the solution at 0 and ∞ (see [5]).¹

¹ Recently, X. Lamy [7] showed the uniqueness and monotonicity of the energy minimizing solution of equation (1.4) for the particular case of $F(u)$ given by (1.5) and on bounded domains by using a different technique.

4. Stability of the melting hedgehog

The goal of this section is to sketch the proof of Theorem 1.1. For that, we study the sign of the second variation \mathcal{Q} at the melting hedgehog H defined at (1.6). The idea is to use a special basis decomposition for $V \in C_c^\infty(\mathbb{R}^3; \mathcal{S}_0)$ and reduce the study of $\mathcal{Q}(V)$ to simpler functionals by separation of variables.

4.1. Decomposition with respect to a special basis

We decompose $V \in C_c^\infty(\mathbb{R}^3; \mathcal{S}_0)$ in a certain orthogonal frame of \mathcal{S}_0 . We use spherical coordinates:

$$x = r(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \in \mathbb{R}^3, \quad r \in \mathbb{R}_+, \quad \theta \in (0, \pi), \quad \varphi \in [0, 2\pi],$$

and the following orthonormal basis in \mathbb{R}^3 :

$$n = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta), \quad m = (\cos \theta \cos \varphi, \cos \theta \sin \varphi, -\sin \theta), \quad p = (\sin \varphi, -\cos \varphi, 0).$$

Now we choose the following orthogonal frame in \mathcal{S}_0 :

$$E_0 = \bar{H}, \quad E_1 = n \otimes p + p \otimes n, \quad E_2 = n \otimes m + m \otimes n, \quad E_3 = m \otimes p + p \otimes m, \quad E_4 = m \otimes m - p \otimes p.$$

Note that $E_i = E_i(\theta, \varphi)$ are independent of r ; moreover, $\{E_1, E_2\}$ (resp., $\{E_0, E_3, E_4\}$) form a basis of the tangent space (resp., the normal space) of the limit target manifold \mathcal{M} at $s_+ \bar{H}$ (defined at (2.1)). Then any \mathcal{S}_0 -valued map V can be represented as the following linear combination:

$$V = \sum_{i=0}^4 w_i(r, \theta, \varphi) E_i. \quad (4.1)$$

with $\{w_i\}_{i=0, \dots, 4}$ scalar functions on \mathbb{R}^3 .

4.2. Instability for a^2 large

The ansatz consists in focusing on axially symmetric perturbations in (4.1), i.e., $w_i = w_i(r, \theta)$ are φ -independent, and moreover, studying the stability only on the subspaces $\{w_i E_i : w_i = w_i(r, \theta) \in C_c^\infty(\mathbb{R}^3)\}$. We obtain stability under such perturbations driven by the uniaxial basis components E_0, E_1 and E_2 , while the stability under perturbations driven by the biaxial basis components E_3 and E_4 holds true for small a^2 and fails for a^2 large (see [6]). We only present here the instability result:

Proposition 4.1 *There exists $a_1^2 > 0$ such that if $a^2 > a_1^2$ then one can find $w \in C_c^\infty(\mathbb{R}^3)$ independent of the φ -variable with $\mathcal{Q}(wE_i) < 0$ for $i = 3, 4$.*

We prove Proposition 4.1 in the special case $b^2 = 0$ corresponding to $a^2 = \infty$ (see Remark 1). For that, we choose $w(r, \theta) = w_*(r) \sin^2 \theta$. Denoting $f(u) = \frac{F(u)}{u} \stackrel{(1.5)}{=} -a^2 + \frac{2e^2 u^2}{3}$, we compute:

$$\mathcal{Q}(wE_3) = \mathcal{Q}(wE_4) = \frac{32\pi}{15} \int_0^\infty \left[|w_*'|^2 + \left(\frac{4}{r^2} + f(u) \right) |w_*|^2 \right] r^2 dr =: \frac{32\pi}{15} \mathcal{E}(w_*).$$

Decomposing $w_*(r) = u(r) \dot{w}(r)$ for u solving (1.4) and $\dot{w} \in C_c^\infty(0, \infty)$, integration by parts yields:

$$\begin{aligned} \mathcal{E}(w_*) &= \int_0^\infty \left\{ |u \dot{w}' + u' \dot{w}|^2 + \frac{4}{r^2} u^2 \dot{w}^2 + f(u) u^2 \dot{w}^2 \right\} r^2 dr \\ &= \int_0^\infty \left\{ |u \dot{w}' + u' \dot{w}|^2 + \frac{4}{r^2} u^2 \dot{w}^2 + (u'' + \frac{2}{r} u' - \frac{6}{r^2} u) u \dot{w}^2 \right\} r^2 dr = \int_0^\infty \left\{ |\dot{w}'|^2 - \frac{2}{r^2} \dot{w}^2 \right\} u^2 r^2 dr. \end{aligned}$$

By (3.3), for small $\epsilon > 0$ there exists $R > 0$ such that $s_+(1 - \epsilon) < u(r) < s_+$ on (R, ∞) . Since the best constant of Hardy's inequality² in \mathbb{R}^3 is $\frac{1}{4} < 2(1 - \epsilon)^2$, one can find³ $\dot{w} \in C_c^\infty(R, \infty)$ with $\mathcal{E}(u\dot{w}) < 0$.

4.3. Stability for a^2 small

Let us briefly explain the strategy of proving stability of the melting hedgehog for small $a^2 > 0$ stated in Theorem 1.1. The first step is to reduce the study of the second variation \mathcal{Q} to the axially symmetric context of φ -independent components $\{w_i\}_{0 \leq i \leq 4}$ in (4.1). Indeed, as in the proof of the stability of the GL vortex (see [10]), we use Fourier decomposition in φ of the components $\{w_i\}_{0 \leq i \leq 4}$; we show that the non-negativity of $\mathcal{Q}(V)$ reduces to proving the non-negativity of three functionals Φ_k ($k = 0, 1, 2$) that correspond to the first three Fourier modes and each Φ_k depends only on three functions $\{v_i(r, \theta)\}_{i=0,1,2}$ (i.e., v_i are φ -independent functions). The second step is to reduce the study of the non-negativity of Φ_k to some new functionals defined on θ -independent components $v_i = v_i(r)$. This separation of variable is much more subtle and uses some orthonormal bases of eigenvectors (depending only on θ) of certain operators coming from the Euler-Lagrange equations associated to the functionals Φ_k . Roughly speaking, this spectral decomposition is similar to sets of spherical harmonics, adapted differently for each of the v_i 's. The last step is to prove non-negativity of the remaining functionals depending only on components $v_i = v_i(r)$. The strategy here relies on a Hardy decomposition (as in Section 4.2) that takes care of the nonlinearity of the problem coming from the bulk energy density.

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² The standard Hardy inequality in \mathbb{R}^3 : $\int_{\mathbb{R}^3} |\nabla \psi|^2 dx \geq \frac{1}{4} \int_{\mathbb{R}^3} \frac{|\psi|^2}{|x|^2} dx$ for every $\psi \in C_c^\infty(\mathbb{R}^3)$.

³ For instance, taking n large enough and defining $\psi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ by $\psi(r) = \frac{1}{R} - \frac{1}{r}$ on $(R, \frac{2nR}{n+1})$, $\psi(r) = \frac{1}{r} - \frac{1}{nR}$ on $(\frac{2nR}{n+1}, nR)$ and $\psi(r) = 0$ elsewhere, we can choose \dot{w} to be a smooth (compactly supported) approximation of ψ .