



## Partial Differential Equations/Calculus of Variations

## Stability of the vortex defect in the Landau–de Gennes theory for nematic liquid crystals



*Stabilité du défaut vortex dans la théorie Landau–de Gennes pour les cristaux liquides*

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## ABSTRACT

We analyze the radially symmetric solution corresponding to the vortex defect (the so-called *melting hedgehog*) in the Landau–de Gennes theory for nematic liquid crystals. We prove the existence, uniqueness and stability results of the melting hedgehog.

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## RÉSUMÉ

Nous étudions la solution à symétrie radiale associée au défaut de type vortex dans la théorie de Landau–de Gennes pour les cristaux liquides. Nous montrons des résultats d'existence, d'unicité et de stabilité de cette solution.

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## 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  $3 \times 3$  à trace nulle. L'énergie LdG est constituée de deux termes : l'énergie élastique et l'énergie potentielles, 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 aux limites correspondant au défaut vortex. Cette solution s'appelle « melting hedgehog » et s'écrit sous la forme  $H(x) = u(|x|)\tilde{H}(x)$  (voir (1.3)), où le profil radial  $u$  satisfait une EDO semilinéaire d'ordre deux (voir (1.4)) avec des conditions aux limites à l'origine 0 et à l'infini. En effet,  $\tilde{H}(x)$  représente le  $Q$ -tenseur associé au champ de vortex singulier  $x/|x|$  dans la théorie de Ginzburg–Landau en 3D, et la fonction scalaire  $u(|x|)$  correspond au profil (scalaire) régulier du vortex, qui s'annule à l'origine.

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

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 non-linéarité  $f_B(Q)$  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

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

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 Eq. (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:

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

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 in (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 the Landau–de Gennes (LdG) model with 2D and 3D Ginzburg–Landau (GL) systems [2,9,10]. 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), if  $b^2 > 0$ , homeomorphic to the projective plane  $\mathbb{RP}^2 \subset \mathbb{R}^3$ :

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

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 with 3D GL, since variations in LdG are allowed in 5D and the target limit manifolds ( $\mathbb{RP}^2$  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  $f_B$  in 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:

$$\begin{cases} F(0) = F(s_+) = 0, & F'(s_+) > 0, \\ F(t) < 0 & \text{if } t \in (0, s_+), \\ F(t) > 0 & \text{if } t > s_+, \end{cases} \quad (3.1)$$

for some  $s_+ > 0$ . (See Fig. 1.)

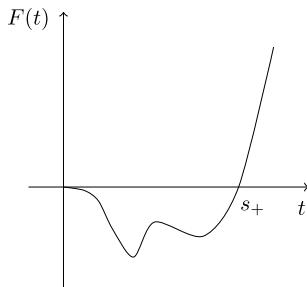


Fig. 1. A schematic graph of  $F$  on  $\mathbb{R}_+$ .

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:

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

We will present the result for the case of finite domains (i.e.,  $(0, R)$  with  $R \in (0, +\infty)$ ) and of 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 toward 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  $\infty$  (see [5]).<sup>1</sup>

#### 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 in [\(1.6\)](#). 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  $V \in C_c^\infty(\mathbb{R}^3; \mathcal{S}_0)$  into a certain orthogonal frame of  $\mathcal{S}_0$ . We use spherical coordinates:

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

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  $\mathcal{S}_0$ :

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

Note that  $E_i = E_i(\theta, \varphi)$  are independent of  $r$ ; moreover, if  $b^2 > 0$ , then  $\{E_1, E_2\}$  (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  $s_+ H$  (defined in [\(2.1\)](#)). 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  $\varphi$ -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 the 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 large  $a^2$  (see [\[6\]](#)). We only present here the instability result:

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

**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  $\varphi$ -variable with  $\mathcal{D}(wE_i) < 0$  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  $f(u) = \frac{F(u)}{u}$  ([1.5](#))  $= -a^2 + \frac{2c^2 u^2}{3}$ , we compute:

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

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:

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

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

#### 4.3. Stability for small $a^2$

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  $\mathcal{D}$  to the axially symmetric context of  $\varphi$ -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 a Fourier decomposition in  $\varphi$  of the components  $\{w_i\}_{0 \leq i \leq 4}$ ; we show that the non-negativity of  $\mathcal{D}(V)$  reduces to proving the non-negativity of the three functionals  $\Phi_k$  ( $k = 0, 1, 2$ ) corresponding to the first three Fourier modes and that each  $\Phi_k$  depends only on three functions  $\{v_i(r, \theta)\}_{i=0,1,2}$  (i.e.,  $v_i$  are  $\varphi$ -independent functions). The second step consists in reducing the study of the non-negativity of  $\Phi_k$  to some new functionals defined on the  $\theta$ -independent components  $\tilde{v}_i = \tilde{v}_i(r)$ . This separation of variables is much more subtle and uses some orthonormal bases of eigenvectors (depending only on  $\theta$ ) of certain operators coming from the Euler-Lagrange equations associated with the functionals  $\Phi_k$ . Roughly speaking, this spectral decomposition is similar to sets of spherical harmonics, adapted differently for each of the  $\tilde{v}_i$ 's. The last step is to prove the non-negativity of the remaining functionals, depending only on the components  $\tilde{v}_i = \tilde{v}_i(r)$ . 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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<sup>2</sup> 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  $\psi \in C_c^\infty(\mathbb{R}^3)$ .

<sup>3</sup> 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  $\psi$ .