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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\textbf{A B S T R A C T}

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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\textbf{R É S Ü M É}

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 potentielle, dont la densité est donnée par un polynôme $f_0(Q)$ 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 $H(x) = u(|x|) \overline{H}(x)$ (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, $\overline{H}(x)$ 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 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 \( \mathcal{D}(V) \) pour toute perturbation V autour de H : nous utilizons 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 \( f_0(Q) \) 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:

\[
\mathcal{S}_0 \equiv \left\{ Q \in \mathbb{R}^{3 \times 3}, \quad Q = Q^t, \quad \text{tr}(Q) = 0 \right\}
\]

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:

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

(1.1)

where \( a^2, c^2 > 0 \) and \( b^2 \geq 0 \) are constants and \( |Q|^2 \) is the tracelessness constraint. A critical point of the functional \( \mathcal{F} \) satisfies the Euler–Lagrange equation

\[
\Delta Q = -a^2 Q - b^2 \left[ Q^2 - \frac{1}{3} |Q|^2 \text{Id} \right] + c^2 |Q|^2 Q,
\]

(1.2)

where the term \( \frac{1}{2} b^2 |Q|^2 \text{Id} \) 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 \( Q : \mathbb{R}^3 \to \mathcal{S}_0 \) 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 \( u : (0, +\infty) \to \mathbb{R} \) for a.e. \( x \in \mathbb{R}^3 \), such that \( Q(x) = u(|x|)\tilde{H}(x) \) for a.e. \( x \in \mathbb{R}^3 \), where \( \tilde{H} \) is the so-called hedgehog:

\[
\tilde{H}(x) = \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} \text{Id}
\]

and the radial scalar profile \( u \) of \( Q \) is given by \( u(|x|) = \frac{1}{2} \text{tr}(Q(x)\tilde{H}(x)) \) 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:

\[
H(x) = u(|x|)\tilde{H}(x)
\]

(1.3)

where the radial scalar profile \( u \) is the unique positive solution of the following semilinear ODE:

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

(1.4)

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

\[
F(u) = -a^2 u - \frac{b^2}{3} u^2 + \frac{2 c^2}{3} u^3
\]

(1.5)

and \( s_+ \) 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 $V \in C_c^\infty(\mathbb{R}^3; \mathcal{J}_0)$, denoted by $\mathcal{D}(V)$:

$$\mathcal{D}(V) = \frac{1}{2} \frac{d^2}{dt^2} \int_{\mathbb{R}^3} \left[ \frac{1}{2} |\nabla (H + tV)|^2 + f_b(H + tV) - \frac{1}{2} |\nabla H|^2 - f_b(H) \right] dx$$

$$= \int_{\mathbb{R}^3} \left[ \frac{1}{2} |\nabla V|^2 + \left( \frac{a^2}{2} + \frac{c^2 u^2}{3} \right) |V|^2 - b^2 u \, \text{tr}(H V^2) + c^2 u^2 \, \text{tr}^2(H V) \right] dx. \quad (1.6)$$

**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., $\mathcal{D}(V) \geq 0$ for all $V \in C_c^\infty(\mathbb{R}^3; \mathcal{J}_0)$. Moreover, $\mathcal{D}(V) = 0$ if and only if $V \in \text{span}(\partial_n H)^i \in \mathcal{J}_0$, i.e., the kernel of the second variation is generated by translations of $H(x)$.

There exists $a_0^2 > 0$ so that for any $a^2 > a_0^2$ there exists $V_* \in C_c^\infty(\mathbb{R}^3; \mathcal{J}_0)$ such that $\mathcal{D}(V_*) < 0$. 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 $N$-dimensional 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 $\mathcal{J}_0$ of $Q$-tensors and the global minimizing $Q$-tensors of the bulk potential $f_b$, as defined in (1.1), form a 2D manifold $\mathcal{M} \subset \mathcal{J}_0$ (the limit target manifold), if $b^2 > 0$, homeomorphic to the projective plane $\mathbb{R}P^2 \subset \mathbb{R}^3$:

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

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 ($\mathbb{R}P^2$ 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 $f_b$ in the LdG model: in that case, the global minimizing $Q$-tensors form a 4D sphere ($Q \in \mathcal{J}_0 : \text{tr}(Q^2) = a^2/c^2$); 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 $a^2 \to \infty$, 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 $F : \mathbb{R}_+ \to \mathbb{R}$ 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 $\mathbb{R}_+$](image)
We will focus on the following semilinear ODE:
\[ u''(r) + \frac{p}{r} u'(r) - \frac{q}{r^2} u(r) = F(u(r)) \] on \((0, R)\)
(3.2)
where we assume:
\(p, q \in \mathbb{R}\) and \(q > 0\).

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:
\[ u(0) = 0, \quad u(R) = s_+, \] (3.3)
with the standard convention \(u(\infty) = \lim_{r \to \infty} u(r) = s_+\) 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]).

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 \(Q(V)\) under the limit conditions:
\[ \lim_{r \to \infty} \frac{Q(V)}{r^2} = \pm \infty, \] (3.3)
and reduce the study of \(Q(V)\) to simpler functionals by separation of variables.

4.1. Decomposition with respect to a special basis

We decompose \(V \in C_\infty^r(\mathbb{R}^3; \mathcal{H}_0)\) into a certain orthogonal frame of \(\mathcal{H}_0\). 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 orthonormal frame in \(\mathcal{H}_0\):
\[ E_0 = \tilde{H}, \quad E_1 = n \otimes p + p \otimes n, \quad E_2 = n \otimes m + m \otimes n, \quad E_3 = m \otimes p + p \otimes m, \quad E_4 = m \otimes m - p \otimes p. \]

Note that \(E_1 = E_1(\theta, \varphi)\) 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 \(\mathcal{H}_0\)-valued map \(V\) can be represented as the following linear combination:
\[ V = \sum_{i=0}^{4} w_i(r, \theta, \varphi) E_i, \]
(4.1)
with \(\{w_i\}_{i=0,4}\) 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 \(\{w_i E_i: w_i = w_i(r, \theta) \in C_\infty^r(\mathbb{R}^3)\}\). 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:

\[ \text{Recently, X. Lamy [7] showed the uniqueness and monotonicity of the energy-minimizing solution of Eq. (1.4) for the particular case of } F(u) \text{ given by (1.5) and on bounded domains by using a different technique.} \]
Proposition 4.1. There exists $a_i^2 > 0$ such that if $a^2 > a_i^2$ then one can find $w \in C^1_0(\mathbb{R}^3)$ independent of the $\varphi$-variable with $\mathcal{D}(\phi E_i) < 0$ 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 $w(r, \theta) = w_0(r) \sin^2 \theta$. Denoting $f(u) = \frac{f(u)}{u}$ by $a^2 + \frac{2a^2}{3}$, we compute:

$$\mathcal{D}(\phi E_3) = \mathcal{D}(\phi E_4) = \frac{32\pi}{15} \int_0^\infty \left[ |w_0'|^2 + \left( \frac{4}{r^2} + f(u) \right) |w_0|^2 \right] r^2 \, dr = \frac{32\pi}{15} \mathcal{E}(w_0).$$

Decomposing $w_0(r) = u(r) w(r)$ for $u$ solving (1.4) and $\phi \in C^1_0(0, \infty)$, integration by parts yields:

$$\mathcal{E}(w_0) = \frac{32\pi}{15} \int_0^\infty \left[ |u w' + u' w|^2 + \frac{4}{r^2} u^2 w^2 + f(u) u'^2 w^2 \right] r^2 \, dr$$

$$= \frac{32\pi}{15} \int_0^\infty \left[ |u w'|^2 + \frac{4}{r^2} u^2 w^2 + \left( u'' + \frac{2}{r} u' - 6 \frac{u}{r^2} \right) u w^2 \right] r^2 \, dr = \frac{32\pi}{15} \int_0^\infty \left[ |w'|^2 + \frac{2}{r^2} w^2 \right] u^2 r^2 \, dr.$$

By (3.3), for small $\epsilon > 0$, there exists $R > 0$ such that $s_\epsilon(1 - \epsilon) < u(r) < s_\tilde{w}$ on $(R, \infty)$. Since the best constant of Hardy’s inequality in $\mathbb{R}^3$ is $\frac{1}{2} < 2(1 - \epsilon)^2$, one can find $\tilde{w} \in C^1_0(R, \infty)$ with $\mathcal{E}(u \tilde{w}) < 0$.

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. The first step is to reduce the study of the second variation $\mathcal{D}$ to the axially symmetric context of $\varphi$-independent components $\{w_1, \ldots, w_4\}$ 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 $\{w_1, \ldots, w_4\}$: we show that the non-negativity of $\mathcal{D}(V)$ reduces to proving the non-negativity of the three functions $\Phi_k (k = 0, 1, 2)$ corresponding to the first three Fourier modes and that each $\Phi_k$ depends only on three functions $\{\psi_0(r, \theta), \psi_1(r, \theta), \psi_2(r, \theta)\}$ (i.e., $\psi_i$ are $\varphi$-independent functions). The second step consists in reducing the study of the non-negativity of $\Phi_k$ to some new functions defined on the $\theta$-independent components $\tilde{\psi}_i = \psi_i(r)$. 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 functions $\Phi_k$. Roughly speaking, this spectral decomposition is similar to sets of spherical harmonics, adapted differently for each of the $\tilde{\psi}_i$’s. The last step is to prove the non-negativity of the remaining functions, depending only on the components $\tilde{\psi}_i$. 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 $\mathbb{R}^3$: $f(\varphi) |\nabla \varphi|^2 \, dx \geq \frac{1}{4} \int_{\mathbb{R}^3} \frac{|\nabla \varphi|^2}{r^2} \, dx$ for every $\varphi \in C^1_0(\mathbb{R}^3)$.

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

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