Existence of Surface Smectic States of Liquid Crystals

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Abstract

The Landau-de Gennes model of liquid crystals is a functional acting on wave functions (order parameters) and vector fields (director fields). In a specific asymptotic limit of the physical parameters, we construct critical points such that the wave function (order parameter) is localized near the boundary of the domain, and we determine a sharp localization of the boundary region where the wave function concentrates. Furthermore, we compute the asymptotics of the energy of such critical points along with a boundary energy that may serve in localizing the director field. In physical terms, our results prove the existence of a surface smectic state.

Contents

1 Introduction 2
1.1 The model ................................. 2
1.2 Limiting Dirichlet condition for the director field ................................. 4
1.3 Critical points and boundary energy for the director field ................................. 6

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1.3.1 The boundary energy ........................................ 7
1.3.2 Concentration of the order parameter ....................... 7
1.4 Behavior of the ground state energy .......................... 10

2 Behavior of the director field ............................... 11

3 Preliminaries .................................................. 13
  3.1 An $L^\infty$ bound for order parameters ..................... 13
  3.2 A spectral estimate ........................................ 14
  3.3 Reduced Ginzburg-Landau energy ........................... 14
  3.4 Boundary coordinates ....................................... 15
  3.5 Gauge transformation ....................................... 21
    3.5.1 Gauge for fields in $C(\tau)$ ......................... 22
    3.5.2 Gauge for $S^2$-valued fields ........................ 23
  3.6 Energy of a boundary trial state ............................ 26

4 Upper bound for the energy ................................ 29

5 Lower bound for the energy ................................ 32
  5.1 The field $n_0$ ............................................. 33
  5.2 Splitting into bulk and surface terms ....................... 35
  5.3 The surface energy ....................................... 36
  5.4 The bulk energy .......................................... 40
  5.5 Proof of Theorem 5.1 ..................................... 43

6 Proof of the main theorems ................................ 43
  6.1 Proof of Theorem 1.4 .................................... 43
  6.2 Proof of Theorem 1.6 .................................... 44
  6.3 Proof of Theorem 1.8 .................................... 47
    6.3.1 Upper bound .......................................... 47
    6.3.2 Lower bound .......................................... 47

1 Introduction .................................................. 4

1.1 The model ................................................ 4

In this paper, we investigate special critical points of the Landau-de Gennes energy functional. These critical points are constructed by minimization over a special class of configurations.

Critical/minimizing configurations of the Landau-de Gennes functional were introduced by De Gennes in [5] to model the nematic-smectic $A^*$ phase transition in a liquid crystal near the critical temperature. The Landau-de Gennes energy functional acts on configurations of the type $(\psi, n)$, where $\psi$ is a complex-valued function and $n$ is a vector field. Both $\psi$ and $n$ are defined in a three dimensional domain $\Omega$, assumed to be the region occupied by the molecules of the liquid crystal. The complex-valued function $\psi$, called the order parameter, detects the nematic/smectic phase as follows: $\psi(x) = 0$ indicates a (chiral) nematic phase near $x$, while $\psi(x) \neq 0$ indicates a (chiral) smectic $A^*$ phase. The
length of the vector field $\mathbf{n}$, also called the director field, is constrained such that $|\mathbf{n}| = 1$. The direction of the director field has a physical meaning: $\mathbf{n}(x)$ is the average direction of the liquid crystal molecules in a small region around $x$.

The Landau-de Gennes energy is given by

$$\mathcal{E}(\psi, \mathbf{n}) = \mathcal{G}(\psi, \mathbf{n}) + \mathcal{F}_N(\mathbf{n}),$$

where

$$\mathcal{G}(\psi, \mathbf{n}) := \int_\Omega |\nabla_{\mathbf{n}} \psi|^2 - \kappa^2 |\psi|^2 + \frac{\kappa^2}{2} |\psi|^4 \, dx,$$

with the notation $\nabla_{\mathbf{n}} := \nabla - i\mathbf{n}$, and

$$\mathcal{F}_N(\mathbf{n}) := \mathcal{F}_N^+(\mathbf{n}) + \mathcal{L}(\mathbf{n}),$$

with

$$\mathcal{F}_N^+(\mathbf{n}) := \int_\Omega \left\{ K_1 |\text{div} \mathbf{n}|^2 + K_2 |(\text{curl} \mathbf{n}) \cdot \mathbf{n} + \tau|^2 + K_3 |\text{curl} \mathbf{n} \times \mathbf{n}|^2 \right\} \, dx,$$

$$\mathcal{L}(\mathbf{n}) := (K_2 + K_4) \int_\Omega \left( \text{tr}(D\mathbf{n})^2 - |\text{div} \mathbf{n}|^2 \right) \, dx.$$

The first term $\mathcal{G}(\psi, \mathbf{n})$ is reminiscent of the energy for the order parameter in the Ginzburg-Landau theory of superconductivity. The term $\mathcal{F}_N(\mathbf{n})$ is the Oseen-Frank energy of the director field and consists of a non-negative part $\mathcal{F}_N^+(\mathbf{n})$ and a part $\mathcal{L}(\mathbf{n})$ which is (a priori) with indefinite sign. The behavior of the minimizers of the functional $\mathcal{F}_N^+$ is well known, this will be recalled in a detailed review below. Moreover these minimizers correspond to the zeros of $\mathcal{F}_N^+$ if no further boundary constraint is imposed on the vector field $\mathbf{n}$. The functional $\mathcal{L}(\mathbf{n})$ is a null Lagrangian, that is, the value of $\mathcal{L}(\mathbf{n})$ is determined by the value of $\mathbf{n}$ on the boundary. In fact if $\mathbf{n}$ is sufficiently regular, then we have

$$\int_\Omega \left( \text{tr}(D\mathbf{n})^2 - |\text{div} \mathbf{n}|^2 \right) \, dx = \int_\Omega \text{div} \left( (\nabla \mathbf{n}) - \text{div}(\mathbf{n}) \mathbf{n} \right) \, dx.$$

If we minimize the Landau-de Gennes functional under a fixed Dirichlet boundary condition on the director field, then the integral of the null Lagrangian will be constant and will not play any role. See [12, 17, 18, 22] for the above mentioned facts and more on the mathematical theory of static nematic liquid crystal configurations in the Oseen-Frank theory, [20, 21, 22, 24] and the references therein for recent progress on the mathematical theory of liquid crystals flows, [3, 2, 26, 16] and the references therein for the mathematical analysis on the Landau-de Gennes model (1.1).

In the expression of the Landau-de Gennes functional, various parameters appear. The parameter $\kappa > 0$ is material dependent and depends on the temperature. That $\kappa > 0$ signifies that the temperature is below the critical temperature responsible for the nematic-smectic transition for a non-chiral material. By analogy with superconductivity, we may call $\kappa$ the Ginzburg-Landau parameter, and we will consider the regime of large $\kappa$.

The two other parameters left in $\mathcal{E}(\psi, \mathbf{n})$ are $q$ and $\tau$. Here $\tau$ is the chiral twist ($\tau = 0$ indicates a non-chiral material). We will suppose that $\tau > 0$. The parameter $q > 0$ measures the density of smectic layering.
The positive constants $K_i$ in the functional $F_N$, $i = 1, 2, 3$, correspond to the splay, twist and bend elasticity constants. The constant $K_4$ is usually selected in $(-\infty, 0]$, see [6, 8], while $K_1, K_2, K_3$ are typically large. We refer to [6] for more details regarding the physics behind the functional in (1.1).

In [5], De Gennes pointed out an analogy between liquid crystals and superconductivity. Guided by this analogy, one might expect to find a surface smectic state for certain values of the various parameters, exactly as one finds a surface superconducting state for type II superconductors. Such a state corresponds to a minimizing/critical configuration $(\psi, n)$ such that $\psi$ is concentrated in a narrow region around the boundary $\partial \Omega$ of the sample, see [26, p.346] and [28, Problem 3.2.4].

This question has been addressed in many papers, see [1, 14, 26] (and the references therein) using techniques developed for the Ginzburg-Landau functional. Loosely speaking, the obtained results for the Landau-de Gennes functional correspond to similar results in superconductivity by understanding the role of $q\tau$ as being the same role played by the intensity of the applied magnetic field in superconductivity (recall that the quantity $q\tau$ involves the chirality constant $\tau$ and the number of smectic layers $q$).

The mathematics behind this is not easy. Using the known techniques from the study of the Ginzburg-Landau functional, we may estimate the energy $G(\psi, n)$ if we know some a priori estimates satisfied by the vector field $n$. In the context of the Ginzburg-Landau functional (as opposed to the Landau-de Gennes functional $E(\psi, n)$) such a priori estimates hold by using PDE techniques, namely the div-curl regularity theorems. This is true since the ‘magnetic energy’ in the Ginzberg-Landau functional is elliptic/coercive, unlike the complicated energy $F_N$ in (1.3). To break this circle, Helffer-Pan [14] dropped the term with the indefinite sign in $F_N$. That can be done either by taking $K_4 = -K_2$ or by imposing a Dirichlet condition on the director field so that the null Lagrangian term is constant. The minimizers of the Landau-de Gennes functional are then analyzed through two successive limits, first a reduced functional is obtained by passing to the limit $\min(K_1, K_2, K_3) \to \infty$, then it is proved that the minimizing order parameter is localized in a thin boundary region by passing to the limit $q \approx \kappa^2$ and $\kappa \to \infty$. Among the results in this paper, we derive additional information about the localization of the minimizing order parameter by passing through one single limit. To do this, we do not drop the null Lagrangian term in order to extract useful estimates about the director field, but we impose a Dirichlet boundary condition. Also, we justify imposing such a Dirichlet boundary condition by proving that it is asymptotically true in a special limit.

The additional estimates we derive allow us to estimate the Ginzburg-Landau energy $G(\psi, n)$ and the concentration of the order parameters using the approach developed recently in [11] for the 3D Ginzburg-Landau functional.

### 1.2 Limiting Dirichlet condition for the director field

Ideally, one would like to minimize the energy in (1.1) without imposing boundary conditions on the configurations $\psi$ and $n$. This leads to the introduction of the following ground state energy,

$$E_{\text{g,s}}^{\text{st}}(\kappa, q, \tau, K_1, K_2, K_3, K_4) = \inf \left\{ E(\psi, n) : (\psi, n) \in H^1(\Omega; \mathbb{C}) \times H^1(\Omega; \mathbb{S}^2) \right\}. \quad (1.6)$$

Notice that the admissible configurations $n$ are constrained, $|n| = 1$. This makes the study of the minimizers more complex. For instance, the Euler-Lagrange equation for the
director field is quite complicated to handle by PDE techniques. The reader is referred to [12, 17, 18, 22] and the references therein for the mathematical analysis on this model, also [29, Sec. 4] for a discussion of the Euler-Lagrange equation for the director fields.

In the mathematical theory of liquid crystals, Dirichlet boundary conditions for \( n \) have been used very often, e.g. [12, 17, 18, 19, 20, 21, 22, 23, 24, 26, 29]. In the physics literature, a boundary condition on the director field models the interaction between the liquid crystal molecules and the molecules near the wall of the container. When the liquid crystal molecules attract the molecules of the container, the director field satisfies the boundary condition \( n \cdot N = 0 \). When the molecules repel each other, the boundary condition becomes \( n \times N = 0 \). Here \( N \) is the unit outward normal vector on the boundary.

In this paper, we will impose a Dirichlet boundary condition on the director field. We will justify imposing such a Dirichlet condition in a specific asymptotic limit (see Theorem 1.3). At the same time, the minimizers obtained under such a Dirichlet condition are still critical points of the functional in (1.1).

We will exhibit an asymptotic limit where we can determine the boundary behavior of the minimizing director field, thereby deriving a limiting form of a Dirichlet boundary condition, that we will impose later in this paper.

The starting point is to find minimizers of the non-negative part of the Oseen-Frank energy, i.e. the functional \( F_N^+ \) in (1.4). Let us introduce the following set,

\[
C(\tau) = \{ n \in H^1(\Omega; S^2) : F_N^+(n) = \min_{u \in H^1(\Omega; S^2)} F_N^+(u) \}.
\]  

In [2], it is proved that:

\[
C(\tau) = \{ n : \text{div } n = 0 \text{ and } \text{curl } n + \tau n = 0 \text{ in } \Omega \} = \{ N_\tau^Q(\cdot) := Q N_\tau(Q^\cdot \cdot) : Q \in SO(3) \},
\]

where

\[
N_\tau(x) = (\cos(\tau x_3), \sin(\tau x_3), 0).
\]

Through (1.9) the set \( C(\tau) \) can be identified with \( SO(3) \), i.e. \( C(\tau) \) is naturally a compact metric space. Hence, continuous functions defined in \( C(\tau) \) have maxima and minima in \( C(\tau) \).

The analysis in this paper is valid when the following two assumptions are satisfied:

**Assumption 1.1.**

1. \( \Omega \subset \mathbb{R}^3 \) is an open domain, \( \partial \Omega \) is \( C^{2,\alpha} \) smooth with \( 0 < \alpha < 1 \), compact and consists of a finite number of connected components.

2. \( M > 1 \) is a constant;

3. \( e(\kappa) \) is a positive function satisfying \( \lim_{\kappa \to \infty} \frac{e(\kappa)}{\kappa^2} = \infty \);

4. \( (\kappa_j, q_j, \tau_j, K_{1,j}, K_{2,j}, K_{3,j}) \) is a sequence in \( \mathbb{R}^6_+ \) such that \( \lim_{j \to \infty} \kappa_j = \infty \) and

\[
\forall j, \quad 0 < e(\kappa_j) \leq \min(K_{1,j}, K_{2,j}, K_{3,j}) \leq \max(K_{1,j}, K_{2,j}, K_{3,j}) \leq Me(\kappa_j).
\]
The Assumption 1.1 is needed for Theorem 1.3 below. For the more detailed convergence results of Theorems 1.4 and 1.6 we will need the additional Assumption 1.2.

**Assumption 1.2.**

1. $b > 1$ and $\tau > 0$ are constants;
2. The function $e(\kappa)$ in Assumption 1.1 satisfies $\lim_{\kappa \to \infty} \frac{e(\kappa)}{\ln \kappa^2 \kappa^3} = \infty$;
3. The sequence in Assumption 1.1 satisfies, for all $j$,
   $$\tau_j = \tau \quad \text{and} \quad q_j \tau = b \kappa_j^2.$$

The asymptotic behavior of the minimizing director fields is contained in:

**Theorem 1.3.** Let $c_2 > c_1 > 0$ be constants. Suppose that Assumption 1.1 is satisfied and $\{K_{ij}\}$ is a sequence in $\mathbb{R}$ satisfying
   $$\forall \ j, \ \ c_1 \kappa_j^3 \leq K_{2,j} + K_{1,j} \leq c_2 \kappa_j^3.$$  

Let $(\psi_j, \mathbf{n}_j)$ be a minimizer of the functional in (1.1) for $(\kappa, q, \tau, K_i) = (\kappa_j, q_j, \tau_j, K_{ij})$. Then there exist $\mathbf{n}_0 \in \mathcal{C}(\tau)$ and a subsequence $\{(\psi_{j_s}, \mathbf{n}_{j_s})\}$ such that, as $s \to \infty$,
   $$\mathbf{n}_{j_s} \to \mathbf{n}_0,$$

where the convergence is in $H^1_{\text{loc}}(\Omega; \mathbb{R}^3) \cap L^p(\Omega; \mathbb{R}^3) \cap W^{1,r}(\Omega; \mathbb{R}^3)$, for all $p \in [1, \infty)$ and $r \in [1, 2)$, and also in $L^r(\partial \Omega; \mathbb{R}^3)$, $1 \leq r < 2$.

Note that Theorem 1.3 adds to the conclusions in [14] since we establish the convergence of $\mathbf{n}_{j_s}$ along the boundary (precisely in the space $W^{1,r}(\Omega; \mathbb{R}^3)$). In [14], the convergence holds in $H^1_{\text{loc}}(\Omega; \mathbb{R}^3)$ and $L^p(\Omega; \mathbb{R}^3)$ only.

### 1.3 Critical points and boundary energy for the director field

In light of Theorem 1.3, we introduce the following admissible class for the director fields,
   $$\mathcal{A} = \{ \mathbf{n} \in H^1(\Omega; \mathbb{S}^2) : \exists \mathbf{n}_0 \in \mathcal{C}(\tau) \text{ such that } \mathbf{n} = \mathbf{n}_0 \text{ on } \partial \Omega \}.$$  

(1.11)

If $\mathbf{n} \in \mathcal{A}$, then $\mathcal{L}(\mathbf{n}) = \mathcal{L}(\mathbf{n}_0) = 0$ by (1.9). Thus, for every $(\psi, \mathbf{n}) \in H^1(\Omega; \mathbb{C}) \times \mathcal{A}$, the expression of the functional in (1.1) simplifies to
   $$\mathcal{E}(\psi, \mathbf{n}) = \mathcal{G}(\psi, \mathbf{n}) + \mathcal{F}_N(\mathbf{n}).$$

(1.12)

Now, we introduce the ground state energy,
   $$\mathcal{E}^{\text{st}}(\kappa, q, \tau, K_1, K_2, K_3) = \inf \{ \mathcal{E}(\psi, \mathbf{n}) : (\psi, \mathbf{n}) \in H^1(\Omega; \mathbb{C}) \times \mathcal{A} \}.$$  

(1.13)

In light of (1.12), the ground state energy $\mathcal{E}^{\text{st}}(\kappa, q, \tau, K_1, K_2, K_3)$ is independent of the coefficient $K_4$. A minimizer $(\psi, \mathbf{n})$ of (1.13) is a critical point of the Landau-de Gennes functional in the following sense:

$$\forall (\phi, \mathbf{w}) \in H^1(\Omega; \mathbb{C}) \times C^\infty(\Omega; \mathbb{R}^3),$$

$$\frac{d}{dt} \mathcal{E}(\psi + t\phi, \mathbf{n}) \big|_{t=0} = 0 \quad \text{and} \quad \frac{d}{dt} \mathcal{E}(\psi, \frac{\mathbf{n} + tw}{|\mathbf{n} + tw|}) \big|_{t=0} = 0.$$

Through the analysis in this paper, we will describe the asymptotic behavior of the ground state energy in (1.13) and its minimizers. Also, we will derive a boundary energy that might hint at the expected profile of the director field of a minimizer.
1.3.1 The boundary energy

The definition of the boundary energy involves many implicit quantities as well as the geometry of the boundary of the domain \( \Omega \). The starting point is a local boundary energy function, which was constructed in [11]. We will recall this construction in Section 3.3 below. Here we just introduce the notation and some basic properties.

For \( b \in (0, 1] \) and \( \nu \in [0, \pi/2] \), let \( E(b, \nu) \) be the quantity defined by (3.10) below. Then \( E(b, \nu) \) is a continuous function of \( (b, \nu) \). In the later use in the paper we have \( b = 1/b \), with \( b \) the constant from Assumption 1.1.

Now we can give the definition of the boundary energy for the direct or field. Let \( n \in C(\tau) \). If \( x \in \partial \Omega \), denote by \( \nu(x; n) \) the angle in \( [0, \pi/2] \) between \( \text{curl} \ n \) (which is equal to \( -\tau n \)) and the tangent plane to \( \partial \Omega \) at \( x \).

Define,

\[
\tilde{E}(b, n) = \int_{\partial \Omega} E(b, \nu(x; n)) \, ds(x),
\]

\[
e_0(b, \tau) = \inf_{n \in C(\tau)} \tilde{E}(b, n),
\]

where \( E(b, \nu) \) is defined in (3.10). Clearly, a minimizer of \( \tilde{E}(b, n) \) in \( C(\tau) \) exists (by continuity and compactness). We therefore introduce

\[
M = M(b, \tau) = \{ \ n \in C(\tau) : \tilde{E}(b, n) = e_0(b, \tau) \}.
\]

The vector fields in \( M \) are determined by the boundary geometry of the domain \( \Omega \). If \( \Omega \) is a ball, then it is invariant by rotation and therefore \( M = C(\tau) \). For general domains, e.g. an ellipsoid, the set of minimizers \( M \) is expected to be a proper subset of \( C(\tau) \). To determine this set is an interesting question. One would expect that ‘generically’, \( M \) consists of a single vector field.

The boundary energy \( e_0(b, \tau) \) might help to determine the behavior of the minimizing director field. If we come back to the content of Theorem 1.3, we find that a sequence of minimizing director fields converges to a vector field \( n_0 \in C(\tau) \). We will localize \( n_0 \) further by proving that \( n_0 \in M \). However, the study of the minimizers of the boundary energy seems complicated, since this energy is defined by implicit quantities.

1.3.2 Concentration of the order parameter

We present here one among the main results proved in this paper. It adds over the results of Helffer-Pan [14] a new formula for the concentration of the minimizing order parameter valid by passing through a single limit (in [14], the concentration is obtained through two successive limits). The starting point is a leading order estimate of the ground state energy.

**Theorem 1.4.** Let \( \tau > 0 \) and \( b > 1 \) be fixed constants and suppose that the conditions in Assumptions 1.1 and 1.2 are satisfied. As \( \kappa_j \to \infty \), the ground state energy in (1.13) satisfies,

\[
\mathcal{E}^\text{st}(\kappa_j, q_j, \tau, K_{1,j}, K_{2,j}, K_{3,j}) = \sqrt{b} \kappa_j e_0\left(\frac{1}{b} \tau\right) + o(\kappa_j),
\]

where \( e_0 \) is defined in (1.15).
The conclusion in Theorem 1.4 shows that the boundary is dominant in the description of $E_{\text{st}}(\kappa_j, q_j, \tau, K_{1,j}, K_{2,j}, K_{3,j})$. In Theorem 1.6 below, we will be more specific regarding the localization near the boundary. In particular, previous results (e.g. [1]) only proved decay of $\psi$ outside a certain ‘allowed’ boundary region. We provide confirmation that $\psi$ is indeed not small in this boundary region.

The statement of Theorem 1.6 below involves a certain class of sub-domains in $\Omega$ that we will call regular domains.

**Definition 1.5.** Let $D \subset \Omega$. We say that $D$ is regular if

1. $D = \tilde{D} \cap \Omega$ where $\tilde{D} \subset \mathbb{R}^3$ is open and has a smooth boundary;
2. If $\tilde{D} \cap \partial \Omega \neq \emptyset$, then it consists of a finite number of connected components;
3. Every connected component of $\tilde{D} \cap \partial \Omega$ is either
   (a) a smooth surface without boundary; or
   (b) a smooth surface with boundary consisting of a finite number of disjoint smooth curves;
4. $\partial \tilde{D}$ intersect $\partial \Omega$ transversally, i.e. the unit normal vectors $N_{\partial \tilde{D}}$ and $N_{\partial \Omega}$ satisfy $N_{\partial \tilde{D}} \times N_{\partial \Omega} \neq 0$.

The assumptions we made on the domain $\Omega$ assert that it is a regular domain. The exterior (in $\Omega$) of a regular domain is a regular domain too (i.e. if $D$ is regular, then $\Omega \setminus D$ is regular). If $B$ is an open ball in $\mathbb{R}^3$ such that $\overline{B} \subset \Omega$ then $B$ is a regular domain. If $\partial \Omega$ is smooth, and if the center of $B$ lies on $\partial \Omega$ and the radius of $B$ is sufficiently small, then the domain $B \cap \Omega$ is another example of a regular domain. Another example of a regular domain is the tubular neighborhood of the boundary of $\Omega$, i.e. $D = \{x \in \Omega : \text{dist}(x, \partial \Omega) < t\}$ where $t > 0$ is sufficiently small.

The results here are valid under the hypotheses in Assumption 1.2. We shall examine the behavior of the minimizers of (1.13) for large $\kappa$, hence $q_{\tau} = b\kappa^2$ increases, and the elastic coefficients $K_1, K_2, K_3$ behave as $e(\kappa) \gg \kappa^3|\ln \kappa|^2$ by the conditions above.

**Theorem 1.6.** Under the conditions of Assumptions 1.1 and 1.2, let $(\psi_j, n_j)$ be a minimizer of the energy in (1.13) for $(\kappa, q, \tau, K_i) = (\kappa_j, q_j, \tau, K_{i,j})$. Then there exists a subsequence $\{(\psi_{j_s}, n_{j_s})\}$ and $n_0 \in \mathcal{M}$ such that, as $s \to \infty$:

1. $n_{j_s} \to n_0$ in $H_{loc}^1(\partial \Omega, \mathbb{R}^3)$ and in every $W^{1,r}(\Omega, \mathbb{R}^3)$ and $L^p(\Omega, \mathbb{R}^3)$, $1 \leq r < 2$ and $2 \leq p < \infty$;
2. The Oseen-Frank energy in (1.4) satisfies,
   $$\mathcal{F}_N^+(n_{j_s}) = o(\kappa_{j_s}).$$
3. If $D \subset \Omega$ is a regular domain, then
   $$\int_D \left\{ |(\nabla - iq_j, \tau n_j)\psi_{j_s}|^2 - \kappa_{j_s}^2|\psi_{j_s}|^2 + \frac{\kappa_{j_s}^2}{2}|\psi_{j_s}|^4 \right\} dx$$
   $$= \sqrt{b}\kappa_{j_s} \int_{D \cap \partial \Omega} E\left(\frac{1}{b}, \nu(x, n_0)\right) ds(x) + o(\kappa_{j_s}), \quad (1.17)$$
where \( E(\cdot, \cdot) \) is defined in (3.10) and \( \nu(x, n_j) \) is the angle in \([0, \pi/2]\) between \( n_j \) and the tangent plane to \( \partial \Omega \) at \( x \).

4. The subsequence \( \{ \psi_j \} \) has the following concentration behavior

\[
\kappa_j |\psi_j|^4 dx \to -2\sqrt{b} E\left(\frac{1}{b}, \nu(x; n_0) \right) ds(x),
\]

which holds in the following sense: If \( D \subset \Omega \) is a regular domain, then

\[
\kappa_j \int_D |\psi_j|^4 dx \to -2\sqrt{b} \int_{\partial D \cap \partial \Omega} E\left(\frac{1}{b}, \nu(x; n_0) \right) ds(x), \tag{1.18}
\]

where \( dx \) is the Lebesgue measure in \( \Omega \), \( ds(x) \) is the surface measure in \( \partial \Omega \), and \( E(\cdot, \cdot) \) is defined in (3.10).

Notice that if \( \mathcal{M} = \{n_0\} \), i.e. if \( \mathcal{M} \) consists of a single field, then there is no need to extract a subsequence.

**Remark 1.7.** Theorem 1.6 indicates that as long as Assumptions 1.1 and 1.2 are satisfied, then as \( \kappa \to \infty \), the order parameter concentrates at the boundary. More precisely, using Remark 3.3 below where the spectral function \( \zeta(\nu) \) is introduced, we see that since \( E\left(\frac{1}{b}, \nu \right) \) vanishes when \( \zeta(\nu) \geq \frac{1}{b} \), we have the following conclusion:

(i) If \( b \geq \frac{1}{\Theta_0} \), then for any \( x \in \partial \Omega \) we have \( \zeta(\nu(x; n_0)) \geq \Theta_0 \geq \frac{1}{b} \), hence

\[
E\left(\frac{1}{b}, \nu(x, n_0) \right) = 0 \quad \text{for any } x \in \partial \Omega.
\]

Therefore, from (1.18) we see that the order parameters \( \psi \) are uniformly small in the sense that for any regular subdomain \( D \)

\[
\int_D |\psi|^4 dx = o(\kappa^{-1}).
\]

This suggests that when \( \kappa \) is large and \( q \tau/\kappa^2 \) is above the critical value \( 1/\Theta_0 \) and kept away from it, the whole liquid crystal sample is in the nematic state.

(ii) If \( 1 < b < \frac{1}{\Theta_0} \), then

\[
E\left(\frac{1}{b}, \nu(x, n_0) \right) < 0 \quad \text{if } \zeta(\nu(x; n_0)) < \frac{1}{b}.
\]

From Theorem 1.6, for \( q \tau = b\kappa^2 \), the order parameter \( \psi \) is localized near the following region:

\[
S_b(n_0) = \left\{ x \in \partial \Omega : \zeta(\nu(x; n_0)) < \frac{1}{b} \right\}, \tag{1.19}
\]

which is a proper subset of \( \partial \Omega \). This suggests that when \( \kappa \) is large and \( q \tau/\kappa^2 \) lies between but away from 1 and \( 1/\Theta_0 \), the liquid crystal is in the surface smectic state, and the surface portion near \( S_b(n_0) \) is in the smectic state, and all the other part of the sample is in the nematic state.
(iii) If $b$ decreases and reaches 1, then $S_b(n_0)$ expands and covers the whole boundary, thus the smectic layer expands and eventually covers the whole surface.

(iv) We expect that when $q\tau = b\kappa^2$ with $0 < b < 1$ then the whole sample is in the smectic state.

The above remark indicates the analogy between the surface superconducting state of type II superconductors (see [25, Theorem 1 and Remark 1.2] and [27, Theorem 2 and Remark 1.2]) and the surface smectic state of liquid crystals. Also, the claim in (iv) is reminiscent of bulk superconductivity in 3D samples [10].

In [14], it is proved that the order parameter decays exponentially fast away from the boundary region $S_b(n_0)$ in (1.19), but (unlike the formula in (1.18)) it is not proved that the order parameter is not small everywhere in $S_b(n_0)$. The result in [14] is valid in the framework of two successive limits. What we prove here is valid in a single limit and yields that the concentration set of the order parameter is exactly the region $S_b(n_0)$.

### 1.4 Behavior of the ground state energy

Here we indicate how our methods improve some of the results of Helffer-Pan [14]. Also, we discuss a possible method for localizing the director field of a minimizing configuration.

We will analyze two successive limits as done by Helffer-Pan in [14]. The analysis here is valid under the assumption that $K_4 = -K_2$ in (1.3) so that the term with indefinite sign is dropped from the Oseen-Frank energy. That is the assumption considered in [14].

The results here will highlight the importance of the boundary energy in (1.15) and are consistent with the contents of Theorems 1.3 and 1.6. The domain $\Omega$ is again supposed bounded, open and regular (see Definition 1.5).

**Theorem 1.8.** Let $b > 1$ and $\tau > 0$ be fixed constants. Suppose that $K_4 = -K_2$ and $q\tau = b\kappa^2$. The ground state energy in (1.13) satisfies,

$$\lim_{\kappa \to \infty} \left[ \lim_{\min(K_1,K_2,K_3) \to \infty} \frac{E^{\text{st}}(\kappa, q, \tau, K_1, K_2, K_3)}{\sqrt{q\tau}} \right] = c_0 \left( \frac{1}{b}, \tau \right),$$

where $c_0\left(\frac{1}{b}, \tau\right)$ is introduced in (1.15).

We stress again that in the limit (1.20), as $\kappa \to \infty$, $q\tau = b\kappa^2$ also goes to $\infty$.

The relevance of the calculation of the limit in (1.20) is more apparent in light of a result by Helffer-Pan [14] that we discuss below.

In [14], it is proved that, as $\min(K_1, K_2, K_3) \to \infty$, the ground state energy

$$E^{\text{st}}(\kappa, q, \tau, K_1, K_2, K_3)$$

converges to the ground state energy of a reduced functional. The reduced functional is defined over configurations in the space $H^1(\Omega; \mathbb{C}) \times C(\tau)$. Furthermore, if $(\psi, n)$ is a minimizer achieving $E^{\text{st}}(\kappa, q, \tau, K_1, K_2, K_3)$, then as $\min(K_1, K_2, K_3) \to \infty$ along a subsequence, the minimizer $(\psi, n)$ converges to $(\psi_0, n_0)$ where $(\psi_0, n_0)$ minimizes the reduced functional. In the specific regime

$$q\tau = b\kappa^2, \quad \Theta_0 < \frac{1}{b} < 1, \quad \text{and} \quad \kappa \to \infty,$$
it is proved that \( \psi_0 \) is localized near the boundary of \( \Omega \) and is exponentially small away from the boundary region \( S_0(\mathbf{n}_0) \) in (1.19). However, the localization of the field \( \mathbf{n}_0 \) is left open. As a byproduct of the proof of Theorem 1.8, we get that \( \mathbf{n}_0 \) is a minimizer of the boundary energy in (1.15).

The results in this paper suggest the following question: Study the minimizers of \( \tilde{E}[\mathbf{b}, \cdot] \) and study the geometric meaning of the minimizers.

## 2 Behavior of the director field

The aim of this section is to prove Theorem 1.3. This is based on the result of the following lemma:

**Lemma 2.1.** Let \( C > 0 \) be a constant and let \( r(\kappa) : \mathbb{R}_+ \to \mathbb{R}_+ \) be a function satisfying \( \lim_{\kappa \to \infty} r(\kappa) = 0 \). Suppose that \( \{ \kappa_j \} \) is a sequence such that \( \kappa_j \to \infty \) and that \( \{ \mathbf{n}_j \} \) is a sequence in \( H^1(\Omega; \mathbb{S}^2) \) satisfying the following estimates,

\[
\| \text{div} \mathbf{n}_j \|_2 + \| \text{curl} \mathbf{n}_j + \tau \mathbf{n}_j \|_2 \leq r(\kappa_j), \quad \text{and} \quad \| \nabla \mathbf{n}_j \|_2 \leq C. \tag{2.1}
\]

Then there exist a subsequence \( \{ (\psi_{j_s}, \mathbf{n}_{j_s}) \} \) and a vector field \( \mathbf{n}_0 \) in the set \( C(\tau) \) introduced in (1.7) such that, as \( s \to \infty \),

\[
\begin{align*}
\mathbf{n}_{j_s} & \to \mathbf{n}_0 \quad \text{in} \quad H^1_{\text{loc}}(\Omega; \mathbb{R}^3), \\
\mathbf{n}_{j_s} & \to \mathbf{n}_0 \quad \text{in} \quad L^p(\Omega; \mathbb{R}^3), \quad 1 \leq p < \infty, \\
\mathbf{n}_{j_s} & \to \mathbf{n}_0 \quad \text{in} \quad W^{1,\tau}(\Omega; \mathbb{R}^3), \quad 1 \leq \tau < 2.
\end{align*}
\]

**Proof.** The proof is similar to that of Theorem 1.1 in [14]. We have from (2.1) and the fact that \( \mathbf{n} \) takes values in \( \mathbb{S}^2 \) that \( \{ \mathbf{n}_j \} \) is bounded in \( H^1(\Omega; \mathbb{R}^3) \), hence there exists a subsequence \( \{ j_s \} \) such that \( \mathbf{n}_{j_s} \) converges weakly to a vector field \( \mathbf{n}_0 \) in \( H^1(\Omega; \mathbb{R}^3) \). By the compact embedding of \( H^1(\Omega; \mathbb{R}^3) \) into \( L^p(\Omega; \mathbb{R}^3) \), \( 2 \leq p \leq 6 \), the convergence is strong in these \( L^p(\Omega; \mathbb{R}^3) \). Passing to a further subsequence, the convergence holds a.e. in \( \Omega \), hence \( \mathbf{n}_0 \) inherits from \( \mathbf{n}_{j_s} \) the constraint \( |\mathbf{n}_0| = 1 \) a.e. in \( \Omega \). By the uniform boundedness in \( L^\infty \) and the convergence in \( L^2(\Omega) \) (and the finiteness of the volume of \( \Omega \) when \( 1 \leq p < 2 \)), we get the convergence in \( L^p \) for all \( 1 \leq p < \infty \) from the Hölder inequality.

By (2.1), \( \| \text{div} \mathbf{n}_{j_s} \|_2 \to 0 \) and \( \| \text{curl} \mathbf{n}_{j_s} + \tau \mathbf{n}_{j_s} \|_2 \to 0 \). Hence

\[
\text{div} \mathbf{n}_0 = 0 \quad \text{and} \quad \text{curl} \mathbf{n}_0 + \tau \mathbf{n}_0 = 0 \quad \text{in} \quad \Omega.
\]

We conclude that \( \mathbf{n}_0 \in C(\tau) \).

Next we prove that \( \mathbf{n}_{j_s} \to \mathbf{n}_0 \) in \( H^1_{\text{loc}}(\Omega; \mathbb{R}^3) \) as \( s \to \infty \). Let \( D \) be an open set such that \( \overline{D} \subset \Omega \). Using local elliptic regularity of the curl-div system (the inequality (A.1) in [14]), we may write,

\[
\| \mathbf{n}_{j_s} - \mathbf{n}_0 \|_{H^1(D)} \leq C(D, \Omega) \left\{ \| \text{div} (\mathbf{n}_{j_s} - \mathbf{n}_0) \|_{L^2(\Omega)} + \| \text{curl} (\mathbf{n}_{j_s} - \mathbf{n}_0) \|_{L^2(\Omega)} + \| \mathbf{n}_{j_s} - \mathbf{n}_0 \|_{L^2(\Omega)} \right\}, \tag{2.2}
\]

where \( C(D, \Omega) \) solely depends on the domains \( D \) and \( \Omega \). The convergence follows in light of the convergence in \( L^2(\Omega; \mathbb{R}^3) \) and the inequality (2.1).
To finish the proof of Lemma 2.1, we need to prove that \( n_j \rightarrow n_0 \) as \( s \rightarrow \infty \) in \( W^{1,r}(\Omega, \mathbb{R}^3) \) for any \( 1 \leq r < 2 \). By the convergence established in \( L^r(\Omega, \mathbb{R}^3) \), we need only prove the convergence of \( Dn_j \) in \( L^r(\Omega, \mathbb{R}^3) \). Let \( \varepsilon_0 > 0 \), \( 0 < \varepsilon < \varepsilon_0 \) and

\[
\Omega_\varepsilon = \{ x \in \Omega : \text{dist}(x, \partial \Omega) > \varepsilon \}.
\]

We may select \( \varepsilon_0 \) sufficiently small such that, for all \( \varepsilon \in (0, \varepsilon_0) \), \( \Omega_\varepsilon \) is a non-empty open set. Smoothness of the boundary of \( \Omega \) ensures that,

\[
|\Omega \setminus \Omega_\varepsilon| = O(\varepsilon), \quad (\varepsilon \rightarrow 0_+).
\]

Now, since \( n_j \) is bounded in \( H^1(\Omega, \mathbb{R}^3) \), there exists \( C > 0 \) such that, for all \( \varepsilon \in (0, \varepsilon_0) \),

\[
\int_{\Omega_\varepsilon} |Dn_j - Dn_0|^r \, dx \leq C \varepsilon^{(2-r)/2}.
\]

By Hölder’s inequality and the local \( H^1 \)–convergence, for all \( \varepsilon \in (0, \varepsilon_0) \),

\[
\int_{\Omega_\varepsilon} |Dn_j - Dn_0|^r \, dx \leq C \varepsilon \| n_j - n_0 \|_{H^1(\Omega_\varepsilon)}^r \rightarrow 0 \quad \text{as} \quad s \rightarrow \infty. \tag{2.3}
\]

Thus, by taking the two successive limits, \( s \rightarrow \infty \) and then \( \varepsilon \rightarrow 0_+ \), we get that,

\[
\limsup_{s \rightarrow \infty} \int_{\Omega} |Dn_j - Dn_0|^r \, dx \leq 0.
\]

\[\square\]

**Lemma 2.2.** Let \( \tau > 0 \). If \( n \in H^1(\Omega; \mathbb{S}^2) \), then with \( F_N^+(n) \) from (1.4),

\[
F_N^+(n) \geq \min(K_1, K_2, K_3) \int_{\Omega} \left\{ |\text{div} \, n|^2 + |\text{curl} \, n + \tau n|^2 \right\} dx,
\]

and

\[
\int_{\Omega} \left\{ |\text{tr}(Dn)|^2 - |\text{div} \, n|^2 \right\} dx \geq \int_{\Omega} \left\{ |Dn|^2 - |\text{div} \, n|^2 \right\} dx - 2 \int_{\Omega} |\text{curl} \, n + \tau n|^2 \, dx - 2|\Omega|\tau^2.
\]

**Proof.** This follows from the following three pointwise identities:

\[
|\text{curl} \, n + \tau n|^2 = |(\text{curl} \, n) \cdot n + \tau|^2 + |(\text{curl} \, n) \times n|^2,
\]

\[
\text{tr}(Dn)^2 = |Dn|^2 - |\text{curl} \, n|^2,
\]

\[
|\text{curl} \, n|^2 = |\text{curl} \, n + \tau n|^2 + \tau^2 - 2\tau \cdot (\text{curl} \, n + \tau n) \leq 2|\text{curl} \, n + \tau n|^2 + 2\tau^2.
\]

\[\square\]

**Proposition 2.3.** Let \( c_2 > c_1 > 0 \) be constants. Suppose that the Assumption 1.1 is satisfied and

\[
c_1 \kappa \leq K_2 + K_4 \leq c_2 \kappa^2.
\]

Then there exist constants \( \kappa_0 > 0 \), \( q > 0 \), \( \tau > 0 \) and \( C > 0 \) such that, if \( \kappa \geq \kappa_0 \) and (\( \psi, n \)) is a minimizer of the functional in (1.1), then

\[
\| \text{div} \, n \|_2 + \| \text{curl} \, n + \tau n \|_2 \leq \sqrt{\frac{C\kappa^2}{2c(\kappa)}} \quad \text{and} \quad \| Dn \|_2 \leq C\tau. \tag{2.4}
\]
Proof. Notice that Lemma 2.2 provides us with a lower bound of the energies $F_N(n)$ and $L(n)$ introduced in (1.4) and (1.5) respectively. With this lower bound, the assumptions on the $K_i$, and the assumption on $e(\kappa) \gg \kappa^2$, we can estimate the energy in (1.3) for large values of $\kappa$ as follows,

$$F_N(n) \geq e(\kappa) \int_{\Omega} |\text{div} n|^2 + |\text{curl} n + \tau n|^2 dx + c_1 \kappa^2 \int_{\Omega} |Dn|^2 dx - 2c_2 |\tau|^2 \kappa^2.$$  \hspace{1cm} (2.5)

Next, by writing

$$-|\psi|^2 + \frac{1}{2} |\psi|^4 = \frac{1}{2} (1 - |\psi|^2)^2 - \frac{1}{2} \geq -\frac{1}{2},$$

we observe that the energy in (1.2) can be estimated from below as follows,

$$G(\psi, n) \geq -\frac{|\Omega|}{2} \kappa^2.$$  \hspace{1cm} (2.6)

Now we insert the estimates in (2.5) and (2.6) into (1.1) to obtain,

$$E(\psi, n) \geq e(\kappa) \int_{\Omega} |\text{div} n|^2 + |\text{curl} n + \tau n|^2 dx + c_1 \kappa^2 \int_{\Omega} |Dn|^2 dx - c_2' \kappa^2,$$ \hspace{1cm} (2.7)

where $c_2' = |\Omega|/2 + 2c_2 |\tau|^2 |\Omega|$.

Let $n_\tau \in C(\tau)$ and let $(\psi, n)$ be a minimizer of the functional in (1.1). We have $E(\psi, n) \leq E(0, n_\tau) = 0$. Thus, we infer the inequalities of (2.4) from (2.7).

$\square$

Proof of Theorem 1.3. By Assumption 1.1, we know that $\lim_{\kappa \to \infty} \kappa^2/e(\kappa) = 0$. Theorem 1.3 therefore follows from Proposition 2.3 and Lemma 2.1. $\square$

3 Preliminaries

3.1 An $L^\infty$ bound for order parameters

Let $(\psi, n)$ be a minimizer of the energy $E(\psi, n)$ in (1.1). Writing the Euler-Lagrange equation for $E(\psi, n)$, we find that the function $\psi$ is a weak solution\(^1\) of

$$\begin{cases} -\nabla_{qn}^2 \psi = \kappa^2 (1 - |\psi|^2) \psi & \text{in } \Omega, \\ N \cdot \nabla_{qn} \psi = 0 & \text{on } \partial \Omega, \end{cases}$$ \hspace{1cm} (3.1)

where $N$ is the interior unit normal vector on $\partial \Omega$. Repeating the argument in [7], we get the following uniform bound.

**Lemma 3.1.** Suppose that $n \in H^1(\Omega; \mathbb{S}^2)$ and $\psi$ is a weak solution of (3.1). Then,

$$\|\psi\|_\infty \leq 1.$$ \hspace{1cm} (3.2)

---

\(^1\)Here we have omitted the equation and boundary condition for $n$. 

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13
3.2 A spectral estimate

We will need the following well-known estimate in (3.3). It follows, for instance, from the min-max principle and the fact that, if \( B = \text{curl} \ A \) is a non-zero constant vector, then the spectrum of the magnetic Laplacian

\[
-(\nabla - iA)^2 \quad \text{in} \quad L^2(\mathbb{R}^3)
\]
is the whole interval \([|B|, \infty)\).

**Lemma 3.2.** Let \( A \) be a vector potential with \( B = \text{curl} \ A \) constant in \( \mathbb{R}^3 \). Let \( u \in L^2(\mathbb{R}^3) \) with \( (\nabla - iA)u \in L^2(\mathbb{R}^3) \). Then

\[
\int_{\mathbb{R}^3} |(\nabla - iA)u|^2 \, dx \geq |B| \int_{\mathbb{R}^3} |u|^2 \, dx,
\]  

(3.3)

3.3 Reduced Ginzburg-Landau energy

Here we recall the definition of the boundary energy \( E(b, \nu) \). This energy was constructed in [11] as the limit of a specific reduced Ginzburg-Landau energy.

Let \( \nu \in [0, \pi/2] \) and \( A_\nu \) be the magnetic potential

\[
A_\nu(x) = (0, 0, x_1 \cos \nu + x_2 \sin \nu), \quad x = (x_1, x_2, x_3) \in \mathbb{R}^3.
\]  

(3.4)

Clearly, the (un-oriented) angle between the vector \( \text{curl} A_\nu = (\sin \nu, -\cos \nu, 0) \) and the plane \( \{x_1 = 0\} \) is \( \nu \) (hence the geometry of the flat boundary of the half space is involved).

For each \( \ell > 0 \), we introduce the domains,

\[
K_\ell = (-\ell, \ell) \times (-\ell, \ell), \quad U_\ell = (0, \infty) \times K_\ell,
\]  

(3.5)

and the space,

\[
S_\ell = \{ u \in L^2(U_\ell, \mathbb{C}) : (\nabla - iA_\nu)u \in L^2(U_\ell, \mathbb{C}^3), \ u = 0 \ on \ (0, \infty) \times \partial K_\ell \}.
\]  

(3.6)

Let \( b \in (0, 1] \) be a given constant—in the later use in the paper we have \( b = 1/b \), with \( b \) the constant from Assumption 1.1 i.e., \( b \) is the ratio of \( \kappa^2 \) to the magnitude of the magnetic field. If \( u \in S_\ell \), we define the reduced Ginzburg-Landau functional,

\[
G_{b,\nu;\ell}(u) = \int_{U_\ell} \left\{|(\nabla - iA_\nu)u|^2 - b|u|^2 + \frac{b}{2}|u|^4\right\} \, dx.
\]  

(3.7)

Associated with \( G_{b,\nu;\ell} \) is the ground state energy,

\[
d(b, \nu; \ell) = \inf_{u \in S_\ell} G_{b,\nu;\ell}(u).
\]  

(3.8)

From [11, Theorem 3.6] we know that a minimizer \( u \) of \( G_{b,\nu;\ell} \) exists and that it satisfies the decay estimate\(^2\), which we recall for later use,

\[
\int_{U_\ell} x_1^p |u(x)|^2 \, dx \leq C_p \ell^2,
\]  

(3.9)

\(^2\)For \( b < 1 \) exponential decay estimates would be possible, but for \( b = 1 \) only weak decay is expected.
for all $0 < p < 1$. In [11], it is proved that the limit of $d(b, \nu; \ell) / \ell^2$ exists (and is finite) as $\ell \to \infty$. Thus we define,

$$E(b, \nu) = \lim_{\ell \to \infty} \frac{d(b, \nu; \ell)}{(2\ell)^2}. \quad (3.10)$$

An explicit formula for $E(b, \nu)$ is not available, but we know the following facts outlined in Remark 3.3 below (see [11]):

**Remark 3.3.**

- $E(b, \nu)$ is a continuous function of $(b, \nu) \in (0, 1] \times [0, \pi/2]$.
- Let $\zeta(\nu)$ be the lowest eigenvalue of the Schrödinger operator in the half-plane

$$\mathcal{P}_\nu = -(\nabla - iF_{\nu})^2 \quad \text{in } L^2(\mathbb{R}_+ \times \mathbb{R}, \mathbb{C}),$$

where

$$F_{\nu}(x) = (0, x_1 \cos \nu + x_2 \sin \nu).$$

Let $\zeta(0) := \Theta_0$. It is known that $\Theta_0 \sim 0.59$ and that $\zeta : [0, \pi/2] \to [\Theta_0, 1]$ is a continuous and increasing bijection. Furthermore, $E(b, \nu)$ vanishes when $\zeta(\nu) \geq b$ and $E(b, \nu) < 0$ otherwise. In particular, $E(\Theta_0, \nu) = 0$ for all $\nu \in [0, \pi/2]$.

- There exist two constants $\ell_0 > 0$ and $C > 0$ such that, for all $\nu \in [0, \pi/2]$, $b \in (0, 1]$ and $\ell \geq \ell_0$,

$$\frac{d(b, \nu; \ell)}{\ell^2} \leq E(b, \nu) \leq \frac{d(b, \nu; \ell)}{\ell^2} + \frac{C}{\ell^{2/3}}. \quad (3.11)$$

### 3.4 Boundary coordinates

In order to analyze the influence of the boundary of the domain $\Omega$ on various quantities, we will carry out the computations in adapted coordinates near the boundary—we will call these coordinates **boundary coordinates**. The specific choice of coordinates has been used in several contexts. In [15] and then in [29], the boundary coordinates are used to estimate the ground state energy of a magnetic Schrödinger operator with large magnetic field (or with small semi-classical parameter). In [11], the boundary coordinates were useful in the computation of the ground state energy of the three dimensional Ginzburg-Landau functional. Here, we will use these coordinates in the same manner as in [11].

Since the boundary $\partial \Omega$ is $C^{2,\alpha}$-smooth, for every point $p \in \partial \Omega$, there exist a neighborhood $\tilde{V}_p \subset \mathbb{R}^3$ of $p$, an open set $\tilde{U}_p$ in $\mathbb{R}^2$ and a $C^{2,\alpha}$-diffeomorphism

$$\tilde{\phi}_p : \tilde{V}_p \cap \partial \Omega \to \tilde{U}_p. \quad (3.12)$$

Furthermore, there exists a $C^{1,\alpha}$ smooth, unit inward pointing normal vector field $N : \partial \Omega \to \mathbb{R}^3$.

This allows us to define,

$$\tilde{\Phi}_p^{-1} : (-\epsilon_p, \epsilon_p) \times \tilde{U}_p \to \mathbb{R}^3,$$

$$(y_1, y_2, y_3) \mapsto \tilde{\phi}_p^{-1}(y_2, y_3) + y_1N(\tilde{\phi}_p^{-1}(y_2, y_3)).$$
For $\epsilon_p$ sufficiently small, $\tilde{\Phi}_p^{-1}$ is a diffeomorphism on its image. Furthermore, we may assume that (after possibly scaling $\tilde{\phi}_p$ and shrinking $\tilde{V}_p$)

$$\frac{1}{2} \leq |D\tilde{\Phi}_p^{-1}(y)| \leq \frac{3}{2}, \quad \forall y \in (-\epsilon_p, \epsilon_p) \times \tilde{U}_p,$$

and that $\tilde{\Phi}_p^{-1}((-\epsilon_p, \epsilon_p) \times \tilde{U}_p) = \tilde{V}_p$.

Clearly, the family $\{\tilde{V}_p : p \in \partial \Omega\}$ is an open cover of $\partial \Omega$. By compactness of $\partial \Omega$, we may extract a finite subcover $\{\tilde{V}_p_i\}_{i=1}^n$ such that

$$\partial \Omega \subset \bigcup_{i=1}^n \tilde{V}_{p_i}.$$  \hspace{1cm} (3.14)

In particular, we may assume that $\epsilon_{p_i} \equiv \epsilon > 0$ is independent of $i$. The collection $(\tilde{V}_{p_i}, \tilde{\phi}_{p_i})_{i=1}^n$ will be fixed once and for all. In particular, it does not depend on the various parameters $(\kappa, \tau, \ldots)$ of our problem. Of course, there is considerable freedom in this choice, but that is not important for our purpose. Different choices can possibly lead to different constants in our error bounds but not affect the overall results.

For convenience in the later use of the coordinates, we proceed to define such boundary coordinates centered around an arbitrary boundary point $x_0$ which might not be one of the $p_i$’s.

Consider a point $x_0 \in \partial \Omega$. There exists $p_i$ such that $x_0 \in \tilde{V}_{p_i}$. Let $V_{x_0}$ be a neighborhood of $x_0$ such that $V_{x_0} \subset \tilde{V}_{p_i}$. Let

$$U_{x_0} := \tilde{\phi}_{p_i}(V_{x_0} \cap \partial \Omega) \quad \text{and} \quad \phi_{x_0} := \tilde{\phi}_{p_i} \big|_{V_{x_0} \cap \partial \Omega}.$$  \hspace{1cm} (3.17)

Clearly, $\phi_{x_0}$ is a diffeomorphism defining local boundary coordinates $(y_2, y_3)$ in

$$W_{x_0} = V_{x_0} \cap \partial \Omega$$

through the relation $\phi_{x_0}(x) = (y_2, y_3)$. After possibly performing a translation and a rotation (notice that this does not affect (3.13)), we may suppose that $0 \in U_{x_0}$, $\phi_{x_0}(x_0) = 0$ and that $N(x_0) = (1, 0, 0)$. We may modify $\phi_{x_0}$ further so that,

$$D\phi_{x_0}(x_0) = I_2,$$  \hspace{1cm} (3.15)

where $I_2$ is the $2 \times 2$ identity matrix—namely (3.15) holds after we replace the map $\phi_{x_0}(x)$ by

$$\phi_{x_0}^{\text{new}}(x) = (D\phi_{x_0}(x_0))^{-1}\phi_{x_0}(x).$$

Notice that, by the choice of $\tilde{\phi}_{p_i}$, we have

$$\frac{1}{3} \leq |D\phi_{x_0}(x)| \leq |(D\phi_{x_0}(x))^{-1}| \leq 3 \quad \text{for all } x \in V_{x_0}, \ x_0 \in \partial \Omega.$$  \hspace{1cm} (3.16)

We define the coordinate transformation $\Phi_{x_0}$ as

$$(x_1, x_2, x_3) = \Phi_{x_0}^{-1}(y_1, y_2, y_3) = \phi_{x_0}^{-1}(y_2, y_3) + y_1 N(\phi_{x_0}^{-1}(y_2, y_3)).$$  \hspace{1cm} (3.17)
In light of (3.15), we have,

\[ D\Phi_{x_0}(x_0) = I, \]

where \( I \) is the \( 3 \times 3 \) identity matrix.

Now the standard Euclidean metric \( g_0 = \sum_{j=1}^{3} dx_j \otimes dx_j \) on \( V_{x_0} \) is transformed to the new metric on \( \Phi_{x_0}(V_{x_0}) \):

\[ g_0 = \sum_{1 \leq j, k \leq 3} g_{jk} dy_j \otimes dy_k \]

\[ = dy_3 \otimes dy_3 + \sum_{2 \leq j, k \leq 3} \left[ G_{jk}(y_2, y_3) - 2y_1 K_{jk}(y_2, y_3) + y_1^2 L_{jk}(y_2, y_3) \right] dy_j \otimes dy_k, \]

where

\[ G = \sum_{2 \leq k, j \leq 3} G_{jk} dy_j \otimes dy_k = \sum_{2 \leq k, j \leq 3} \left( \frac{\partial x_1}{\partial y_j}, \frac{\partial x_1}{\partial y_k} \right) dy_j \otimes dy_k, \]

\[ K = \sum_{2 \leq k, j \leq 3} K_{jk} dy_j \otimes dy_k = \sum_{2 \leq k, j \leq 3} \left( \frac{\partial N_{x_0}}{\partial y_j}, \frac{\partial x}{\partial y_k} \right) dy_j \otimes dy_k \]

\[ L = \sum_{2 \leq k, j \leq 3} L_{jk} dy_j \otimes dy_k = \sum_{2 \leq k, j \leq 3} \left( \frac{\partial N_{x_0}}{\partial y_j}, \frac{\partial N_{x_0}}{\partial y_k} \right) dy_j \otimes dy_k, \]

are the first, second and third fundamental forms on \( \partial \Omega \). We denote by \( g^{jk} \) the entries of the inverse matrix of \( (g_{jk}) \). Its Taylor expansion at \( x_0 \), valid in the neighborhood \( \Phi_{x_0}(V_{x_0}) \), is given by

\[ (g^{jk})_{1 \leq j, k \leq 3} = I + \begin{pmatrix} 0 & 0 & 0 \\ 0 & O(|y|) & O(|y|) \\ 0 & O(|y|) & O(|y|) \end{pmatrix}. \]  

(3.18)

Note that both \( g_{jk} \) and \( g^{jk} \) depend on \( x_0 \) and on the modification of \( \phi_{x_0} \) used to make (3.15) valid.

Similarly, the Lebesgue measure \( dx \) on \( V_{x_0} \) transforms into the measure on \( \Phi_{x_0}(V_{x_0}) \) by the formula

\[ dx = [\det(g_{jk})]^{1/2} dy. \]

For future use, we introduce the notation

\[ \text{Jac}(y) = \det(g_{jk})^{1/2}(y), \quad y \in \Phi_{x_0}(V_{x_0}), \quad x_0 \in \partial \Omega. \]  

(3.19)

This determinant has the Taylor expansion

\[ [\det(g_{jk})]^{1/2} = \text{Jac}(y) = 1 + O(|y|), \]  

(3.20)

which is valid in the neighborhood \( \Phi_{x_0}(V_{x_0}) \).

We may express the integrals over \( \Omega \) and \( \partial \Omega \) using the \( y \)-coordinates as follows. For all \( u \in L^2(\Omega), v \in L^2(\partial \Omega) \), and \( x_0 \in \partial \Omega \), using the above notation, we have

\[ \int_{V_{x_0}} |u(x)|^2 \, dx = \int_{\Phi_{x_0}(V_{x_0})} \det(g_{jk})^{1/2} |u(\Phi_{x_0}^{-1}(y))|^2 \, dy \]

\[ \int_{V_{x_0} \cap \partial \Omega} |v(x)|^2 \, ds(x) = \int_{V_{x_0}} \det(g_{jk})^{1/2} \left| v(\Phi_{x_0}^{-1}(0, y_2, y_3)) \right|^2 \, dy_2 \, dy_3. \]  

(3.21)
In light of (3.20), we may simplify the formulas displayed in (3.21) as follows. There exist two constants \( C > 0 \) and \( \delta_0 > 0 \), independent of the choice of the point \( x_0 \in \partial \Omega \), such that, if \( 0 < \delta < \delta_0 \) and if
\[
\Phi_{x_0}(V_{x_0}) \subset \{ y = (y_1, y_2, y_3) \in \mathbb{R}^3 : |y| < \delta \},
\]
then, for all \( u \in L^2(\Omega) \) and \( v \in L^2(\partial \Omega) \),
\[
\left| \int_{V_{x_0}} |u(x)|^2 \, dx - \int_{\Phi_{x_0}(V_{x_0})} |u(\Phi_{x_0}^{-1}(y))|^2 \, dy \right| \leq C\delta \int_{\Phi_{x_0}(V_{x_0})} |u(\Phi_{x_0}^{-1}(y))|^2 \, dy, \tag{3.22}
\]
and
\[
\left| \int_{V_{x_0} \cap \partial \Omega} |u(x)|^2 \, ds(x) - \int_{U_{x_0}} |u(\Phi_{x_0}^{-1}(0, y_2, y_3))|^2 \, dy_2 dy_3 \right|
\leq C\delta \int_{U_{x_0}} |u(\Phi_{x_0}^{-1}(0, y_2, y_3))|^2 \, dy_2 dy_3. \tag{3.23}
\]

A magnetic potential
\[
F = (F_1, F_2, F_3)
\]
defined in cartesian coordinates in \( V_{x_0} \) is transformed to a magnetic potential \( \tilde{F} \) in \( y \)-coordinates in \( \Phi_{x_0}(V_{x_0}) \). To save notation we shall write the vector field \( \tilde{F} \) in terms of its coefficients associated with the natural (Cartesian) basis:
\[
\tilde{F}(y) = (\tilde{F}_1(y), \tilde{F}_2(y), \tilde{F}_3(y)),
\]
where
\[
\tilde{F}_j(y) := \sum_{k=1}^3 F_k(\Phi_{x_0}^{-1}(y)) \frac{\partial x_k}{\partial y_j}. \tag{3.24}
\]

If \( \text{curl} F \) is constant and has magnitude equal to 1, and if there exists a constant \( C > 0 \) such that,
\[
\sum_{|\alpha| \leq 2} |D^\alpha F| \leq C, \quad x \in V_{x_0}, \tag{3.25}
\]
then a particular choice of a gauge transformation is constructed in [29] so that, in the neighborhood \( \Phi_{x_0}(V_{x_0}) \), the new vector potential \( \tilde{F} \) satisfies,
\[
\tilde{F}_1 = 0, \quad \tilde{F}_2 = O(|y|^2), \quad \tilde{F}_3 = y_1 \cos \nu + y_2 \sin \nu + O(|y|^2). \tag{3.26}
\]
Here, \( \nu = \nu(x_0) \) is the angle between the magnetic field \( \text{curl} F \) and the tangent plane of \( \partial \Omega \) at the point \( x_0 \), i.e.
\[
\sin \nu = |N(x_0) \cdot (\text{curl} F)(x_0)|.
\]
Recall that this equality follows from (3.15), hence it is true after a rotation of the \( (y_2, y_3) \) coordinates, namely after modification of the mapping \( \phi_{x_0} \).

Notice that the constants implicit in the \( O \) notation in (3.18), (3.20) and (3.26) are determined by the domain \( \Omega \) as well as the constant \( C \) in (3.25), i.e. these quantities are independent of the boundary point \( x_0 \) by compactness and regularity of \( \partial \Omega \).
If \( u \) is a function with support in a coordinate neighborhood \( V_{x_0} \), we may express the functional
\[
E_0(u, F) = \int_\Omega \left\{ |(\nabla - iF)u|^2 \, dx - \kappa^2 |u|^2 + \frac{\kappa^2}{2} |u|^4 \right\} \, dx
\]
explicitly in the new coordinates as follows,
\[
E_0(u, F) = \int_{\Phi_{x_0}(V_{x_0})} \det(g_{jk})^{1/2} \left[ \sum_{1 \leq j, k \leq 3} g^{jk}(\partial_j - i\tilde{F}_j)\tilde{u} \times (\partial_k - i\tilde{F}_k)\tilde{u} 
- \kappa^2 |\tilde{u}|^2 + \frac{\kappa^2}{2} |\tilde{u}|^4 \right] \, dy,
\]
where \( \tilde{u} \) denotes the function defined in the new variable \( y \) as follows:
\[
\tilde{u} = \left( \exp(-iq\tau\beta_{x_0})u \right) \circ \Phi_{x_0}^{-1},
\]
(with \( \beta_{x_0} \) the gauge transformation necessary to pass to the \( \tilde{F} \) given in (3.26)).

Using the boundary coordinates, we can give a uniform bound of the integral of a function defined in a tubular neighborhood of the boundary. The bound will involve the Sobolev norm and the thickness of the boundary layer.

For \( t > 0 \) small we denote
\[
\Omega_t = \{ x \in \Omega : \text{dist}(x, \partial \Omega) < t \}.
\]

**Lemma 3.4.** There exist two constants \( t_0 \in (0, 1) \) and \( C > 0 \) such that, for all \( t \in (0, t_0) \) and \( u \in W^{1,1}(\Omega, \mathbb{C}) \), it holds,
\[
\int_{\Omega_t} |u(x)| \, dx \leq C \, t \|u\|_{W^{1,1}(\Omega)}.
\]

If \( u = 0 \) on \( \partial \Omega \), then we get the improved estimate,
\[
\int_{\Omega_t} |u(x)| \, dx \leq C \, t \int_{\Omega_2t} |Du(x)| \, dx.
\]

**Proof.** Let \( (\Phi_{x_j}, V_{x_j})_{j=1}^N \) be a finite collection of local coordinate maps as above such that \( \partial \Omega \subset \bigcup_{j=1}^N V_{x_j} \). Choose \( t_0 \) so small that
\[
\Omega_{2t_0} \subset \bigcup_{j=1}^N V_{x_j}.
\]
For simplicity we write \( \Phi_j \) instead of \( \Phi_{x_j} \), etc. in the rest of the proof.

For all \( j \), the Jacobian of \( \Phi_j \) satisfies (3.20). That way, there exists a constant \( C > 0 \) such that, for all \( t \in (0, t_0) \) and \( u \in C^\infty(\bar{\Omega}) \), (recall that \( \phi_j \) was the boundary part of the coordinate transform \( \Phi_j \))
\[
\int_{\Omega_t \cap V_j} |u(x)| \, dx \leq C \int_0^{2t} \int_{\phi_j(V_j \cap \partial \Omega)} |\tilde{u}_j(y_1, y_2, y_3)| \, dy_2 \, dy_3 \, dy_1,
\]
Lemma 3.5. Let \( \delta > 0 \) and define for \( \eta > 0 \) the set
\[
O_\eta = \{(y_1, y_2, y_3) \in \mathbb{R}^3 : 0 < y_1 < \delta, -\eta < y_1, y_2 < \eta\}.
\]

There exist constants \( C > 0 \) and \( \epsilon_0 \in (0,1) \) such that, for all \( \delta, \alpha \in (0, \epsilon_0) \) the following holds.

There exist a finite sequence of points \( \{x_i\}_{i=1}^N \subset \partial \Omega \) (with \( N \) possibly depending on \( \delta, \alpha \)) and a smooth partition of unity \( \{\tilde{\chi}_i\}_{i=1}^N \), with \( \tilde{\chi}_i \geq 0 \), and
\[
\partial \Omega \subset \bigcup_{i=1}^N \Phi^{-1}_i(O_\delta),
\]
\[
\sum_{i=1}^N \tilde{\chi}_i^2(x) = 1 \quad \text{in} \quad \{x : \text{dist}(x, \partial \Omega) < \delta\},
\]
\[
\tilde{\chi}_i \equiv 1 \quad \text{in} \quad Q_{\delta,i} := \Phi^{-1}_i(O_{(1-\alpha)\delta}),
\]
\[
\sum_{i} |\nabla \tilde{\chi}_i(x)|^2 \leq C(\alpha \delta)^{-2}.
\]

Here \( \Phi_i = \Phi_{x_i} \) is as in (3.17).
Proof. In $\mathbb{R}^2$, we introduce the following partition of unity

$$\sum_l g^2_{l,\delta,\alpha} = 1 \quad \text{and} \quad \sum_l |\nabla g_{l,\delta,\alpha}|^2 \leq \frac{C}{\alpha \delta} \quad \text{in} \quad \mathbb{R}^2,$$

where

$$\text{supp } g_{l,\delta,\alpha} \subset Q_{\delta}(y_{j,\delta,\alpha}), \quad g_{l,\delta,\alpha} = 1 \quad \text{in} \quad Q_{(1-\alpha)\delta}(y_{l,\delta,\alpha}),$$

and, for $u = (u_1, u_2) \in \mathbb{R}^2$, $Q_{\delta}(y) = (y_1 - \delta, y_1 + \delta) \times (y_2 - \delta, y_2 + \delta) \subset \mathbb{R}^2$ is the square of center $y$ and length $\delta$.

Let us introduce the set of indices

$$J = \{l \in \mathbb{Z}^2 : y_{l,\delta,\alpha} \in \bigcup_{i=1}^n \tilde{U}_{p_i}\},$$

where $(\tilde{U}_{p_i} = \phi_{p_i}(\tilde{V}_{p_i}))_{i=1}^n$ is the class of subsets of $\mathbb{R}^2$ satisfying (3.12) and (3.14).

Using the diffeomorphism in (3.12), we get a family of points $(x_l)_{l \in J}$ in $\partial \Omega$ defined as follows

$$x_l = \phi_{p_i}^{-1}(y_{l,\delta,\alpha}) \quad \text{if} \quad y_{l,\delta,\alpha} \in \tilde{U}_{p_i}.$$

Now we define the functions

$$\chi_l(x) = g_{l,\delta,\alpha}(\Phi_{x_l}(p(x))) \quad \text{in} \quad \Phi_{x_l}^{-1}(O_\delta), \quad \chi_l(x) = 0 \quad \text{outside} \quad \Phi_{x_l}^{-1}(O_\delta),$$

$$f(x) = \sum_{j \in J} \chi_j^2(x) \quad \text{in} \quad \{\text{dist}(x, \partial \Omega) < \delta\},$$

where, for $x \in \Omega$ satisfying $\text{dist}(x, \partial \Omega) \leq \epsilon_0$, $p(x) \in \partial \Omega$ is the unique point in $\partial \Omega$ such that $\text{dist}(x, \partial \Omega) = \text{dist}(x, p(x))$. Note that $f(x) \geq 1$ for all $x$.

Now we define the partition of unity $(\tilde{\chi}_l(x))$ as follows,

$$\tilde{\chi}_l(x) = \frac{\chi_l(x)}{\sqrt{f(x)}}.$$

\[\square\]

### 3.5 Gauge transformation

The Ginzburg-Landau energy in (1.2) is gauge invariant, i.e.

$$G(\psi, n) = G(e^{-iq\beta}\psi, n + \nabla \beta)$$

for any real-valued $H^1$-function $\beta$. In order to estimate $G(\psi, n)$, we will replace $n$ with $n_{\text{new}} = n + \nabla \beta$, such that the new field $n_{\text{new}}$ produces small errors in the various calculations. This is easy to do when $n = n_0$ is a fixed smooth field, but is hard to do when $(\psi, n)$ is simply a minimizer of the Landau-de Gennes energy in (1.1) and therefore possibly varies with the various parameters (e.g. $\kappa$). Notice that, the new ‘director field’ $n + \nabla \beta$ will generally not satisfy the pointwise normalization $|n + \nabla \beta| = 1$. 

21
3.5.1 Gauge for fields in $C(\tau)$

In this section, we fix a vector field $n_0 \in C(\tau)$. By definition of $C(\tau)$ (recall (1.8)), we may write,

$$n_0(x) = N^Q(x) = QN_{\tau}(Q^tx),$$  \hspace{1cm} (3.30)

where $N_{\tau}$ has been given in (1.10) and $Q$ is an orthogonal matrix such that det $Q = 1$.

For all $x_0 \in \Omega$, define the magnetic potential,

$$\left(n_0\right)_{\text{cst}} = \int_0^1 s(x - x_0) \times n_0(x_0) \, ds.$$  \hspace{1cm} (3.31)

Note that $(n_0)_{\text{cst}}$ generates a constant magnetic field,

$$\text{curl} \left( n_0 \right)_{\text{cst}} = -n_0(x_0) = \tau^{-1}(\text{curl} \, n_0)(x_0).$$  \hspace{1cm} (3.32)

In Lemma 3.6, we explain how to pass from the field $n_0$ to the field $(n_0)_{\text{cst}}$.

**Lemma 3.6.** There exists a constant $C > 0$ such that, if

- $x_0 \in \Omega$,
- $U \subset \Omega$ is a simply connected domain,
- $x_0 \in U$ and $\delta := \text{diam}(U)$,

then there exists a smooth function $\bar{f}_0 : U \to \mathbb{R}$ such that,

$$|n_0(x) - \tau(n_0)_{\text{cst}}(x) - \nabla \bar{f}_0| \leq C\delta^2 \quad \text{in} \ U.$$  \hspace{1cm} (3.33)

Here $(n_0)_{\text{cst}}$ is the vector field introduced in (3.31).

**Proof.** Let

$$a_0(x) = \tau \int_0^1 s(x - x_0) \times n_0(s(x - x_0) + x_0) \, ds.$$  

It is clear that

$$\text{curl} \, a_0 = -\tau n_0 = \text{curl} \, n_0 \quad \text{and} \quad \text{curl} \left( n_0 \right)_{\text{cst}} = -n_0(x_0).$$

In the simply connected domain $U$ containing $x_0$, there exists a smooth function $\bar{f}_0$ such that, we have,

$$a_0 = n_0 - \nabla \bar{f}_0 \quad \text{in} \ U.$$  

Using (3.31) and the smoothness of the vector field $n_0$, we have,

$$|a_0 - \tau(n_0)_{\text{cst}}| \leq \|Dn_0\|_{\infty} |x - x_0|^2 \leq C |x - x_0|^2 \quad \text{in} \ U.$$  

As we shall see in Lemma 3.7 below, if the point $x_0 \in \partial \Omega$, then it is possible to apply a further gauge transformation to transform $(n_0)_{\text{cst}}$ to a magnetic potential of the form in (3.4). In the statement of Lemma 3.7, we will use the following notation:
\( \nu_0 := \nu(n_0; x_0) \in [0, \pi/2] \) is the non-oriented angle between \( n_0(x_0) \) and the tangent plane to \( \partial \Omega \) at \( x_0 \);

- \( \Phi_0 \) is the coordinate transformation that straightens a neighborhood \( V_0 \) of the point \( x_0 \) such that \( \Phi_0(x_0) = 0 \) (see Sec. 3.4).

- For every \( x \in V_0, (x_1, x_2, x_3) \) are the standard cartesian coordinates of \( x \) in \( \mathbb{R}^3 \) and 
\[
(y_1, y_2, y_3) = \Phi_0^{-1}(x_1, x_2, x_3), \quad y_1 \geq 0.
\]

- For every vector field \( a \) defined in \( V_0 \) by the cartesian coordinates \( (x_1, x_2, x_3) \), we denote by \( \tilde{a} \) the corresponding vector field defined via the boundary coordinates \( (y_1, y_2, y_3) = \Phi_0^{-1}(x_1, x_2, x_3) \), i.e. \( \tilde{a}(y_1, y_2, y_3) = a(x_1, x_2, x_3) \).

- \( A_{\nu_0} \) is the vector potential (in boundary coordinates) introduced in (3.4).

Now we can state Lemma 3.7:

**Lemma 3.7.** There exist two constants \( C, \delta_0 > 0 \) such that, if

- \( x_0 \in \partial \Omega \),
- \( U \subset \overline{\Omega} \) is a simply connected domain,
- \( x_0 \in U \) and \( \delta := \text{diam}(U) \in (0, \delta_0] \),

then there exists a smooth function \( \beta_0 \) such that,

\[
\left| \tilde{(n_0)_{\text{cst}}} - (A_{\nu_0} + \nabla \beta_0) \right| \leq C\delta^2, \quad \text{in } \Phi_0(V_0). \tag{3.34}
\]

Here \( (n_0)_{\text{cst}} \) is the vector field introduced in (3.31).

**Proof.** Choose \( \delta_0 \) small enough such that \( B(x_0, \delta_0) \cap \overline{\Omega} \subset V_0 \). Hence, for \( \delta \in (0, \delta_0], U \subset V_0 \).

Notice that, in light of (3.32), \( |\text{curl}(n_0)_{\text{cst}}| = 1 \) and, the (non-oriented) acute angle between the fields \( n_0, (n_0)_{\text{cst}} \) and the tangent plane to \( \partial \Omega \) at \( x_0 \) are equal, i.e.

\[
\nu((n_0)_{\text{cst}}; x_0) = \nu(n_0; x_0) = \nu_0.
\]

The equation \( y_1 = 0 \) defines part of the boundary of \( \partial \Omega \). Since \( \text{curl}(n_0)_{\text{cst}} \) is a constant vector and makes an angle \( \nu_0 \) with \( \partial \Omega \), it follows from (3.26) that we may find a smooth function \( \beta_0(y) \) such that (3.34) holds. \( \square \)

### 3.5.2 Gauge for \( S^2 \)-valued fields

Let \( n \in H^1(\Omega; S^2) \). We will describe a procedure allowing us to go from the field \( n \) (with a variable curl) to a field \( n_{\text{cst}} \) (with a constant curl). The errors produced by this procedure will be uniformly controlled by \( \| \text{curl } n + \tau n \|_2 \). (\( \tau > 0 \) is supposed a fixed constant, hence we do not seek estimates that are valid uniformly with respect to \( \tau \)).
Approximation by a field in $C(\tau)$

**Lemma 3.8.** Let $C_0 > 0$. There exists a constant $C > 0$ such that, if

- $\mathbf{n} \in H^1(\Omega; \mathbb{S}^2)$, $\mathbf{n}_0 \in C(\tau)$, $x_0 \in \overline{\Omega}$, $\delta > 0$,
- $Q_\delta \subset \overline{\Omega}$ is starshaped with respect to $x_0$ and $Q_\delta \subset B(x_0, C_0 \delta)$,

then, there exists a function $f \in H^1(Q_\delta)$ such that

$$\|\mathbf{n} - \tau(\mathbf{n}_0)\|_{L^2(Q_\delta)} - \nabla f_0\|_{L^2(Q_\delta)} \leq 3\delta \sqrt{|\ln \delta|} \left( \|\text{curl } \mathbf{n} + \tau \mathbf{n}\|_{L^2(Q_\delta)} + \tau \|\mathbf{n} - \mathbf{n}_0\|_{L^2(Q_\delta)} \right) + C\delta^3. \quad (3.35)$$

*Here $(\mathbf{n}_0)_{\text{cst}}$ is the field defined as in (3.31)*

**Proof.** Define the vector fields

$$\mathbf{a}(x) = -\int_{\eta}^1 s(x - x_0) \times (\text{curl } \mathbf{n}) \left( s(x - x_0) + x_0 \right) ds, \quad (3.36)$$

$$\mathbf{a}^0(x) = -\int_{\eta}^1 s(x - x_0) \times (\text{curl } \mathbf{n}_0) \left( s(x - x_0) + x_0 \right) ds, \quad (3.37)$$

$$\mathbf{c}(x) = (\mathbf{n} - \mathbf{n}_0) \left( \eta(x - x_0) + x_0 \right). \quad (3.38)$$

It is easy to check that in $Q_\delta$,

$$\text{curl } \mathbf{c}(x) = \eta \text{curl } (\mathbf{n} - \mathbf{n}_0) \left( \eta(x - x_0) + x_0 \right),$$

$$\text{curl } (\mathbf{a} - \mathbf{a}^0)(x) = \text{curl } (\mathbf{n} - \mathbf{n}_0)(x) - \eta \text{curl } \mathbf{c}(x). \quad (3.39)$$

Consequently, since $Q_\delta$ is simply-connected, there exists a function $f_0 \in H^1(Q_\delta)$ such that,

$$\mathbf{n} - \mathbf{n}_0 - \nabla f_0 = \mathbf{a} - \mathbf{a}^0 + \eta \mathbf{c} \quad \text{in } Q_\delta. \quad (3.40)$$

Now, we estimate $\|\mathbf{a} - \mathbf{a}^0\|_{L^2(Q_\delta)}$ and $\|\mathbf{c}\|_{L^2(Q_\delta)}$. We have, for all $x \in Q_\delta$,

$$|\mathbf{a}(x) - \mathbf{a}^0(x)|^2 \leq \delta^2 \int_{\eta}^1 s^2 \left( \text{curl } \mathbf{n} - \text{curl } \mathbf{n}_0 \right) \left( s(x - x_0) + x_0 \right)^2 ds$$

and, performing the change of variable $y = s(x - x_0) + x_0$ (using that $Q_\delta$ is star-shaped),

$$\int_{Q_\delta} |\mathbf{a}(x) - \mathbf{a}^0(x)|^2 dx \leq \delta^2 \int_{\eta}^{\frac{1}{s}} \frac{1}{s} \int_{Q_\delta} \left( \text{curl } \mathbf{n} - \text{curl } \mathbf{n}_0 \right)(y)^2 dy ds$$

$$\leq \delta^2 |\ln \eta| \|\text{curl } (\mathbf{n} - \mathbf{n}_0)\|_{L^2(Q_\delta)}^2.$$

Using the fact that $\text{curl } \mathbf{n}_0 = -\tau \mathbf{n}_0$, the norm of $\text{curl } (\mathbf{n} - \mathbf{n}_0)$ can be estimated by the triangle inequality,

$$\|\text{curl } (\mathbf{n} - \mathbf{n}_0)\|_{L^2(Q_\delta)} \leq \|\text{curl } \mathbf{n} + \tau \mathbf{n}\|_{L^2(Q_\delta)} + \tau \|\mathbf{n} - \mathbf{n}_0\|_{L^2(Q_\delta)}.$$  

This yields

$$\|\mathbf{a} - \mathbf{a}^0\|_{L^2(Q_\delta)} \leq \delta \sqrt{|\ln \eta|} \left( \|\text{curl } \mathbf{n} + \tau \mathbf{n}\|_{L^2(Q_\delta)} + \tau \|\mathbf{n} - \mathbf{n}_0\|_{L^2(Q_\delta)} \right). \quad (3.41)$$

24
At the same time, the identities $|\mathbf{n}| = |\mathbf{n}_0| = 1$ yield,

$$\|\mathbf{c}\|_{L^2(Q_\delta)}^2 \leq 4|Q_\delta| \leq C\delta^3,$$

where $C$ is a constant independent of $\delta$ and $\eta$. Inserting this estimate and the one in (3.41) into (3.40), we deduce that,

$$\|\mathbf{n} - \mathbf{n}_0 - \nabla f_0\|_{L^2(Q_\delta)} \leq \delta \sqrt{|\ln \eta|} \left( \|\text{curl } \mathbf{n} + \tau \mathbf{n}\|_{L^2(Q_\delta)} + \tau \|\mathbf{n} - \mathbf{n}_0\|_{L^2(Q_\delta)} \right) + C\eta^{3/2}. \quad (3.42)$$

We can choose $\eta = \delta^{3/2}$ and get,

$$\|\mathbf{n} - \mathbf{n}_0 - \nabla f_0\|_{L^2(Q_\delta)} \leq 3\delta \sqrt{|\ln \delta|} \left( \|\text{curl } \mathbf{n} + \tau \mathbf{n}\|_{L^2(Q_\delta)} + \tau \|\mathbf{n} - \mathbf{n}_0\|_{L^2(Q_\delta)} \right) + C\delta^3. \quad (3.43)$$

In light of (3.33), we may modify the function $f_0$ in (3.43) so that (3.35) holds. □

**Approximation by a constant field**

In the interior of $\Omega$, we can pass from a general $\mathbf{n} \in H^1(\Omega; \mathbb{S}^2)$ to a vector field with constant curl in a manner more efficient than Lemma 3.8, in the sense better errors are produced. This is the purpose of Lemma 3.9 below.

**Lemma 3.9.** There exists a constant $C > 0$ such that, if

- $\mathbf{n} \in H^1(\Omega; \mathbb{S}^2)$, $\mathbf{n}_0 \in C(\tau)$, $x_0 \in \Omega$, $\ell \in (0, 1)$,
- $Q_\delta \subset \Omega$ is a cube of side-length $\ell$ and center $x_0$,

then there exist $f_0 \in H^1(Q_\delta)$ and a vector field $\mathbf{a}_{\text{av}} : \mathbb{R}^3 \to \mathbb{R}^3$ such that,

$$\text{curl } \mathbf{a}_{\text{av}} \text{ is constant},$$

$$|\text{curl } \mathbf{a}_{\text{av}}| \geq 1 - C\ell^6 - C\ell \|D\mathbf{n}\|_{L^2(Q_\ell)}, \quad (3.44)$$

and

$$\|\mathbf{n} - \tau \mathbf{a}_{\text{av}} - \nabla f_0\|_{L^2(Q_\ell)}^2 \leq C\ell^2 |\ln \ell| \left( \|\text{curl } \mathbf{n} + \tau \mathbf{n}\|_{L^2(Q_\delta)}^2 + \ell^2 \|D\mathbf{n}\|_{L^2(Q_\delta)}^2 \right) + C\ell^3. \quad (3.45)$$

**Proof.** We introduce the two vector fields

$$\mathbf{c} = \mathbf{n}(\ell^3(x - x_0) + x_0), \quad \mathbf{n}_{\text{av}} = \frac{1}{|Q_\ell|} \int_{Q_\ell} \mathbf{n} \, dx.$$ 

By the Poincaré inequality, there exists a universal constant $C_0 > 0$ such that

$$\|\mathbf{n} - \mathbf{n}_{\text{av}}\|_{L^2(Q_\ell)} \leq C_0 \ell \|D\mathbf{n}\|_{L^2(Q_\ell)}. \quad (3.46)$$

Define $\mathbf{a}_{\text{av}}$ as follows

$$\mathbf{a}_{\text{av}} = -\int_{-\eta}^1 s(x - x_0) \times \mathbf{n}_{\text{av}} \, ds.$$ 

Clearly

$$\text{curl } \mathbf{a}_{\text{av}} = (1 - \ell^6)\mathbf{n}_{\text{av}} \quad (3.47)$$
is constant and by (3.46)
\[ |n_{av}| = \|n_{av}\|_{L^2(Q)} \geq \|n\|_{L^2(Q)} - \|n - n_{av}\|_{L^2(Q)} \geq 1 - C\ell\|Du\|_{L^2(Q)}, \]
thereby giving (3.44).

Now, we introduce the 'magnetic potential'
\[ a = -\int_1^1 s(x - x_0) \times (\text{curl } n)(s(x - x_0) + x_0) \, ds. \]
Clearly,
\[ \text{curl } a = \text{curl } n - \ell^3 \text{curl } c \text{ in } Q. \]
This yields the existence of a function \( f_0 \in H^1(Q) \) such that
\[ n - a - \nabla f_0 = \ell^3 c \text{ in } Q. \quad (3.48) \]
On the other hand, we observe that,
\[ a(x) - \tau a_{av}(x) = -\int_1^1 s(x - x_0) \times (\text{curl } n + \tau n)(s(x - x_0) + x_0) \, ds \\
+ \tau \int_1^1 s(x - x_0) \times (n - n_{av})(s(x - x_0) + x_0) \, ds. \]
After applying the change of variables \( y = s(x - x_0) + x_0 \), we observe that,
\[ \|a - \tau a_{av}\|_{L^2(Q)} \leq \ell^2 \ln(\ell^3) \left( \|\text{curl } n + \tau n\|_{L^2(Q)}^2 + \tau^2 \|n - n_{av}\|_{L^2(Q)}^2 \right) \\
\leq C\ell^2 \ln(\ell^3) \left( \|\text{curl } n + \tau n\|_{L^2(Q)}^2 + \tau^2 \|Dn\|_{L^2(Q)}^2 \right), \]
Inserting this into (3.48) then using that \( |c| = 1 \), we obtain the conclusion in (3.45). \( \Box \)

3.6 Energy of a boundary trial state

In this subsection we shall estimate the local energy of a test function in a specific domain \( Q_\delta \). For every \( D \subset \Omega \), we introduce the following 'local' energy in \( D \),
\[ G(\psi, n; D) = \int_D \left\{ |(\nabla - iqn)|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2} |\psi|^4 \right\} \, dx. \quad (3.49) \]
We suppose that \( \tau > 0 \) and \( n_0 \in C(\tau) \) are fixed (cf. (1.8)). Let \( x_0 \in \partial \Omega \) and \( \Phi \) be the coordinate transformation defined in (3.17) that straightens a neighborhood \( V \) of the point \( x_0 \) such that \( \Phi(x_0) = 0 \). Let \( \delta_0 > 0 \) and \( \delta \in (0, \delta_0) \). We select \( \delta_0 \) sufficiently small such that,
\[ \forall \delta \in (0, \delta_0), \quad (0, \delta) \times (-\delta, \delta)^2 \subset \Phi(V). \]
From the discussion in subsection 3.4, the constant \( \delta_0 \) can be selected in a manner independent of the variation of the point \( x_0 \in \partial \Omega \).

Let \( Q_\delta = \Phi^{-1}\{(0, \delta) \times (-\delta, \delta)^2\}, \) \( (n_0)_{\text{cst}} \) be the vector field in (3.31) and \( \beta_0 \) be the function in (3.34). Notice that the vector field \( (n_0)_{\text{cst}} \) generates a constant magnetic field,
\[
\text{curl}(n_0)_{\text{est}} = -n_0(x_0). \text{ Let } \nu_0 = \nu(x_0; n_0) \text{ be the angle in } [0, \pi/2] \text{ between the vector } n_0(x_0) \text{ and the tangent plane to } \partial \Omega \text{ at } x_0. \text{ This is the same angle in } [0, \pi/2] \text{ between the vector } \text{curl}(n_0)_{\text{est}} \text{ and the tangent plane to } \partial \Omega \text{ at } x_0.
\]

Let \( \tilde{\beta}_0 = \beta_0 \circ \Phi^{-1} \), where \( \beta_0 \) is the function introduced in Lemma 3.7. We have,
\[
\left| \left( \widehat{n_0} \right)_{\text{est}} - (A_{\nu_0} + \nabla \beta_0) \right| \leq C\delta^2 \quad \text{in } Q_\delta,
\]  
where \( A_{\nu_0} \) is the vector field defined in (3.4).

Let \( b = \frac{1}{b}, \ell = \delta \sqrt{q\tau} = \delta \sqrt{b\kappa} \), and \( u \) be a minimizer of the functional \( G_{b,\nu_0,\ell} \) introduced in (3.7). For all \( x = \Phi^{-1}(y) \in Q_\delta \), we define the trial function \( \psi(x; x_0) \) as follows,
\[
\psi(x; x_0) = \exp \left( iqg_0(x) \right) u \left( y \sqrt{q\tau} \right),
\]  
where \( g_0 = \bar{f}_0 + \beta_0 \circ \Phi^{-1} \) and \( \bar{f}_0 \) is the function introduced in Lemma 3.6 and satisfying (3.33). Note that \( \psi(x; x_0) \) is well-defined in \( Q_\delta \). Recall that \( u = 0 \) on \((0, \infty) \times \partial K_\ell \), see (3.6). Hence \( \psi(x; x_0) = 0 \) on \( \Omega \cap \partial Q_\delta \).

Near \( x_0 \), we expect that \( \psi(x; x_0) \) is an approximation of the actual minimizing order parameter, that is why we refer to it as trial function.

Computing the energy of \( \psi(x; x_0) \) in \( Q_\delta \) is easy by converting to boundary coordinates and dilating the variables.

**Lemma 3.10.** Let \( b > 1 \) be a fixed constant and \( n_0 \in C(\tau) \). There exists a constant \( C > 0 \) such that, for all \( \eta \in (0, 1), \delta \in (0, \delta_0), \kappa \geq 1, q\tau = b\kappa^2 \) and \( x_0 \in \partial \Omega \), the function \( \psi(x; x_0) \) in (3.51) satisfies,
\[
\frac{G(\psi(\cdot; x_0), n_0; Q_\delta)}{|Q_\delta \cap \partial \Omega|} \leq (1 + C\eta + C\delta) \sqrt{q\tau} E\left(b^{-1}, \nu_0 \right) + r,
\]  
where the constant \( r \) satisfies,
\[
|r| \leq C\eta^{-1} q^2 \delta^4 + C \sqrt{q\tau} \left( \delta + \eta + \eta^{-1} q \delta^4 + \frac{|\ln \kappa|}{\delta \sqrt{q\tau}} \right).
\]  
Here, \( E(\cdot, \cdot) \) is the energy introduced in (3.10), and \( \nu_0 = \nu(x_0; n_0) \) is the angle in \([0, \pi/2]\) between the vector \( n_0(x_0) \) and the tangent plane to \( \partial \Omega \) at \( x_0 \).

Furthermore, for \( \frac{1}{\sqrt{q\tau}} \leq \epsilon \leq \delta \), we have
\[
\int_{\{x \in Q_\delta, \text{dist}(x, \partial \Omega) \geq \epsilon\}} |\psi(\cdot, x_0)|^2 \, dx \leq C_p \frac{\delta^2}{\sqrt{q\tau}(\sqrt{q\tau} \epsilon)^p},
\]  
for all \( 0 < p < 1 \).
Proof. The estimate (3.53) is immediate, using the decay of \( u \) in the normal coordinate (see (3.9)). For simplicity, we will omit \( x_0 \) from the notation of the trial function and write \( \psi = \psi(\cdot; x_0) \). Let \( \eta \in (0, 1) \). We write by the Cauchy-Schwarz inequality,

\[
\int_{Q_\delta} |(\nabla - iqn_0)\psi|^2 \, dx \leq (1 + \eta) \int_{Q_\delta} |(\nabla - i\tau q\tau(n_0)_{\text{cat}})e^{-iqf_0}\psi|^2 \, dx
\]

\[
+ C\eta^{-1}q^2 \int_{Q_\delta} |n - \tau(n_0)_{\text{cat}} - \nabla f_0|^2 |e^{-iqf_0}\psi|^2 \, dx.
\]

Now, using the bound \( |\psi| \leq 1 \) and the estimate in (3.33), we get further,

\[
\int_{Q_\delta} |(\nabla - iqn_0)\psi|^2 \, dx \leq (1 + \eta) \int_{Q_\delta} |(\nabla - i\tau q\tau(n_0)_{\text{cat}})e^{-iqf_0}\psi|^2 \, dx + C\eta^{-1}q^2\delta^6.
\]

We convert to integration in boundary coordinates (by using (3.20) and (3.27)). Using the estimate in (3.34) and the Cauchy-Schwarz inequality, we may write,

\[
G(\psi, n_0; Q_\delta)
\]

\[
\leq (1 + C\eta + C\delta) \int_{\Phi(Q_\delta)} \left\{ |(\nabla - i\tau q\tau A_{n_0})u(y\sqrt{q\tau})|^2 - \kappa^2 |u(y\sqrt{q\tau})|^2 + \frac{\kappa^2}{2} |u(y\sqrt{q\tau})|^4 \right\} \, dy
\]

\[
+ C\eta^{-1}q^2\delta^6 + r_1,
\]

where

\[
r_1 = C(\delta + \eta)\kappa^2 \int_{\Phi(Q_\delta)} \left\{ |u(y\sqrt{q\tau})|^2 + |u(y\sqrt{q\tau})|^4 \right\} \, dx + C\eta^{-1}q^2\delta^4 \int_{\Phi(Q_\delta)} |u(y\sqrt{q\tau})|^2 \, dy.
\]

Recall that \( q\tau = \kappa^2 \) and \( \ell = \delta\sqrt{q\tau} \). We perform the change of variable \( z = y\sqrt{q\tau} \) and use that the function \( u \) decays at infinity (see [11, Thm. 3.6]) to write,

\[
G(\psi, n_0; Q_\delta) \leq (1 + C\eta + C\delta) \frac{(2b^{-1}; \nu_0; \ell)}{\sqrt{q\tau}} + \frac{C|\ln \kappa|}{\ell} \delta^2 \sqrt{q\tau} + C\eta^{-1}q^2\delta^6 + r_1,
\]

and

\[
r_1 \leq C(\delta + \eta)\delta^2 \sqrt{q\tau} + C\eta^{-1}q\delta^6 \sqrt{q\tau}.
\]

Thanks to (3.11) and the fact that \( \ell = \delta\sqrt{q\tau} \), we get,

\[
G(\psi, n_0; Q_\delta) \leq (1 + C\eta + C\delta) \sqrt{q\tau} (2\delta)^2 E(b^{-1}; \nu_0) + \frac{C|\ln \kappa|}{\ell} \delta^2 \sqrt{q\tau} + C\eta^{-1}q^2\delta^6 + r_1.
\]

This finishes the proof of Lemma 3.10, thanks to (3.55), the boundedness of the function \( E(\cdot, \cdot) \) and the following estimate that results from (3.23),

\[
|Q_\delta \cap \partial \Omega| \leq C\delta^3.
\]

\[
\square
\]
4 Upper bound for the energy

In this section we derive an upper bound estimate of the value of \( E(\psi, n) \), where \((\psi, n)\) is a minimizer of the Landau-de Gennes energy \( E \) given in (1.1) and the Assumption 1.1 is satisfied.

For every \( x \in \partial \Omega \), recall the definition of \( E(b, \nu(x; n)) \) and \( e_0(\frac{1}{b}, \tau) \) (see (3.10), (1.14) and (1.15)).

Proposition 4.1. Let \( b > 1 \) and \( \tau > 0 \) be fixed constants. There exists a function \( \text{err} : [1, \infty) \to \mathbb{R}_+ \) such that \( \lim_{\kappa \to \infty} \text{err}(\kappa) = 0 \) and the following is true. For all \( \kappa \geq 1 \), \( q\tau = b\kappa^2 \), \( K_1, K_2, K_3 \geq 0 \), the ground state energy in (1.13) satisfies,

\[
E_{g,st}(\kappa, q, \tau, K_1, K_2, K_3) \leq \sqrt{q\tau} e_0\left(\frac{1}{b}, \tau\right) + \kappa \text{err}(\kappa). \tag{4.1}
\]

To prove Proposition 4.1, we need:

Lemma 4.2. Let \( b \in (1, \Theta_0^{-1}) \), \( \tau > 0 \) and \( n_0 \in C(\tau) \) (defined in (1.8)). There exist constants \( \kappa_0 \geq 1 \), \( C > 0 \) and \( \eta_0 \in (0, 1) \) such that, for all \( \eta \in (0, \eta_0) \), \( \kappa \geq \kappa_0 \), there exists a function \( \psi_{\text{trial}} \in H^1(\Omega; \mathbb{C}) \) satisfying,

\[
\limsup_{\kappa \to \infty} \frac{G(\psi_{\text{trial}}, n_0)}{\sqrt{q\tau}} \leq (1 + C\eta) E\left(\frac{1}{b}, n_0\right) + C\eta. \tag{4.2}
\]

Here, \( G(\cdot, \cdot) \) and \( E(\cdot, \cdot) \) are introduced in (1.2) and (1.14).

Proof of Proposition 4.1. Let \( n_0 \in C(\tau) \) and \( \psi_{\text{trial}} \) be the trial function in Lemma 4.2. We may write the following upper bound for the full Landau-de Gennes functional,

\[
E(\psi, n) = E_{g,st}(\kappa, q, \tau, K_1, K_2, K_3) \leq E(\psi_{\text{trial}}, n_0) = G(\psi_{\text{trial}}, n_0),
\]

using that the Oseen-Frank energy of \( n_0 \) vanishes, since \( n_0 \in C(\tau) \). Using the conclusion of Lemma 4.2 we get

\[
\limsup_{\kappa \to \infty} \frac{E_{g,st}(\kappa, q, \tau, K_1, K_2, K_3)}{\sqrt{q\tau}} \leq (1 + C\eta) E\left(\frac{1}{b}, n_0\right) + C\eta.
\]

The term in the left side above is independent of \( \eta \). Taking the limit as \( \eta \to 0_+ \), we get

\[
\limsup_{\kappa \to \infty} \frac{E_{g,st}(\kappa, q, \tau, K_1, K_2, K_3)}{\sqrt{q\tau}} \leq E\left(\frac{1}{b}, n_0\right). \tag{4.2}
\]

Since (4.2) is true for all \( n_0 \in C(\tau) \), then by definition of \( e_0(\frac{1}{b}, \tau) \) in (1.15), we get

\[
\limsup_{\kappa \to \infty} \frac{E_{g,st}(\kappa, q, \tau, K_1, K_2, K_3)}{\sqrt{q\tau}} \leq e_0\left(\frac{1}{b}, \tau\right).
\]

Proof of Lemma 4.2. The proof consists of two parts. The first part is devoted to the construction of the trial function \( \psi_{\text{trial}} \) and the second part is devoted to computation of the corresponding energy, \( G(\psi_{\text{trial}}, n_0) \).
Step 1. Splitting the boundary region into small disjoint boxes.

Let $\eta > 0$ be small but fixed. We will choose another parameter $\delta > 0$ which will be specified as a negative power of $\kappa$ below.

Choose a finite collection of points $\{x_j : 1 \leq j \leq m\} \subset \partial \Omega$ such that

$$
\forall j \neq k : \eta/2 \leq \text{dist}(x_j, x_k), \quad \forall j : \min_{k \neq j} \text{dist}(x_j, x_k) \leq 2\eta \quad \text{and} \quad \partial \Omega \subset \bigcup_{j=1}^{m} B(x_j, 4\eta).
$$

Define $U_j$ as

$$
U_j = \{x \in \partial \Omega : \forall k \neq j, \text{dist}(x, x_j) < \text{dist}(x, x_k)\}.
$$

Clearly the $U_j$'s are disjoint and

$$
\partial \Omega = \bigcup_{j=1}^{m} U_j.
$$

Next, we construct a family of sets that cover a tubular neighborhood of $\partial \Omega$. That will be done by using the boundary coordinates $(y_1, y_2, y_3)$ introduced in Sec. 3.4 (where the equation $y_1 = 0$ defines the corresponding part in $\partial \Omega$). Let $\Phi_j$ be the coordinate transformation that straightens a neighborhood $V_j$ of the point $x_j$ such that $\Phi_j(x_j) = 0$.

We may assume that $U_j \subset V_j$ for all $j = 1, \cdots, m$ (this amounts to selecting $\eta$ sufficiently small). Let

$$
O_j = \{x = \Phi_j^{-1}(y_1, y_2, y_3) : \Phi_j^{-1}(0, y_2, y_3) \in U_j \quad \text{and} \quad 0 < y_1 < \delta\}, \quad j = 1, \cdots, m.
$$

We impose the following condition on $\delta$:

$$
\frac{1}{\sqrt{\kappa H}} \ll \delta \ll \eta.
$$

The number $m$ of the sets $U_j$ is independent of $\delta$ (but depends on $\eta$). Define

$$
\tilde{O}_j^{2D} = \Phi_j(O_j) \cap \{y \in \mathbb{R}^3 : y_1 = 0\}.
$$

For fixed $\delta$ and for each $1 \leq j \leq m$ we may cover $\tilde{O}_j^{2D}$ by a tiling of non-overlapping squares $\{K_{j,i}\}, i = 1, \cdots, n_j$, where $K_{j,i}$ is centered at the point $y_{j,i}$ and has side-length $2\delta$ i.e., $K_{j,i} = y_{j,i} + [-\delta, \delta]^2$, with $y_{j,i} \in \{0\} \times 2\delta \mathbb{Z}^2$.

Let

$$
\mathcal{J}_j = \{i : K_{j,i} \subset \tilde{O}_j^{2D}\}, \quad N_j = \text{Card } \mathcal{J}_j, \quad N = \sum_{j=1}^{m} N_j.
$$

Note that both $N_j$ and $N$ depend on $\delta$. We combine the coordinate transformation $\Phi_j$ by a translation taking the point $y_{j,i}$ to 0. Thus, we let $\Phi_{j,i}$ be the resulting coordinate transformation defined by

$$
\Phi_{j,i}^{-1}(y) = \Phi_j^{-1}(y_{j,i} + y),
$$

for $y = (y_1, y_2, y_3) \in (0, \delta) \times (-\delta, \delta)^2$.

As a result of the construction of the transformations $\Phi_{j,i}$, we get a tiling of (most of) the three dimensional domain $O_j$ by the ‘cube-like’ sub-domains

$$
Q_{j,i} = \Phi_{j,i}^{-1}(\{0\} \times (-\delta, \delta)^2).
$$

We restrict to the indices $(j, i)$ such that $1 \leq j \leq m$ and $i \in \mathcal{J}_j$. By construction the $Q_{j,i}$'s are non-overlapping. Let $x_{j,i} = \Phi_{j,i}^{-1}(0)$.
Step 2. Splitting the energy.

Our trial state will have the structure

$$\psi_{\text{trial}}(x) = h_\delta(x) u_{\text{trial}}(x), \quad u_{\text{trial}}(x) = \sum_{j=1}^{n} \sum_{i=1}^{N_j(\delta)} \psi_{j,i}^{\text{trial}}(x),$$

where

$$h_\delta(x) = h \left( \frac{\text{dist}(x, \partial \Omega)}{\delta} \right).$$

Here $h$ is a smooth cut-off function satisfying

$$\text{supp } h \subset [-1, 1], \quad 0 \leq h \leq 1 \text{ in } \mathbb{R}, \quad h(x) = 1 \text{ in } [-1/2, 1/2],$$

and, for all $(j, i)$,

$$\psi_{j,i}^{\text{trial}}(x) = \psi(x; x_{j,i}),$$

is the function introduced in (3.51) with $x_0 = x_{j,i}$, $Q_\delta = Q_{j,i}$ and $\Phi = \Phi_{j,i}$. Recall that $\psi(x; x_{j,i})$ is well-defined in $Q_{j,i}$ and $\psi(x; x_{j,i}) = 0$ on $\Omega \cap \partial Q_{j,i}$. Hence we may extend it over $\Omega$ by letting it equal zero outside of $Q_{j,i}$. The energy of this function is estimated in Lemma 3.10.

Let us start by observing that

$$|u_{\text{trial}}| \leq 1 \text{ in } \Omega. \quad (4.4)$$

The function $u_{\text{trial}}$ inherits this bound from the definition of the functions $\psi_{j,i}^{\text{trial}}$ and the fact that these functions have mutually disjoint supports.

From the disjoint supports of the summands and by the Cauchy-Schwarz inequality, we get for any $\eta \in (0, 1),

$$G(\psi_{\text{trial}}, n_0) = \sum_{j=1}^{n} \sum_{i=1}^{N_j(\delta)} G(h_\delta \psi_{j,i}^{\text{trial}}, n_0; Q_{j,i})$$

$$\leq (1 + \eta) \sum_{j=1}^{n} \sum_{i=1}^{N_j(\delta)} \int_{Q_{j,i}} \left| h_\delta(\nabla - iq_0) \psi_{j,i}^{\text{trial}} \right|^2 - \kappa^2 |h_\delta \psi_{j,i}^{\text{trial}}|^2 + \frac{\kappa^2}{2} h_\delta^4 |\psi_{j,i}^{\text{trial}}|^4 \, dx + \frac{C}{\eta \delta^2} \, dx$$

$$\leq (1 + \eta) \sum_{j=1}^{n} \sum_{i=1}^{N_j(\delta)} \left\{ G(\psi_{j,i}^{\text{trial}}, n_0; Q_{j,i}) + C(\kappa^{1/2} \delta^{3/2} + \eta^{-1} \delta) \right\}. \quad (4.5)$$

Here we also used (3.53) (with $p = 1/2$ for concreteness), that the volume of $Q_{j,i}$ is controlled by $C\delta^3$ and that $\tau = b\kappa^2$. We use the estimate in Lemma 3.10 to estimate $G(\psi_{j,i}^{\text{trial}}, n_0; Q_{j,i})$ and find with the remainder $r$ from (3.52),

$$G(\psi_{\text{trial}}, n_0) \leq (1 + C \eta + C \delta) \times$$

$$\sum_{j=1}^{n} \sum_{i=1}^{N_j(\delta)} \int_{Q_{j,i} \cap \partial \Omega} \sqrt{q_\tau E(b^{-1}, \nu_{j,i}) + r + C(\kappa^{1/2} \delta^{-1/2} + \eta^{-1} \delta^{-1})} \, d\sigma(x), \quad (4.6)$$
where $d\sigma$ is the surface measure, and where we used that $\sigma(Q_{j,i} \cap \partial \Omega)/\delta^2$ is bounded from above and below.

We choose

$$\delta = \kappa^{-4/5}. $$

The remainder term $r$ now satisfies,

$$r \leq C(\eta^{-1}\kappa^{-4/5} + |\ln \kappa|\kappa^{-4/5} + \eta\kappa),$$

and since the $Q_{j,i}$ are disjoint, we may estimate

$$\sum_{j=1}^{N} \sum_{i=1}^{N_j(\delta)} |Q_{j,i} \cap \partial \Omega| E(b^{-1}, \nu_{j,i}) \leq \int_{\partial \Omega} E(b^{-1}, \nu(x; n_0)) ds(x) + o(1),$$

as $\delta \to 0$. We insert this into (4.7) to obtain,

$$\mathcal{G}(\psi_{\text{trial}}, n_0) \leq (1 + C\eta + C\kappa^{-4/5} \sqrt{q\tau} \left( \int_{\partial \Omega} E\left(\frac{1}{b}, \nu(x; n_0)\right) ds(x) + o(1) \right) + C(\eta^{-1}\kappa^{-4/5} + \eta\kappa + \kappa^{-9/10}). \quad (4.8)$$

We take $\limsup_{\kappa \to \infty}$ to get,

$$\limsup_{\kappa \to \infty} \frac{\mathcal{G}(\psi_{\text{trial}}, n_0)}{\sqrt{q\tau}} \leq (1 + C\eta) \int_{\partial \Omega} E\left(\frac{1}{b}, \nu(x; n_0)\right) ds(x) + C\eta. $$

Recalling the definition of $\tilde{E}(\cdot, \cdot)$ in (1.14), this finishes the proof of Lemma 4.2.

5 Lower bound for the energy

In this section, we derive a lower bound of the ground state energy in (1.13) under the Assumptions 1.1 and 1.2.

Let $D \subset \Omega$ be a regular set as in Definition 1.5. We introduce the local Ginzburg-Landau energy as follows (compare with (1.2)),

$$\mathcal{G}(\psi, n; D) = \int_D \left\{ |(\nabla - iqn)|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4 \right\} dx. \quad (5.1)$$

The main result in this section is:
Theorem 5.1. Suppose that the Assumptions 1.1 and 1.2 are satisfied, and let \((\psi_j, n_j)\) be a minimizer of the energy in (1.13) corresponding to \(\kappa = \kappa_j\) (and \(q = q_j = b\kappa_j^2/\tau\) with \(\tau > 0\) and \(b > 1\) being fixed by Assumptions 1.1 and 1.2).

There exist \(n_0 \in C(\tau)\) and a subsequence \(\{\kappa_j\}\) such that, for every regular subset \(D \subset \Omega\), and for every \(h \in H^1(D)\) satisfying \(\|h\|_\infty \leq 1\), it holds,

\[
G(h\psi_j, n_j; D) \geq \sqrt{q_j} \int_{D \cap \partial \Omega} E \left( \frac{1}{b}, \nu(x; n_0) \right) ds(x) + o(\sqrt{q_j}) \quad (\kappa_j \to \infty),
\]

where \(E(\cdot, \cdot)\) is the energy function introduced in (3.10).

Before presenting the proof of Theorem 5.1, we discuss an easy consequence of it by taking \(D = \Omega\) and \(h = 1\):

Corollary 5.2. Under the assumptions in Theorem 5.1,

\[
G(\psi_j, n_j) \geq \sqrt{q_j} \int_{\partial \Omega} E \left( \frac{1}{b}, \nu(x; n_0) \right) ds(x) + o(\sqrt{q_j}) \quad (\kappa_j \to \infty).
\]

To prove the lower bound in Theorem 5.1, we shall split the energy into two parts, the surface energy and the bulk energy, and they will be estimated separately.

5.1 The field \(n_0\)

Here, we will construct the subsequence \(\{\psi_j, n_j, \kappa_j\}\) and the vector field \(n_0\) appearing in Theorem 5.1. This is the content of:

Lemma 5.3. Under the assumptions in Theorem 5.1, there exist \(n_0 \in C(\tau)\) and a subsequence \(\{n_{j_s}\}\) such that, as \(s \to \infty\),

\[
n_{j_s} \to n_0 \quad \text{in} \quad H^1_{\text{loc}} \cap L^p \cap W^{1,r}(\Omega, \mathbb{R}^3),
\]

for \(1 \leq p < \infty\) and \(1 \leq r < 2\), and also pointwise a.e. in \(\Omega\). Furthermore, as \(s \to \infty\),

\[
n_{j_s} \to n_0 \quad \text{uniformly on} \quad \partial \Omega.
\]

Note that we work under the assumptions in Theorem 5.1, in particular,

\[
n_j \in \mathcal{A} \quad \text{and} \quad \mathcal{E}(\psi_j, n_j) = E^{\kappa,\text{st}}(\kappa_j, q_j, \tau, K_{1,j}, K_{2,j}, K_{3,j}),
\]

where the admissible class \(\mathcal{A}\) is introduced in (1.11) and the energy \(E^{\kappa,\text{st}}(\kappa, q, \tau, K_1, K_2, K_3)\) is introduced in (1.13). By definition of the admissible class \(\mathcal{A}\), there exists a sequence of vector fields, \(\{n_{j_s}^{\partial \Omega}\} \subset C(\tau)\) such that

\[
n_j = n_{j_s}^{\partial \Omega} \quad \text{on} \quad \partial \Omega.
\]

In the sequel, we will fix the choice of the sequence \(\{n_{j_s}^{\partial \Omega}\}\) such that (5.4) holds.
Proof of Lemma 5.3. Since \( n_j \in \mathcal{A} \), we know that \( \mathcal{L}(n_j) = 0 \). In light of (1.12), we get,

\[
\mathcal{E}(\psi_j, n_j) = \mathcal{G}(\psi_j, n_j) + \mathcal{F}^+_n(n_j) + \kappa_j^2 \int_\Omega \left\{ \text{tr}(Dn_j)^2 - |\text{div}\ n_j|^2 \right\} \, dx.
\]

We write a lower bound for \( \mathcal{E}(\psi_j, n_j) \) using Lemma 2.2 and the inequality in (2.6),

\[
\mathcal{E}(\psi_j, n_j) \geq \left( \min(K_{1,j}, K_{2,j}, K_{3,j}) - 2\kappa_j^2 \right) \int_\Omega \left\{ |\text{div}\ n_j|^2 + |\text{curl}\ n_j + \tau n_j|^2 \right\} \, dx + \kappa_j^2 \int_\Omega |Dn_j|^2 \, dx - C|\Omega|\kappa_j^2.
\]

Note that, if \( n_r \in \mathcal{C}(\tau) \), then it is in the admissible class \( \mathcal{A} \) in (1.11) and

\[
\mathcal{E}(\psi_j, n_j) \leq \mathcal{E}(0, n_r) = 0.
\]

Furthermore, using Assumptions 1.1 and 1.2, we see that \((n_j)_j\) satisfy for all \( j \),

\[
\|\text{div}\ n_j\|_2 + \|\text{curl}\ n_j + \tau n_j\|_2 \leq C\kappa_j^{-1/2} \ln \kappa_j^{-1} = o(1) \quad \text{and} \quad \|Dn_j\|_2 \leq C. \quad (5.5)
\]

We can now apply Lemma 2.1 to extract a vector field \( n_0 \in \mathcal{C}(\tau) \) and a subsequence \( n_{j_0} \to n_0 \) with convergence in \( H^1(\Omega; \mathbb{R}^3) \), in \( L^p(\Omega; \mathbb{R}^3) \) for all \( 1 \leq p < \infty \), and in \( W^{1,r}(\Omega; \mathbb{R}^3) \) for all \( 1 \leq r < 2 \). We can still refine the subsequence and get the additional convergence

\[
n_{j_0} \to n_0 \quad \text{in} \quad L^r(\partial\Omega; \mathbb{R}^3) \quad \text{and} \quad n_{j_0} \to n_0 \quad \text{a.e. in} \quad \Omega.
\]

We will refine the subsequence one more time to get that \( n_{j_0}^{30} \) converges uniformly to \( n_0 \) on the boundary. Here \( \{n_j\} \) is the sequence in \( \mathcal{C}(\tau) \) and satisfying (5.4). The class \( \mathcal{C}(\tau) \) is defined in (1.8).

Since \( n_{j_0}^{30} \in \mathcal{C}(\tau) \), \( n_{j_0}^{30}(x) = Q_{j_0}N_{\tau}(Q_{j_0}x) \) where \( Q_{j_0} \in SO(3) \) is an orthogonal matrix and \( N_{\tau}(\cdot) \) is the smooth vector field introduced in (1.10).

By compactness of the orthogonal group \( SO(3) \), we may extract a subsequence and an orthogonal matrix \( Q_0 \) such that \( Q_{j_0} \to Q_0 \) in the sense of matrices. Consequently, by defining the vector field

\[
n_*(x) = Q_0N_{\tau}(Q_0'x),
\]

we infer from the \( L^r \) convergence and (5.4)

\[
n_*(x) = n_0(x) \quad \text{on} \quad \partial \Omega.
\]

The compactness of \( \overline{\Omega} \) allows us to refine the subsequence further and get

\[
\sup_{x \in \overline{\Omega}} |n_{j_0}^{30}(x) - n_*(x)| \to 0.
\]

Actually, by smoothness of \( N_{\tau}(\cdot) \), we may define \( x_{j_0} \in \overline{\Omega} \) such that

\[
\sup_{x \in \overline{\Omega}} |n_{j_0}^{30}(x) - n_*(x)| = |n_{j_0}^{30}(x_{j_0}) - n_*(x_{j_0})| = |Q_{j_0}N_{\tau}(Q_{j_0}'x_{j_0}) - Q_0N_{\tau}(Q_0'x_{j_0})|.
\]

The compactness of \( \overline{\Omega} \) ensures that \( x_{j_0} \to x_* \) along a subsequence, and (5.3) follows.
In the rest of this section, we will skip the reference to the subsequence and write

\[ \kappa = \kappa_j, \quad q = b\kappa^2_j/\tau, \quad (\psi, \mathbf{n}) = (\psi_j, n_j), \quad \mathbf{n}^\Omega = n^\Omega_j. \quad (5.6) \]

We mention one more useful estimate:

**Lemma 5.4.** Using the convention in (5.6), we have two constants \( C > 0 \) and \( t_0 > 0 \) such that, for all \( t \in (0, t_0) \),

\[ \| \mathbf{n} - \mathbf{n}^\Omega \|_{L^2(\Omega_t)} \leq C t^{3/4}, \]

where \( \Omega_t \) is defined in (3.28).

**Proof.** Let \( t_0 > 0 \) be the constant in Lemma 3.4. Our assumption on the vector fields \( \mathbf{n} \) and \( \mathbf{n}^\Omega \) say that \( |\mathbf{n}| = |\mathbf{n}^\Omega| = 1 \) a.e. and \( \mathbf{n} = \mathbf{n}^\Omega \) along the boundary of \( \Omega \). Consequently, for all \( t \in (0, t_0) \),

\[ \| \mathbf{n} - \mathbf{n}^\Omega \|_{L^2(\Omega_t)}^2 \leq 2\| \mathbf{n} - \mathbf{n}^\Omega \|_{L^1(\Omega_t)} \leq C t \| D\mathbf{n} - D\mathbf{n}^\Omega \|_{L^1(\Omega_{2t})}. \]

By compactness of the orthogonal group \( SO(3) \), we get that \( \| D\mathbf{n}^\Omega \|_\infty \) is bounded (recall that \( \mathbf{n}^\Omega \in C(\tau) \) and \( C(\tau) \) is defined in (1.8)). We use the Cauchy-Schwarz inequality and the estimate in (5.5) to write

\[ \| D\mathbf{n} - D\mathbf{n}^\Omega \|_{L^1(\Omega_{2t})} \leq |\Omega_{2t}|^{1/2} \| D\mathbf{n} - D\mathbf{n}^\Omega \|_{L^2(\Omega)} \leq C t^{1/2}. \]

\[ \square \]

### 5.2 Splitting into bulk and surface terms

We will split the energy

\[ \mathcal{G}(h\psi, \mathbf{n}; D) := \int_D \left\{ |(\nabla - i\mathbf{n})\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4 \right\} dx. \quad (5.7) \]

into boundary and bulk parts.

We introduce three parameters \( \alpha, \delta, \varepsilon \in (0, 1) \) depending on \( \kappa \) that will be used along the proof. Different conditions on these parameters will arise so as to control the error terms correctly. We work with the concrete choice.

\[ \delta = \kappa^{-1} |\ln \kappa|^{1/2}, \quad \alpha = |\ln \kappa|^{-1/16}, \quad \varepsilon = |\ln \kappa|^{-1} \quad (5.8) \]

for concreteness. Notice in particular, that the parameter \( \delta \) will have a different value than was the case for the upper bound.

We introduce smooth real-valued functions \( \chi_1 \) and \( \chi_2 \) such that \( \chi^2_1 + \chi^2_2 = 1 \) in \( \Omega \),

\[ \chi_1(x) = \begin{cases} 1, & \text{if dist}(x, \partial\Omega) < \delta/2, \\ 0, & \text{if dist}(x, \partial\Omega) > \delta, \end{cases} \]
and \(|\nabla \chi_j| \leq C/\delta\) for \(j = 1, 2\) and some constant \(C\) independent of \(\delta\). Notice that 
\[
\chi_1 \nabla \chi_1 + \chi_2 \nabla \chi_2 = 0.
\]
Therefore, we get the localization formula,
\[
\mathcal{G}(h\psi, n; D) = \mathcal{G}(\chi_1 h\psi, n; D) + \mathcal{G}(\chi_2 h\psi, n; D) + 2\sum_{j=1}^2 \int_D (\chi_j(x)^2 - \chi_j(x)^4) |h\psi|^4 \, dx - \sum_{j=1}^2 \int_D |\nabla \chi_j|^2 |h\psi|^2 \, dx.
\]

We will use the facts that
\[
\int_D (\chi_j(x)^2 - \chi_j(x)^4) |h\psi|^4 \, dx \geq 0,
\]

since \(0 \leq \chi_j(x) \leq 1\), that \(||h\psi||_\infty \leq 1\), and that the measure of the support of \(\nabla \chi_j\) is bounded by \(C\delta\) for some constant \(C\). Therefore,
\[
\mathcal{G}(h\psi, n; D) \geq \mathcal{G}(\chi_1 h\psi, n; D) + \mathcal{G}(\chi_2 h\psi, n; D) - C\delta^{-1}.
\]

In the following we estimate separately the terms \(\mathcal{G}(\chi_1 h\psi, n; D)\) (surface energy) and \(\mathcal{G}(\chi_2 h\psi, n; D)\) (bulk energy).

### 5.3 The surface energy

Let \(n_0\) be the vector field constructed in Lemma 5.3 along with the two subsequences \(\kappa = \kappa_j \to \infty\) (as \(s \to \infty\)) and \((\psi, n) = (\psi_j, n_j)\). From here till the end of subsection 6.2, we use the convention in (5.6) and write “\(\kappa \to \infty\)” for “\(\kappa_j \to \infty\)”. This section is devoted to the proof of

**Lemma 5.5.** The surface energy satisfies the following lower bound (as \(\kappa \to \infty\))

\[
\mathcal{G}(\chi_1 h\psi, n; D) \geq \sqrt{q} \int_{\Omega} E(\frac{1}{b}, \nu(x; n_0)) \, ds(x) - o(\kappa).
\]

**Proof.** The estimate of the surface energy requires two steps, a decomposition of the energy via a partition of unity, then passing to local boundary coordinates (introduced in Section 3.4) that allow us to compare with the reduced Ginzburg-Landau energy (introduced in Section 3.3).

**Step 1.** Let \(\alpha = \alpha(\kappa) \ll 1\) be a parameter that will be explicitly chosen below. Let, for \(\delta > 0\),

\[
O_\delta := \{(y_1, y_2, y_3) \mid 0 < y_1 < \delta, -\delta < y_2 < \delta, -\delta < y_3 < \delta\}.
\]

Consider the family \(\{x_{0,l}\} \subset \partial \Omega\) introduced in Lemma 3.5. For each point \(x_{0,l}\), we may introduce a coordinate transformation \(\Phi_l\) valid near the point \(x_{0,l}\) (see (3.17)). In light of Lemma 3.5, we introduce a partition of unity \(\{\tilde{\chi}_l\}\) covering the set

\[
\Omega_{\text{bnd}} := \text{supp} \chi_1,
\]

such that

\[
\begin{cases}
\sum_l \tilde{\chi}_l^2(x) = 1 \text{ and } \tilde{\chi}_l \geq 0 \text{ in } \Omega_{\text{bnd}}, \\
\tilde{\chi}_l \equiv 1 \text{ in the set } Q_{\delta,l} := \Phi_l^{-1}(O_{\{(l-\alpha)\delta\}}), \\
\exists C > 0, \forall x \in \Omega_1, \sum_l |\nabla \tilde{\chi}_l(x)|^2 \leq C(\alpha \delta)^{-2}.
\end{cases}
\]
We write the following decomposition formula
\[
G(\chi_1 h\psi, n; D) = \sum_l \left\{ G(\tilde{\chi}_l \chi_1 h\psi, n; D) + \int_D (\tilde{\chi}_l(x)^2 - \tilde{\chi}_l(x)^4) |\chi_1 h\psi|^4 dx - \int_{D\cap \Omega_l} |\nabla \tilde{\chi}_l|^2 |\chi_1 h\psi|^2 dx \right\}.
\]
By this and an inequality similar to (5.9) we get the following lower bound of the surface energy,
\[
G(\chi_1 h\psi, n; D) \geq \sum_l \left\{ G(\tilde{\chi}_l \chi_1 h\psi, n; D) - \int_{D\cap \Omega_{\text{bnd}}} |\nabla \tilde{\chi}_l|^2 |\chi_1 h\psi|^2 dx \right\}.
\]
Using the bound on $\nabla \tilde{\chi}_l$ from (5.12), the lower bound of the surface energy becomes
\[
G(\chi_1 h\psi, n; D) \geq \sum_l G(\tilde{\chi}_l \chi_1 h\psi, n; D) - C_\alpha^{-2}\delta^{-1}.
\] (5.13)

**Step 2.** Now we derive estimates for the terms in the right side of (5.13). In the following we estimate the terms of the form $G(\tilde{\chi}_l \chi_1 h\psi, n; D)$. As we shall see, the approximation relies on the construction of a suitable gauge transformation and using the local boundary coordinates.

The first step is to restrict the summation over the cells in $D$ by writing
\[
G(\chi_1 h\psi, n; D) \geq \sum_{l, Q_{\delta, l} \subset D} G(\tilde{\chi}_l \chi_1 h\psi, n; D) - C(\delta^2 k^2 + \alpha^{-2}\delta^{-1})
\] (5.14)
The lower bound in (5.14) is a simple consequence of the fact that
\[
|(D \cap \Omega_{\text{bnd}}) \setminus \bigcup_{Q_{\delta, l} \subset D} Q_{\delta, l}| \leq C_\delta^2,
\] (5.15)
which is a consequence of the assumption that the domain $D$ is regular (see Definition 1.5).

In light of (5.14), we only deal with cells $Q_{\delta, l} \subset D$. In each cell $Q_{\delta, l}$, we will apply Lemma 3.8 to obtain an estimate as in (3.35). That way, we get a function $f_{0,l} \in H^1(Q_{\delta, l})$ such that the vector field $n$ satisfies
\[
\|n - \tau(n^{\Omega})_{\text{cst,l}} - \nabla f_{0,l}\|_{L^2(Q_{\delta, l})} \leq 3\delta \sqrt{\ln \delta} \left( \|\text{curl } n + \tau n\|_{L^2(Q_{\delta, l})} + \|n - n^{\Omega}\|_{L^2(Q_{\delta, l})} \right) + C_\delta^3.
\] (5.16)
Here, $n^{\Omega} \in C(\tau)$ is the field constructed satisfying (5.4) and $(n^{\Omega})_{\text{cst,l}}$ is defined as follows,
\[
(n^{\Omega})_{\text{cst,l}} = \int_0^1 s(x - x_{0,l}) \times n^{\Omega}(x_{0,l}) \, ds.
\] (5.17)
Note that
\[
\text{curl}(n^{\Omega})_{\text{cst,l}} = -n^{\Omega}(x_{0,l}) = \tau^{-1} \text{curl } n^{\Omega}(x_{0,l}).
\] (5.18)
In light of the estimate in (5.16) we have, for all \( \varepsilon \in (0, 1/2) \),
\[
\int_D |(\nabla - i q n)\tilde{\chi}_l \chi_1 h \psi|^2 \, dx \\
\geq (1 - \varepsilon) \int_D |(\nabla - i q \tau (n^{\beta l})_{\text{est},l}) e^{-i q f_{0,l}} \tilde{\chi}_l \chi_1 h \psi|^2 \, dx \\
- C \varepsilon^{-1} q^2 \delta^2 |\ln \delta| \left( \| \text{curl} n + \tau n \|_{L^2(Q_{\delta,l})} + \| n - n^{\beta l} \|_{L^2(Q_{\delta,l})} \right) - C \varepsilon^{-1} q^2 \delta^6.
\]
(5.19)

As indicated in (5.17), the magnetic field curl \( n^{\beta l}(x_{0,l}) \) is constant. At each point \( x_{0,l} \), the director field \( n^{\beta l}(x_{0,l}) \) forms an angle
\[
\nu_{0,l} = \nu(x_{0,l}) = \arcsin(n^{\beta l}(x_{0,l}) \cdot N(x_{0,l})) \in [0, \pi/2]
\]
with the tangent plane to \( \partial \Omega \); \( N(x) \) denotes the outward normal to \( \partial \Omega \) at \( x \).

We apply the result in Lemma 3.7 to obtain a real valued smooth function \( \beta_{0,l} \) such that, if \( (n^{\beta l})_{\text{est},l} \) is the vector field defined in \( y \)-coordinates by the relation in (3.24) (with \( F = (n^{\beta l})_{\text{est},l} \)), then it holds in \( Q_{\delta,l} \),
\[
\left| (n^{\beta l})_{\text{est},l} - (A_{\nu_{0,l}} + \nabla \beta_{0,l}) \right| \leq C \delta^2,
\]
(5.20)
where \( A_{\nu_{0,l}} \) is the magnetic potential from (3.4). We introduce the function
\[
v_l = \tilde{\chi}_l \chi_1 h \psi \exp(-i q f_{0,l}) \circ \Phi_l^{-1} \times \exp(-i q \beta_{0,l}),
\]
(5.21)
and the vector field \( F \) defined in \( y \)-coordinates by the relation \( \tilde{F} = (n^{\beta l})_{\text{est},l} - \nabla \beta_{0,l} \). We mention again that for a given vector field \( F \) defined in the \( x \)-variable, we use \( \tilde{F} \) to denote the new vector field in the \( y \)-variables corresponding to \( F \) via the formula (3.24). Let \( (\tilde{F}_1, \tilde{F}_2, \tilde{F}_3) \) be the components of the vector field \( \tilde{F} \) in \( y \)-coordinates. Also, let \( \tilde{v}_l \) be the function obtained from the function \( v_l \) by converting to \( y \)-coordinates. Using (3.27) we get,
\[
\mathcal{G}(\tilde{\chi}_l \chi_1 v_l, (n^{\beta l})_{\text{est},l}; D) = \int_{O_{\delta}} \det(g_{jk})^{1/2} \left[ \sum_{1 \leq j, k \leq 3} g^{jk} (\partial_{y_j} - i q \tau \tilde{F}_j) \tilde{v}_l \times (\partial_{y_k} - i q \tau \tilde{F}_k) \tilde{v}_l - \kappa^2 |\tilde{v}_l|^2 + \frac{\kappa^2}{2} |\tilde{v}_l|^4 \right] dy.
\]
(5.23)
Inserting the estimates (3.18) and (3.20) into the above equality we obtain (again it is assumed that \( \delta \) is sufficiently small)
\[
\mathcal{G}(\tilde{\chi}_l \chi_1 v_l, (n^{\beta l})_{\text{est},l}; D)
\geq (1 - C \delta) \int_{O_{\delta}} \left\{ \left| (\nabla_y - i q \tau ((n^{\beta l})_{\text{est},l} - \nabla \beta_{0,l})) \tilde{v}_l \right|^2 - \kappa^2 |\tilde{v}_l|^2 + \frac{\kappa^2}{2} |\tilde{v}_l|^4 \right\} dy
- C \delta \kappa^2 \int_{O_{\delta}} |\tilde{v}_l|^2 \, dx.
\]
To estimate the first term in the right side of the above inequality, we use (5.21) to write the pointwise inequality (with \( \varepsilon \in (0, 1/2) \) arbitrary)
\[
\left| (\nabla_y - i q \tau ((n^{\beta l})_{\text{est},l} - \nabla \beta_{0,l})) \tilde{v}_l \right|^2 \geq (1 - \varepsilon) \left| (\nabla_y - i q \tau A_{\nu_{0,l}}) \tilde{v}_l \right|^2 + (1 - \varepsilon^{-1})(q \tau)^2 \delta^4.
\]
That way we infer from (5.19)
\[
\mathcal{G}(\tilde{v}_l, \chi_l \psi, n; D) \geq (1 - C\varepsilon - C\delta)\tilde{g}(\tilde{v}_l, A_{\nu_0})
\]
\[
- C\varepsilon^{-1}(q\tau)^2\delta^4 \int_{O_\delta} |\tilde{v}_l|^2 \, dy - C(\varepsilon + \delta)\kappa^2 \int_{O_\delta} |\tilde{v}_l|^2 \, dy
\]
\[
- C\varepsilon^{-1}q^2\delta^2 |\ln \delta| \left( \| \nabla \times n + \tau \mathbf{n} \|^2_{L^2(Q_{\delta,l})} + \| n - n^\Omega \|^2_{L^2(Q_{\delta,l})} \right) - C\varepsilon^{-1}q^2\delta^6,
\]
where
\[
\tilde{g}(\tilde{v}_l, A_{\nu_0}) = \int_{O_\delta} \left\{ |(\nabla_y - i q\tau A_{\nu_0}(y))\tilde{v}_l|^2 - \kappa^2|\tilde{v}_l|^2 + \kappa^2 |\nabla \times \tilde{v}_l|^2 \right\} \, dy.
\]
(5.24)
Recall that \(\kappa^2/(q\tau) = \frac{1}{b}\) where \(b\) is a constant in \((1, \infty)\). As a consequence, we get,
\[
\mathcal{G}(\chi_l h\psi, n; D)
\]
\[
\geq (1 - C\varepsilon - C\delta)\tilde{g}(\tilde{v}_l, A_{\nu_0}) - C(\delta + \varepsilon + \varepsilon^{-1}\kappa^2\delta^4)\kappa^2 \int_{O_\delta} |\tilde{v}_l|^2 \, dy
\]
\[
- C\varepsilon^{-1}\kappa^4\delta^2 |\ln \delta| \left( \| \nabla \times n + \tau \mathbf{n} \|^2_{L^2(Q_{\delta,l})} + \| n - n^\Omega \|^2_{L^2(Q_{\delta,l})} \right) - C\varepsilon^{-1}\kappa^4\delta^6.
\]
(5.25)
After applying the re-scaling \(y = (q\tau)^{-1/2} z\), we obtain
\[
\tilde{g}(v_l, A_n) = \frac{1}{\sqrt{q\tau}} \int_{O_{\sqrt{q\tau}}} \left\{ |(\nabla_z - i A_n(z))v_l|^2 - \frac{1}{b} |v_l|^2 + \frac{1}{2b} |v_l|^4 \right\} \, dz,
\]
(5.26)
where \(v_l(z) = v_l((q\tau)^{-1/2} z)\). Notice that our parameters satisfy \(\delta, \varepsilon \ll 1, \sqrt{q\tau} \delta \gg 1\). By using (3.11) (with \(\ell = \sqrt{q\tau} \delta\)) we conclude that,
\[
\tilde{g}(v_l, A_{\nu_0}) \geq (1 - C\varepsilon - C\delta)\sqrt{q\tau} E\left(\frac{1}{b}, \nu_0, l\right) (4\delta^2),
\]
(5.27)
provided that \(q\) is large enough (and \(\kappa^2/(q\tau) = \frac{1}{4}\)). We combine the estimates in (5.13)-(5.27) to get,
\[
\mathcal{G}(\chi_l h\psi, n; D)
\]
\[
\geq \sum_{Q_{\delta,l} \subset D} (1 - C\varepsilon - C\delta)\sqrt{q\tau} E\left(\frac{1}{b}, \nu_0, l\right) (4\delta^2) - C(\delta + \varepsilon + \varepsilon^{-1}\kappa^2\delta^4)\kappa^2 \int_{O_\delta} |\tilde{v}_l|^2 \, dy
\]
\[
- C\varepsilon^{-1}\kappa^4\delta^2 |\ln \delta| \left( \| \nabla \times n + \tau \mathbf{n} \|^2_{L^2(\Omega)} + \| n - n^\Omega \|^2_{L^2(\{\text{dist}(x,\partial\Omega) \leq C\delta\})} \right)
\]
\[
- C\varepsilon^{-1}\kappa^4\delta^4 - C\alpha^{-2}\delta^{-1}.
\]
To control the error terms in the right side of the above inequality, we estimate as before using the finite overlap of the supports of the partition of unity, and we get
\[
\sum_{l} \int_{O_\delta} |\tilde{v}_l|^2 \, dy \leq C \int_{\Omega_{\text{bnd}}} |\psi|^2 \, dx = C \int_{\Omega_{\text{bnd}}} |\psi|^2 \, dx \leq C\delta.
\]
(5.28)
The terms \( \| \text{curl} \mathbf{n} + \tau \mathbf{n} \|_2 \) is estimated in (5.5). The term \( \| \mathbf{n} - \mathbf{n}^{\Omega} \|_{L^2(\{ \text{dist}(x, \partial \Omega) \leq C\delta \})} \) is estimated by Lemma 5.4. That way we get,

\[
\mathcal{G}(\chi_1 h\psi, \mathbf{n}; D) \geq \sum_{Q_{\delta,l} \subset D} (1 - C \varepsilon - C \delta) \sqrt{q_T} E \left( \frac{1}{b}, \nu_{0,l} \right) (4\delta^2) - C(\delta + \varepsilon + \varepsilon^{-1} \kappa^2 \delta^4) \delta \kappa^2
\]

\[ - C \varepsilon^{-1} \kappa^4 \delta^2 | \ln \delta | (\kappa^{-1} | \ln \kappa^{-2} (\delta + \varepsilon) + \delta^{3/2}) - C \varepsilon^{-1} \kappa^4 \delta^4 - C \alpha^{-2} \delta^{-1}. \] (5.29)

With the choice (5.8) of the parameters we find that all the error terms in (5.29) are of order \( o(\kappa) \) when \( \kappa \to \infty \). Thus,

\[
\mathcal{G}(\chi_1 h\psi, \mathbf{n}; D) \geq \sum_{l_0} (1 - C \varepsilon - C \delta) \sqrt{q_T} E \left( \frac{1}{b}, \nu_{0,l} \right) (4\delta^2) - o(\kappa). \] (5.30)

where the sum over all \( l_0 \) such that \( Q_{\delta,l} \subset D \).

Now we estimate the sum in (5.30). Recall the definition of the angle \( \nu_{0,l} \) in (5.20). By Lemma 5.3, we get that, as \( \kappa \to \infty \),

\[
E \left( \frac{1}{b}, \nu_{0,l} \right) - E \left( \frac{1}{b}, \nu(x_0,l; \mathbf{n}_0) \right) \to 0 \quad \text{uniformly in } l. \]

Here \( \mathbf{n}_0 \) is the vector field constructed in Sec. 5.1 and satisfying (5.2). The angle \( \nu(x_0,l; \mathbf{n}_0) \in [0, \pi/2] \) is

\[
\arcsin(\mathbf{n}_0(x_0,l) \cdot \mathbf{N}(x_0,l)),
\]

where \( \mathbf{N} \) is the unit outward normal vector on \( \partial \Omega \).

That way, the sum in (5.30) can be estimated as follows

\[
\sum_{l_0} (1 - C \varepsilon - C \delta) \sqrt{q_T} E \left( \frac{1}{b}, \nu_{0,l} \right) (4\delta^2) = \sum_{l_0} (1 - C \varepsilon - C \delta) \sqrt{q_T} E \left( \frac{1}{b}, \nu(x_0,l; \mathbf{n}_0) \right) (4\delta^2) + o(1).
\]

The sum on the right side can be estimated via a Riemann sum of the continuous function \( \partial \Omega \ni x \mapsto E \left( \frac{1}{b}, \nu(x; \mathbf{n}_0) \right) \). That way we obtain that, as \( \kappa \to \infty \),

\[
\sum_{l_0} \left\{ E \left( \frac{1}{b}, \nu_{0,l} \right) (4\delta^2) \right\} = \int_{\partial \Omega} E \left( \frac{1}{b}, \nu(x; \mathbf{n}_0) \right) ds(x) + o(1). \] (5.31)

We insert (5.31) into (5.30), to get (5.11). \( \square \)

### 5.4 The bulk energy

Compared to the estimate of the surface energy, the estimation of the term \( \mathcal{G}(\chi_2 h\psi, \mathbf{n}; D) \) is easy. Recall the choice of parameters (5.8) involved in the definition of \( \chi_2 \). We will prove that

**Lemma 5.6.** Under the assumptions in Theorem 5.1, the subsequence in Lemma 5.5 \( (\psi, \mathbf{n}, \kappa) = (\psi_j, \mathbf{n}_j, \kappa_j) \) satisfies,

\[
\int_{\{ \text{dist}(x, \partial \Omega) \geq \kappa^{-1} | \ln \kappa^{1/2} \}} |\psi|^2 dx = o(\kappa^{-1}), \] (5.32)

and

\[
\mathcal{G}(\chi_2 h\psi, \mathbf{n}; D) \geq -o(\kappa) \quad \text{as } \kappa \to \infty. \] (5.33)
Proof. Step 1. The first step in the proof of Lemma 5.6 consists of determining a lower bound to $G(\chi_2 h\psi, n)$. Let $\delta, \varepsilon$ and $\alpha$ be the positive parameters introduced in (5.8). We cover $\mathbb{R}^3$ by cubes $\{Q_1(x_j, \alpha)\}_j$, where for all $j \in \mathbb{Z}^3$, $y = (y_1, y_2, y_3) \in \mathbb{R}^3$ and $\delta > 0$, we define,

$$x_{j, \alpha} = (1 - \alpha)j, \quad Q_\ell(y) = \prod_{k=1}^3 \left( y_k - \frac{\delta}{2}, y_k + \frac{\delta}{2} \right).$$

Let $(g_j)$ be a partition of unity in $\mathbb{R}^3$ such that,

$$\sum_j g_j^2 = 1, \quad \text{supp} g_j \subset Q_1(x_{j, \alpha}), \quad |\nabla g_j| \leq \frac{C}{\alpha},$$

for some universal constant $C$.

Defining the re-scaled functions,

$$\forall x \in \mathbb{R}^3, \quad g_{j, \delta}(x) = g_j(x/\delta),$$

we get a new partition of unity $(g_{j, \delta})_j$ such that each $g_{j, \delta}$ has support in the cube $Q_{j, \delta} := Q_\delta(x_{j, \alpha})$ of side length $\delta$ and,

$$\sum_j g_{j, \delta}^2 = 1, \quad |\nabla g_{j, \delta}| \leq \frac{C}{\alpha \delta}.$$

Let

$$\mathcal{J} = \{j \in \mathbb{Z}^3 : \text{supp} \chi_2 \cap \text{supp} g_{j, \delta} \neq \emptyset\}, \quad \text{and} \quad N_\delta = \text{Card} \mathcal{J}.$$

Then we know that, for $\delta$ and $\alpha$ sufficiently small,

$$|\Omega| \leq N_\ell \times \delta^3 \leq |\Omega| + O(\delta) + O(\alpha). \quad (5.34)$$

We have the localization formula, with arguments as before,

$$G(\chi_2 h\psi, n) \geq \sum_{j \in \mathcal{J}} G(g_{j, \delta} \chi_2 h\psi, n) - \sum_j \int_\Omega |\nabla g_{j, \delta}|^2 |\chi_2 h\psi|^2 \, dx$$

$$\geq \sum_{j \in \mathcal{J}} G(g_{j, \delta} \chi_2 h\psi, n) - \frac{C}{\alpha^2 \delta^2} \int_\Omega |h\psi|^2 \, dx, \quad (5.35)$$

using that $\chi_2 \leq 1$ and the finite overlap of the $g_{j, \delta}$'s.

Now we estimate the first term in the right side of (5.35). We define the constant vector field

$$n_{av,j} = \frac{1}{|Q_{j, \delta}|} \int_{Q_{j, \delta}} n \, dx,$$

along with magnetic potential

$$a_{av,j} = -\int_0^1 s(x - x_{j, \delta}) \times n_{av,j} \, ds.$$

We apply Lemma 3.9 in $Q_{j, \delta}$ to obtain a function $f_{j, \delta}$ such that,

$$\|n - \tau a_{av,j} - \nabla f_{j, \delta}\|^2_{L^2(Q_{j, \delta})} \leq C\delta^2 |\ln \delta| \left( \|\text{curl} n + \tau n\|^2_{L^2(Q_{j, \delta})} + \delta^2 \|Dn\|^2_{L^2(Q_{j, \delta})} \right) + C\delta^9.$$
It is therefore possible to estimate the ‘kinetic energy’ term in $G(g_{j,\delta}\chi_2 h\psi, n)$ from below as follows:

$$
\int_{\Omega} |(\nabla - iq\mathbf{n})g_{j,\delta}\chi_2\psi|^2 \, dx \geq (1 - \varepsilon) \int_{\Omega} |(\nabla - iq\tau\mathbf{a}_{av,j})e^{-qf_{j,\delta}}g_{j,\delta}\chi_2\psi|^2 \, dx
- C\varepsilon^{-1}q^2\delta^2|\ln \delta| (\|\text{curl } \mathbf{n} + \tau \mathbf{n}\|_{L^2(Q_{j,\delta})}^2 + \delta^2\|D\mathbf{n}\|_{L^2(Q_{j,\delta})}^2) + C\varepsilon^{-1}q^2\delta^6. \tag{5.36}
$$

Here $\varepsilon$ is an arbitrary real number in $(0, 1)$ whose choice will be specified later.

Referring to (5.5), we know that $\|D\mathbf{n}\|_{L^2(Q_{j,\delta})} \leq C$ where $C$ is a constant independent of $\delta$, $\kappa$ and $q$. By Lemma 3.9, $\text{curl } \mathbf{a}_{av,j}$ is constant and has magnitude $\geq 1 - C\ell$. Since every function $g_{j,\delta}\chi_2\psi$ has compact support in $\Omega$, we may write using (3.3),

$$
\int_{\Omega} |(\nabla - iq\mathbf{n})g_{j,\delta}\chi_2\psi|^2 \, dx \geq q\tau(1 - C\delta) \int_{\Omega} |g_{j,\delta}\chi_2\psi|^2 \, dx. \tag{5.37}
$$

Inserting (5.37), (5.36) into (5.35), we get,

$$
G(\chi_2 h\psi, \mathbf{n}) \geq [q\tau(1 - C\delta)(1 - \varepsilon) - \kappa^2 - \frac{C}{\alpha^2\delta^2}] \int_{\Omega} |\chi_2\psi|^2 \, dx
- C\varepsilon^{-1}q^2\delta^2|\ln \ell| (\|\text{curl } \mathbf{n} + \tau \mathbf{n}\|_{L^2(\Omega)}^2 + \delta^2\|D\mathbf{n}\|_{L^2(\Omega)}^2) + C\varepsilon^{-1}q^2\delta^6. \tag{5.38}
$$

We estimate the error term using the inequalities in (5.5) to obtain,

$$
G(\chi_2 h\psi, \mathbf{n}) \geq [q\tau(1 - \varepsilon)(1 - C\delta) - \kappa^2 - \frac{C}{\alpha^2\delta^2}] \int_{\Omega} |\chi_2\psi|^2 \, dx
- C\varepsilon^{-1}q^2\delta^2|\ln \ell| (\kappa^{-1}|\ln \kappa|^{-2}o(1) + \delta^2) - C\varepsilon^{-1}q^2\delta^6. \tag{5.39}
$$

By assumption, the parameters $q$, $\tau$ and $\kappa$ satisfy

$$
q\tau = b\kappa^2, \quad b > 1.
$$

Consequently, when $\kappa$ is sufficiently large, the choice of the parameters $\delta$, $\alpha$, $\varepsilon$ in (5.8) yields

$$
q\tau(1 - \varepsilon)(1 - C\delta) - \kappa^2 - \frac{C}{\alpha^2\delta^2} \geq (b - 1)\kappa^2 - \kappa^2o(1) \geq \frac{(b - 1)}{2}\kappa^2 > 0,
$$

and

$$
\varepsilon^{-1}q^2\delta^2|\ln \delta| (\kappa^{-1}|\ln \kappa|^{-2}o(1) + \delta^2) + \varepsilon^{-1}q^2\delta^6 = o(\kappa).
$$

Inserting this into (5.39), we get, as $\kappa \to \infty$,

$$
G(\chi_2 h\psi, \mathbf{n}) \geq \frac{(b - 1)}{2}\kappa^2 \int_{\Omega} |\chi_2\psi|^2 \, dx + o(\kappa). \tag{5.40}
$$

**Step 2.** Now, we insert (5.40) and the lower bound in Lemma 5.11 (used with $D = \Omega$) into (5.10). We get that,

$$
G(\psi, \mathbf{n}) \geq \sqrt{q\tau} \int_{\partial\Omega} E(b, \nu(x; \mathbf{n}_0)) \, ds(x) + \frac{(b - 1)}{2}\kappa^2 \int_{\Omega} |\chi_2\psi|^2 \, dx + o(\kappa).
$$
We insert the upper bound for $G(\psi, n)$ given in Proposition 4.1, then we cancel the matching terms in the resulting inequality to get,

$$
\int_{\Omega} |\chi_2 \psi|^2 dx \leq o(\kappa^{-1}).
$$

(5.41)

Dropping the positive terms in the energy $G(\chi h \psi, n; D)$ and using (5.41) to estimate the negative term, we get the inequality in (5.33).

The estimate in (5.32) results from (5.41) by recalling that $\chi_2 = 1$ in $\{\text{dist}(x, \partial \Omega) \geq \delta\}$ and that $\delta = |\ln \kappa|^{1/2} \kappa^{-1}$.

### 5.5 Proof of Theorem 5.1

The proof of Theorem 5.1 follows by collecting the estimates in (5.10) and Lemmas 5.5 and 5.6.

### 6 Proof of the main theorems

In this section, we will present the proof of Theorems 1.4 and 1.6.

#### 6.1 Proof of Theorem 1.4

Proposition 4.1 yields

$$
\limsup_{\kappa \to \infty} \frac{E^{\text{st}}(\kappa, q, \tau, K_1, K_2, K_3)}{\sqrt{q\tau}} \leq \epsilon_0 \left(\frac{1}{b}, \tau\right).
$$

Suppose the conclusion in Theorem 1.4 were false, then there exists a sequence $\kappa_j \to \infty$ such that

$$
\lim_{j \to \infty} \frac{E^{\text{st}}(\kappa_j, q_j, \tau, K_{1,j}, K_{2,j}, K_{3,j})}{\sqrt{q\tau}} < \epsilon_0 \left(\frac{1}{b}, \tau\right).
$$

Let $(\psi_j, n_j)$ be a minimizer of the energy in (1.13) with $\kappa = \kappa_j$ and $q = q_j$. By the assumption in Theorem 1.4, we know that

$$
\mathcal{G}(\psi_j, n_j) \leq \mathcal{E}(\psi_j, n_j) = E^{\text{st}}(\kappa_j, q_j, \tau, K_{1,j}, K_{2,j}, K_{3,j})).
$$

Owing to Corollary 5.2, there exists a subsequence $\kappa_{j_*} \to \infty$ and a vector field $n_0 \in C(\tau)$ such that

$$
\int_{\partial\Omega} E\left(\frac{1}{b}, \nu(x, n_0)\right) ds(x) \leq \lim_{s \to \infty} \frac{E^{\text{st}}(\kappa_{j_*}, q_b, \tau, K_1, K_2, K_3)}{\sqrt{q\tau}} < \epsilon_0 \left(\frac{1}{b}, \tau\right).
$$

This violates the definition of $\epsilon_0$ in (1.15).
6.2 Proof of Theorem 1.6

The first assertion is proved in Sec. 5.1, namely in (5.2). Using the inequality,
\[ G(\psi_j, n_{js}) \leq \mathcal{E}(\psi_j, n_{js}) , \]  
(6.1)
we infer from Theorem 1.4 and Corollary 5.2 that the vector field \( n_0 \) satisfies the additional property \( n_0 \in M \), where \( M \) is the set introduced in (1.16).

The second assertion in Theorem 1.6 is obtained by combining the results in Theorems 1.4 and 5.1 (and Corollary 5.2).

The rest of this section is devoted to the lengthy proof of the last assertions in Theorem 1.6. We will split the proof into several steps. In the sequel, following the convention in (5.6), \((\psi, n) = (\psi_j, n_{js})\) is the subsequence of minimizers of the functional in (1.1), and \( D \subset \Omega \) is a regular domain as in Definition 1.5.

**Step 1. Local energy estimate**

We have the simple decomposition of the energy in (1.2),
\[ G(\psi, n) = G(\psi, n; D) + G(\psi, n; \overline{D}) , \]  
(6.2)
where \( \overline{D} = \Omega \setminus D \).

Using Theorem 5.1 for the domain \( \overline{D} \) and with \( h = 1 \), we get,
\[ G(\psi, n; \overline{D}) \geq \sqrt{qT} \int_{\overline{D} \cap \partial \Omega} E\left(\frac{1}{b}, \nu(x; n_0)\right) ds(x) + o(\kappa) . \]  
(6.3)

In light of the inequality in (6.1) and the result in Proposition 4.1, we get an upper bound for \( G(\psi, n) \). Using this and the lower bound for \( G(\psi, n; \overline{D}) \) in (6.3), we infer from (6.2),
\[ G(\psi, n; D) \leq \sqrt{qT} \int_{D \cap \partial \Omega} E\left(\frac{1}{b}, \nu(x; n_0)\right) ds(x) + o(\kappa) . \]

Combining this upper bound and the lower bound (6.3), we get the asymptotics in (1.17).

**Step 2. Global estimate of the \( L^4 \)-norm**

The order parameter \( \psi \) satisfies the equation
\[-(\nabla - iq n)^2 \psi = \kappa^2 (1 - |\psi|^2) \psi \quad \text{in} \ \Omega , \]
with magnetic Neumann boundary conditions on \( \partial \Omega \). Multiplying both sides of the equation by \( \psi \) and integrating by parts, we get,
\[ \frac{\kappa^2}{2} \int_{\Omega} |\psi|^4 dx = -G(\psi, n) . \]

Using the estimate for \( G(\psi, n) \) in (1.17) (with \( D = \Omega \)), we get,
\[ \kappa \int_{\Omega} |\psi|^4 dx = -\frac{2\sqrt{qT}}{\kappa} \int_{\partial \Omega} E\left(\frac{1}{b}, \nu(x; n_0)\right) ds(x) + o(1) . \]  
(6.4)

44
Step 3. Local estimate of the $L^4$ norm

Here we use a method in [13] to determine an upper bound for $\int_D |\psi|^4 \, dx$ for any sub-domain $D$ of $\Omega$. This is a new ingredient in the proof compared to the similar statements for the Ginzburg-Landau order parameter in [11]. The novelty is that we do not use elliptic a priori estimates satisfied by $\psi$.

By the assumption that the domain $D$ is regular in the sense described in Definition 1.5, we may reduce the analysis to distinguish between the case when $D \cap \partial \Omega$ is empty and the case when $D \cap \partial \Omega$ is a smooth surface without boundary (or a smooth surface with a piece-wise smooth boundary). In general, $D$ will be the union of a finite number of sub-domains satisfying the aforementioned assumptions.

**Case 1.** $D \cap \partial \Omega = \emptyset$.

In this case, the integral on $\partial \Omega \cap D$ vanishes. So we have to prove that

$$\kappa \int_D |\psi|^4 \, dx = o(1) \quad \text{as } \kappa \to \infty.$$

Since $D \subset \Omega$, then for $\kappa$ sufficiently large, $D \subset \{ \text{dist}(x, \partial \Omega) \geq \kappa^{-1/2} \}$. That way, in virtue of (5.32), we write,

$$\int_D |\psi|^4 \, dx \leq \int_{\{\text{dist}(x, \partial \Omega) \geq \kappa^{-1/2}\}} |\psi|^4 \, dx = o(\kappa^{-1}).$$

**Case 2.** $D \cap \partial \Omega$ is a smooth surface (without boundary or with a piece-wise smooth boundary).

In this case, the assumption on $D = \tilde{D} \cap \Omega$ guarantees that $D \cap \partial \Omega$ is a finite union of smooth surfaces in $\partial \Omega$.

Let

$$\ell = \kappa^{-1/2} \ln \kappa \quad \text{and} \quad D_\ell = \{ x \in D : \text{dist}(x, \partial D) \geq \ell \}.$$ 

Consider a cut-off function $\chi_\ell \in C_0^\infty(D)$ such that,

$$\|\chi_\ell\|_\infty \leq 1, \quad \|\nabla \chi_\ell\|_\infty \leq \frac{C}{\ell}, \quad \chi_\ell = 1 \text{ in } D_\ell, \quad \text{and } \text{supp } \chi_\ell \subset \overline{D_\ell/2}.$$ 

The function $\chi_\ell^2 \psi$ is easily seen to belong to $H^1_0(D)$. Multiplying both sides of the equation in (1.2) by $\chi_\ell^2 \overline{\psi}$ then integrating over $D$, we get,

$$\int_D \{ |(\nabla - iqn)\chi_\ell \psi|^2 - \kappa^2 \chi_\ell^2 |\psi|^2 + \kappa^2 \chi_\ell^2 |\psi|^4 \} \, dx = \int_D |\nabla \chi_\ell|^2 |\psi|^2 \, dx. \quad (6.5)$$

We estimate using the bounds $\|\psi\|_\infty \leq 1$, $|\nabla \chi_\ell| \leq C/\ell$ and the condition on the support of $\nabla \chi_\ell$,

$$\int_D |\nabla \chi_\ell|^2 |\psi|^2 \, dx \leq C \ell^{-2} \int_{\{\text{dist}(x, \partial D) \leq \ell\}} \, dx = C \ell^{-1} = o(\kappa).$$

That way, we infer from (6.5) that, as $\kappa \to \infty$,

$$\int_D \{ |(\nabla - iqn)\chi_\ell \psi|^2 - \kappa^2 \chi_\ell^2 |\psi|^2 + \kappa^2 \chi_\ell^2 |\psi|^4 \} \, dx = o(\kappa). \quad (6.6)$$
We estimate \( \int_D \chi_\ell^2 |\psi|^4 \, dx \) as follows. We write
\[
\int_D \chi_\ell^2 |\psi|^4 \, dx = \int_D |\psi|^4 \, dx + \int_D (1 - \chi_\ell^2)|\psi|^4 \, dx.
\] (6.7)

Since \( \ell = \kappa^{-1} \ln \kappa \geq \kappa^{-1} \ln \kappa^{1/2} \), we may use the estimate in (5.32) to write
\[
\int_{D \cap \{ \text{dist}(x, \partial \Omega) \geq \ell \}} (1 - \chi_\ell^2)|\psi|^4 \, dx = o(\kappa^{-1}).
\] (6.8)

The condition on the support of \( 1 - \chi_\ell \) and the assumption on the regularity of \( D \) imply that (see Definition 1.5)
\[
|D \cap (\text{supp}(1 - \chi_\ell)) \cap \{ \text{dist}(x, \partial \Omega) \leq \ell \}| = O(\ell^2) = o(\kappa^{-1}),
\]

and consequently
\[
\int_{D \cap \{ \text{dist}(x, \partial \Omega) \leq \ell \}} (1 - \chi_\ell^2)|\psi|^4 \, dx = o(\kappa^{-1}).
\]

Inserting this estimate and (6.8) into (6.7), we get
\[
\int_D \chi_\ell^2 |\psi|^4 \, dx = \int_D |\psi|^4 \, dx + o(\kappa^{-1}).
\] (6.9)

Since \( 1 \geq \chi_\ell^2 \geq \chi_\ell^4 \), the estimates (6.6) and (6.9) imply,
\[
-\frac{\kappa^2}{2} \int_D \chi_\ell^2 |\psi|^4 \, dx \geq \mathcal{G}(\chi_\ell \psi, n; D) - o(\kappa)
\]
\[
\geq \sqrt{q} \tau \kappa \int_{D \cap \partial \Omega} E \left( \frac{1}{b}, \nu(x; n_0) \right) \, ds(x) - o(\kappa),
\] (6.10)

where we used that Theorem 5.1 and that \( \|\chi_\ell\|_\infty \leq 1 \). That way, we infer from (6.9) and (6.10) that, as \( \kappa \to \infty \),
\[
\int_D |\psi(x)|^4 \, dx \leq -\frac{2\sqrt{q} \tau}{\kappa^2} \int_{D \cap \partial \Omega} E \left( \frac{1}{b}, \nu(x; n_0) \right) \, ds(x) + o(\kappa^{-1}).
\] (6.11)

**Step 4: Lower bound**

Notice that (6.11) is valid when \( D \) is replaced by the complementary of \( D \) in \( \Omega \), i.e. \( \overline{\Omega} \). We have the simple decomposition,
\[
\int_D |\psi(x)|^4 \, dx = \int_\Omega |\psi(x)|^4 \, dx - \int_{\overline{\Omega}} |\psi(x)|^4 \, dx
\]
\[
\geq \int_\Omega |\psi(x)|^4 \, dx - \frac{2\sqrt{q} \tau}{\kappa^2} \int_{\overline{\Omega} \cap \partial \Omega} E \left( \frac{1}{b}, \nu(x; n_0) \right) \, ds(x) + o(\kappa^{-1}).
\]

Using the asymptotics in (6.4) obtained in Step 2, we deduce that, as \( \kappa \to \infty \),
\[
\int_D |\psi(x)|^4 \, dx \geq -\frac{2\sqrt{q} \tau}{\kappa^2} \int_{\overline{\Omega} \cap \partial \Omega} E \left( \frac{1}{b}, \nu(x; n_0) \right) \, ds(x) + o(\kappa^{-1}).
\]

Combining this lower bound and the upper bound in (6.11), we obtain the asymptotics announced in the fourth assertion of Theorem 1.6. This finishes the proof of Theorem 1.6. \(\square\)

46
6.3 Proof of Theorem 1.8

Here we present the proof of Theorem 1.8 which is relatively easier than that of Theorem 1.6. The proof is along similar calculations done in [11], so we will be rather succinct here.

6.3.1 Upper bound

Recall that \( b > 1 \) is a fixed constant and \( q\tau = b\kappa^2 \). Since \( C(\tau) \) is a closed set in a finite dimensional space, then we can choose \( n_0 \in C(\tau) \) such that

\[
\tilde{E}\left(\frac{1}{b}, n_0 \right) = e_0\left(\frac{1}{b}, \tau \right),
\]

where \( \tilde{E} \) and \( e_0 \) are the energies in (1.14) and (1.15).

We have, for all \( \psi \in H^1(\Omega; \mathbb{C}) \)

\[
E(\psi, n_0) = G(\psi, n_0) = \int_{\Omega} \left\{|\nabla q_{n_0}\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4\right\} dx. \tag{6.12}
\]

Upon minimizing this energy over \( \psi \), we will get an upper bound to the full energy in (1.1). This will be done through the computation of the energy of a relevant test configuration, whose construction hints at the expected behavior of the actual minimizers of the energy in (1.1). We take the same trial function \( \psi_{\text{trial}} \) in the proof of Lemma 4.2. Thanks to Lemma 4.2, we get, for all \( K_1, K_2, K_3 \geq 0 \),

\[
E_{\text{g},\ast}(\kappa, q, \tau, K_1, K_2, K_3) \leq (1 + C\eta)\sqrt{q\tau}e_0\left(\frac{1}{b}, \tau \right) + C\eta + \kappa f(\kappa),
\]

where the function \( f(\cdot) \) is independent of \( K_1, K_2, K_3 \) and \( f(\kappa) = o(1) \) as \( \kappa \to \infty \). Taking successively the limit as \( \min(K_1, K_2, K_3) \to \infty \) then as \( \kappa \to \infty \), we get,

\[
\limsup_{\kappa \to \infty} \left( \limsup_{\min(K_1, K_2, K_3) \to \infty} \frac{E_{\text{g},\ast}(\kappa, q, \tau, K_1, K_2, K_3)}{\sqrt{q\tau}} \right) \leq (1 + C\eta)\sqrt{q\tau}e_0\left(\frac{1}{b}, \tau \right) + C\eta.
\]

Sending \( \eta \to 0_+ \), we get

\[
\limsup_{\kappa \to \infty} \left( \limsup_{\min(K_1, K_2, K_3) \to \infty} \frac{E_{\text{g},\ast}(\kappa, q, \tau, K_1, K_2, K_3)}{\sqrt{q\tau}} \right) \leq e_0\left(\frac{1}{b}, \tau \right),
\]

which can be re-written in the form,

\[
\limsup_{\min(K_1, K_2, K_3) \to \infty} E_{\text{g},\ast}(\kappa, q, \tau, K_1, K_2, K_3) \leq \sqrt{q\tau}e_0\left(\frac{1}{b}, \tau \right) + o(\kappa). \tag{6.13}
\]

6.3.2 Lower bound

It is proved in [14] that,

\[
\lim_{\min(K_1, K_2, K_3) \to \infty} E_{\text{g},\ast}(\kappa, q, \tau, K_1, K_2, K_3) = \inf_{(\psi, n_0) \in H^1(\Omega; \mathbb{C}) \times C(\tau)} G(\psi, n_0), \tag{6.14}
\]
where $C(\tau)$ is introduced in (1.8) and $G$ is the functional in (1.2). Since the Oseen-Frank energy in (1.3) vanishes for all $n_0 \in C(\tau)$, we get, for all $(\psi, n_0) \in H^1(\Omega; \mathbb{C}) \times C(\tau)$ and $K_1, K_2, K_3 \geq 0$,

$$G(\psi, n_0) \geq E^{g, st}(\kappa, q, \tau, K_1, K_2, K_3).$$

In particular, when $K_1 = K_2 = K_3 = \kappa^4$ and $q \tau = b \kappa^2$, Assumptions 1.1 and 1.2 are satisfied and we can use Theorem 1.4 to write a lower bound for $E^{g, st}(\kappa, q, \tau, K_1, K_2, K_3)$. That way we get,

$$G(\psi, n_0) \geq \sqrt{q \tau} e_0\left(\frac{1}{b}, \tau\right) + \kappa f(\kappa),$$

where $f(\kappa)$ is a function satisfying $f(\kappa) = o(1)$ as $\kappa \to \infty$. Consequently, (6.14) yields,

$$\lim_{\min(K_1, K_2, K_3) \to \infty} E^{g, st}(\kappa, q, \tau, K_1, K_2, K_3) \geq \sqrt{q \tau} e_0\left(\frac{1}{b}, \tau\right) + \kappa f(\kappa). \quad (6.15)$$

Combining the upper and lower bounds in (6.13) and (6.15) finishes the proof of Theorem 1.8.

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