

Thin film liquid crystals with oblique anchoring and boojums

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Abstract

We study a two-dimensional variational problem which arises as a thin-film limit of the Landau-de Gennes energy of nematic liquid crystals. We impose an oblique angle condition for the nematic director on the boundary, via boundary penalization (weak anchoring.) We show that for strong anchoring strength (relative to the usual Ginzburg-Landau length scale parameter), defects will occur in the interior, as in the case of strong (Dirichlet) anchoring, but for weaker anchoring strength all defects will occur on the boundary. These defects will each carry a fractional winding number; such boundary defects are known as “boojums”. The boojums will occur in ordered pairs along the boundary; for angle $\alpha \in (0, \frac{\pi}{2})$, they serve to reduce the winding of the phase by steps of 2α and $(2\pi - 2\alpha)$ in order to avoid the formation of interior defects. We determine the number and location of the defects via a Renormalized Energy and numerical simulations.

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1. Introduction

In this paper we study minimizers of a variational problem motivated by the study of defects in a nematic liquid crystal. We consider a two-dimensional setting, arising in a thin-film reduction of the three dimensional Landau–de Gennes model to two dimensions. The special feature of our problem is in the boundary condition imposed, in which energy minimization prefers that the nematic director be oblique to the normal to the boundary with a prescribed angle. In three dimensions, such a fixed angle condition constrains the nematic director to lie on a cone coaxial with the boundary normal; in the plane, this reduces to demanding that the director make an angle of $\pm\alpha$ with respect to the normal vector at each boundary point. In our model this will be accomplished by imposing *weak anchoring conditions* on the domain boundary, that is, by adding a penalization term to the energy which favors oblique director configurations. We refer the reader to [21,20,19] for the detailed discussion of anchoring within the context of the Landau-de Gennes theory and relevant physical observations.

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We begin by describing the variational problem in mathematical terms, and stating our main result in Theorem 1.1. Let $\Omega \subset \mathbb{R}^2$ be a bounded, simply connected domain with C^2 boundary $\Gamma := \partial\Omega$, carrying unit exterior normal vector ν . Our energy functional is the classical Ginzburg-Landau functional, modified by the addition of a surface energy term which enforces the desired weak anchoring. Let $\alpha \in (0, \frac{\pi}{2})$ be fixed throughout the paper. As usual, we associate $\mathbb{C} \simeq \mathbb{R}^2$, with scalar product $(u, v) = \Re[u \bar{v}]$ and wedge product $u \wedge v = (iu, v)$ for $u, v \in \mathbb{C}$. Let $g : \Gamma \rightarrow \mathbb{S}^1 \subset \mathbb{C}$ be a given C^1 smooth function on the boundary. We assume that

$$\mathcal{D} = \deg(g; \Gamma) > 0,$$

and take a smooth lifting $\gamma : \Gamma \rightarrow \mathbb{R}$, $g = e^{i\gamma}$. In the physical context, g would represent the unit normal vector field on Γ ; in the orientable GL or Ericksen models, it would then have degree $\mathcal{D} = 1$. In the reduction from the 3D Landau-de Gennes model the complex order parameter doubles the phase of the director, and so we would have $\mathcal{D} = 2$. (See the discussion below.) However, we may take g to be any smooth \mathbb{S}^1 -valued map in our analysis.

Our energy then takes the form:

$$E_\varepsilon^{g,\alpha}(u) := \frac{1}{2} \int_{\Omega} \left(|\nabla u|^2 + \frac{1}{2\varepsilon^2} (|u|^2 - 1)^2 \right) dx + \frac{\Upsilon}{2} \int_{\Gamma} W(u, g) ds, \quad (1.1)$$

with boundary anchoring energy density W given by:

$$W(u, g) := \frac{1}{2} (|u|^2 - 1)^2 + [(u, g) - \cos \alpha]^2. \quad (1.2)$$

The weak anchoring strength Υ is assumed to depend on the length scale parameter ε ,

$$\Upsilon = \Upsilon(\varepsilon) = \varepsilon^{-s} \quad \text{for } s \in (0, 1].$$

The effect of the weak anchoring may be inferred from the form of W . As $\varepsilon \rightarrow 0$ we expect that $W(u_\varepsilon, g) \rightarrow 0$ almost everywhere on Γ . At points $y \in \Gamma$ at which $W(u_\varepsilon(y), g(y)) \rightarrow 0$, we would have $|u_\varepsilon| \rightarrow 1$ and $(u, g) \rightarrow \cos \alpha$, that is, $u_\varepsilon \simeq g \exp(\pm i\alpha)$. If g represents the unit normal vector field, this is the desired cone condition for a nematic. If there are no defects on Γ then the phase shift $\pm\alpha$ is uniformly chosen on Γ , and u_ε will effectively satisfy a Dirichlet boundary condition with degree \mathcal{D} , for which there must be interior defects, which will be vortices. However, energy minimization may prefer to accept defects on Γ in order to avoid the energy cost of interior vortices. In this case, the phase of u_ε must jump at defect points in order to “unwind” its phase so as to have degree zero on Γ . The form of W allows the phase to unwind by steps of 2α , $(2\pi - 2\alpha)$ or 2π . This suggests that there are *three* distinct types of boundary defects. The first two are *boojums*—defects with fractional degree. In correspondence with the size of the jump in angle, we call these a “light” boojum and a “heavy” boojum, respectively. The last type is a boundary vortex, of the sort studied in [1], with integer degree. Our result states that for very strong anchoring (larger s), minimizers prefer interior vortices, while for milder anchoring (smaller s), we will obtain light-heavy boojum pairs on Γ and no interior vortices. The threshold value for s will depend on the angle α . In no case are boundary vortices (of integer degree) preferred.

In order to state our result, we define

$$C_\alpha := \left\{ \left(\frac{\alpha}{\pi} \right)^2 + \left(1 - \frac{\alpha}{\pi} \right)^2 \right\}, \quad (1.3)$$

a constant which will appear often in our calculations of the energy of boundary defects of solutions. Note that $\frac{1}{2} < C_\alpha < 1$ for all $\alpha \in (0, \pi/2)$.

Theorem 1.1.

- (a) If $1 \geq s > \frac{1}{2C_\alpha}$, then $\exists \mathcal{D}$ points, $p_1, \dots, p_{\mathcal{D}} \in \Omega$ and a subsequence $\varepsilon_n \rightarrow 0$ such that the minimizers u_{ε_n} of $E_{\varepsilon_n}^{g,\alpha}$ satisfy

$$u_{\varepsilon_n} \rightarrow u_* \text{ in } H_{loc}^1 \cap C_{loc}^{1,\alpha}(\bar{\Omega} \setminus \{p_1, \dots, p_{\mathcal{D}}\}),$$

with u_* an \mathbb{S}^1 -valued harmonic map with $W(u, g) = 0$ on Γ , and p_i is a vortex of degree 1, $\forall i$.

(b) If $s < \frac{1}{2C_\alpha}$, there $\exists (2\mathcal{D})$ points $y_1, \tilde{y}_1, y_2, \tilde{y}_2, \dots, y_{\mathcal{D}}, \tilde{y}_{\mathcal{D}} \in \Gamma$, ordered along the boundary curve, and a subsequence $\varepsilon_n \rightarrow 0$ such that the minimizers u_{ε_n} of $E_{\varepsilon_n}^{g,\alpha}$ satisfy

$$u_{\varepsilon_n} \rightarrow u_* \text{ in } H_{loc}^1 \cap C_{loc}^{1,\alpha}(\bar{\Omega} \setminus \{y_1, \tilde{y}_1, \dots, y_{\mathcal{D}}, \tilde{y}_{\mathcal{D}}\}),$$

with u_* an S^1 -valued harmonic map with $W(u, g) = 0$ on $\Gamma \setminus \{y_1, \tilde{y}_1, \dots, y_{\mathcal{D}}, \tilde{y}_{\mathcal{D}}\}$, and y_j, \tilde{y}_j is a boojum pair of total degree -1 .

In the critical case $s = \frac{1}{2C_\alpha}$ the situation is more delicate, as interior and boundary defects will have the same energy to highest order $O(|\ln \varepsilon|)$, and one may have coexistence of the two species of defect depending on the geometry of the domain and choice of boundary map g . As in [1] we expect that by introducing a coefficient $\Upsilon = K\varepsilon^{-s}$ in the weak anchoring strength, the cross-over between boundary and interior vortices may be observed by varying K when $s = \frac{1}{2C_\alpha}$, but we do not pursue this direction in the present paper.

As in the classical work [4] on the Ginzburg–Landau model with Dirichlet boundary conditions, the location of the defects may be determined by minimizing a finite dimensional Renormalized Energy. This will be briefly discussed in Section 8, after the proof of Theorem 1.1.

A related model is that of a thin ferromagnetic film as obtained in appropriate limiting regime by DeSimone, Kohn, Muller and Otto ([5]). This limiting ferromagnetic thin film was studied by Moser ([11]), and by Kurzke ([9]) in certain settings. In those problems, they impose tangential weak anchoring conditions (i.e. $\alpha = 0$) and find critical anchoring strength (though with a different critical exponent), at which boundary vortices are favored over interior vortices. In our case we impose oblique anchoring conditions which reveal boojums defects.

In the context of nematic liquid crystals, boojums were also observed in [12,13] at interfaces between the nematic and the isotropic phases. In the limit of the small nematic correlation length, the assumption of a large splay elastic constant in [12,13] led to the tangency condition of the director on the interface and appearance of boojums. In this setting, the boojums are also associated with interface singularities because the interface location is one of the unknowns of the problem.

The rest of the paper is organized as follows: in Section 2 we describe how to obtain the above variational problem as a thin-film limit of the Landau-de Gennes energy of nematic liquid crystals. In Section 3, we present an upper bound on the energy of minimizers, as well as *a priori* pointwise bounds for all solutions of the Euler-Lagrange equations. In Section 4, we present an η compactness result adapted to handle boundary defects and use it to define the “bad balls” and show that they are contained in a finite number of very small balls. Next in Section 5, we classify the “bad balls” as interior vortex, boundary vortex, light and heavy boojums. In Section 6, we obtain an energy lower bound for each type of defects and prove an important new “degree Lemma” (Lemma 6.3) which will be essential in proving the lower bound on the energy of boundary defects in terms of the degree of the boundary data. In section 7, we put everything together and prove our main theorem, modifying the technique of vortex ball analysis introduced by Jerrard [8] and Sandier [17]. In Section 8, we formally derive the associated Renormalized Energy and, finally, in Section 9 we present numerical examples of possible defect configurations.

2. Modeling nematic thin films

In this section we motivate our variational problem via the Landau-de Gennes theory of nematic liquid crystals, in a limiting thin-film regime.

2.1. The Q -tensor

A nematic liquid crystal occupying a region $\Omega \in \mathbb{R}^3$ can be described by a 2-tensor-valued field which can be thought of as the field $Q: \mathbb{R}^3 \rightarrow M_{sym}^{3 \times 3}$ of 3×3 symmetric, traceless matrices [15]. It immediately follows that Q has a mutually orthonormal eigenframe $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and three real eigenvalues satisfying $\lambda_1 + \lambda_2 + \lambda_3 = 0$. The tensor $Q(x)$ represents the second moment of the orientational distribution in \mathbb{S}^2 of the nematic molecules near $x \in \mathbb{R}^3$, hence its eigenvalues must satisfy the constraints

$$\lambda_i \in [-1/3, 2/3], \text{ for } i = 1, 2, 3. \quad (2.1)$$

Suppose that $\lambda_1 = \lambda_2 = -\lambda_3/2$. Then the liquid crystal is in a *uniaxial nematic* state and

$$Q = -\frac{\lambda_3}{2} \mathbf{e}_1 \otimes \mathbf{e}_1 - \frac{\lambda_3}{2} \mathbf{e}_2 \otimes \mathbf{e}_2 + \lambda_3 \mathbf{e}_3 \otimes \mathbf{e}_3 = S \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right), \quad (2.2)$$

where $S := \frac{3\lambda_3}{2}$ is the uniaxial nematic order parameter and $\mathbf{n} = \mathbf{e}_3 \in \mathbb{S}^2$ is the nematic director. If there are no repeated eigenvalues, the liquid crystal is said to be in a *biaxial nematic* state and

$$Q = \lambda_1 \mathbf{I} \otimes \mathbf{I} + \lambda_3 \mathbf{n} \otimes \mathbf{n} - (\lambda_1 + \lambda_3) (\mathbf{I} - \mathbf{I} \otimes \mathbf{I} - \mathbf{n} \otimes \mathbf{n}) = S_1 \left(\mathbf{I} \otimes \mathbf{I} - \frac{1}{3} \mathbf{I} \right) + S_2 \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right), \quad (2.3)$$

where $S_1 := 2\lambda_1 + \lambda_3$ and $S_2 = \lambda_1 + 2\lambda_3$ are biaxial order parameters.

For so-called *thermotropic* liquid crystals nematic states are typically observed at low temperatures. On the contrary, at high temperatures, these materials loose orientational order and become *isotropic*. The corresponding state is represented by $Q = 0$ so that $\lambda_1 = \lambda_2 = \lambda_3 = 0$.

2.2. Landau-de Gennes model

Within the Q -tensor theory, the bulk elastic energy density of a nematic liquid crystal is given by

$$f_e(\nabla Q) := \sum_{j=1}^3 \left\{ \frac{L_1}{2} |\nabla Q_j|^2 + \frac{L_2}{2} (\operatorname{div} Q_j)^2 + \frac{L_3}{2} \nabla Q_j \cdot \nabla Q_j^T \right\}, \quad (2.4)$$

while the bulk Landau-de Gennes energy density is

$$f_{LdG}(Q) := a \operatorname{tr}(Q^2) + \frac{2b}{3} \operatorname{tr}(Q^3) + \frac{c}{2} \left(\operatorname{tr}(Q^2) \right)^2, \quad (2.5)$$

cf. [15]. Here Q_j , $j = 1, 2, 3$ is the j -th column of the matrix Q and $A \cdot B = \operatorname{tr}(B^T A)$ is the dot product of two matrices $A, B \in M^{3 \times 3}$. The coefficient $a = a_0(T - T_*)$ in (2.5) is temperature-dependent and negative for sufficiently low temperatures, while $c > 0$. The potential (2.5) is designed to depend only on the eigenvalues of Q and its form guarantees that the isotropic state $Q \equiv 0$ yields the global minimum of f_{LdG} at high temperatures while a uniaxial state of the form (2.2) gives the global minimum when temperature is sufficiently low, cf. [10, 15]. In what follows we set the temperature to be low enough so that the minimizers of f_{LdG} are uniaxial. Note that by adding an appropriate constant to f_{LdG} we can assume the global minimum value of zero for f_{LdG} .

Now consider a nematic sample occupying a thin domain $\Omega_h := \Omega \times (-h, h) \subset \mathbb{R}^3$, where $\Omega \subset \mathbb{R}^2$ and $h \ll 1$. The equilibrium nematic configuration should minimize the bulk energy subject to the appropriate boundary conditions on $\partial\Omega_h$. There are two possible alternatives. The first option is to impose Dirichlet boundary conditions on Q —also known as strong anchoring conditions—that fix the alignment of nematic molecules on $\partial\Omega_h$. The second option is to consider *weak anchoring*, that is, to specify the surface energy on the boundary of the nematic sample. The molecular orientations on the boundary are then determined as a part of the minimization procedure.

In this paper we consider a two-dimensional variational problem for Q that can be obtained—following [7]—via a rigorous dimension reduction procedure by taking the limit $h \rightarrow 0$. Briefly, as in [7], suppose that weak anchoring conditions are specified on the top and the bottom surfaces $\Omega \times \{-h, h\}$ of the nematic film Ω_h . The anchoring energy density has the form

$$f_s^{(1)}(Q, \hat{z}) = \alpha \left([(Q\hat{z} \cdot \hat{z}) - \beta]^2 + |(\mathbf{I} - \hat{z} \otimes \hat{z}) Q \hat{z}|^2 \right), \quad (2.6)$$

for any $Q \in \mathcal{A}$, where $\alpha > 0$, $\beta \in \mathbb{R}$,

$$\mathcal{A} := \left\{ Q \in M_{sym}^{3 \times 3} : \operatorname{tr} Q = 0 \right\}, \quad (2.7)$$

and \hat{z} is normal to the surface of the film. This form of the anchoring energy requires that a minimizer of $f_s^{(1)}$ has \hat{z} as an eigenvector with corresponding eigenvalue equal to β .

On the remaining part $\Gamma \times (-h, h)$ of $\partial\Omega_h$ we impose different weak anchoring conditions with the nonnegative surface energy density $f_s^{(2)}(Q, g)$, where $\Gamma = \partial\Omega$, the uniaxial data $g \in H^{1/2}(\Gamma \times (-h, h); \mathcal{A})$ does not vary in the direction normal to Γ , and $f_s^{(2)}$ is a smooth function of its arguments.

The Landau-de Gennes energy can then be obtained by combining together (2.4), (2.5), and (2.6) so that

$$E_h(Q) := \int_{\Omega_h} \{f_e(\nabla Q) + f_{LdG}(Q)\} dV + \int_{\Omega \times \{-h, h\}} f_s^{(1)}(Q, \hat{z}) dS + \int_{\Gamma \times (-h, h)} \tilde{f}_s^{(2)}(Q, g) dS. \quad (2.8)$$

In what follows we will assume that the elastic constants $L_2 = L_3 = 0$ and $L_1 = L > 0$; this corresponds to the so called equal elastic constants case where the equality of the constants refers to those in the Oseen-Frank model. The elastic energy density we consider is thus given by

$$f_e(\nabla Q) := \frac{L}{2} |\nabla Q|^2. \quad (2.9)$$

The problem can be nondimensionalized by scaling the spatial coordinates

$$\tilde{x} = \frac{x}{D}, \quad \tilde{y} = \frac{y}{D}, \quad \tilde{z} = \frac{z}{h},$$

where $D := \text{diam}(\omega)$. Set $\xi = \frac{L}{2D^2}$, $\delta = \frac{h}{D}$ and introduce $\tilde{f}_e(\nabla Q) := \frac{1}{\xi} f_e(\nabla Q)$. Dropping tildes, we obtain

$$f_e(\nabla Q) := Q_{im,j} Q_{im,j} + \frac{1}{\delta^2} Q_{im,3} Q_{im,3},$$

where the indices $i, m = 1, 2, 3$, and $j = 1, 2$. Rescaling the Landau-de Gennes potential $\tilde{f}_{LdG}(Q) := \frac{\varepsilon^2}{\xi} f_{LdG}(Q)$ and ignoring tildes again gives

$$f_{LdG}(Q) = 2A \operatorname{tr}(Q^2) + \frac{4}{3} B \operatorname{tr}(Q^3) + \left(\operatorname{tr}(Q^2) \right)^2, \quad (2.10)$$

where $A = \frac{a}{c}$, $B = \frac{b}{c}$, and $\varepsilon = \sqrt{\frac{2\xi}{c}}$. We also let $\tilde{\alpha} = \frac{\alpha}{\xi D}$ and set

$$\tilde{f}_s^{(1)}(Q, \hat{z}) := \frac{1}{\xi D} f_s^{(1)}(Q, \hat{z}), \quad \tilde{f}_s^{(2)}(Q, g) := \frac{1}{\xi D} f_s^{(2)}(Q, g)$$

to obtain the expressions for the nondimensionalized surface energies.

Finally, introducing the non-dimensional energy $F_\delta[Q] := \frac{2}{Lh} E[Q]$ and dropping all tildes, we find that

$$\begin{aligned} F_\delta(Q) = & \int_{\Omega \times (-1, 1)} \left(f_e(\nabla Q) + \frac{1}{\varepsilon^2} f_{LdG}(Q) \right) dV \\ & + \frac{1}{\delta} \int_{\Omega \times \{-1, 1\}} f_s^{(1)}(Q, \hat{z}) dA + \int_{\Gamma \times \{-1, 1\}} f_s^{(2)}(Q, g) dA. \end{aligned} \quad (2.11)$$

We now define the space

$$\mathcal{H} := \left\{ Q \in H^1(\Omega \times (-1, 1); \mathcal{A}) : \frac{\partial Q}{\partial z} \equiv 0 \text{ a.e.}, f_s(Q(x), \hat{z}) = 0 \text{ a.e. in } \Omega \right\} \quad (2.12)$$

and let $F_0 : H^1(\Omega \times (-1, 1); \mathcal{A}) \rightarrow \mathbb{R}$ be given by

$$F_0(Q) := \begin{cases} 2 \int_\Omega \left\{ |\nabla_{xy} Q|^2 + \frac{1}{\varepsilon^2} f_{LdG}(Q) \right\} dx + 2 \int_\Gamma f_s^{(2)}(Q, g) dA & \text{if } Q \in \mathcal{H}, \\ +\infty & \text{otherwise.} \end{cases} \quad (2.13)$$

The following theorem can be proved in the same way as its analog in [7].

Theorem 2.1. Fix $g \in H^{1/2}(\partial\Omega; \mathcal{A})$ that does not vary in the direction normal to Γ . Let F_δ be given by (2.11). Then $\Gamma\text{-}\lim_\delta F_\delta = F_0$ in the weak H^1 topology. Furthermore, if a sequence $\{Q_\delta\}_{\delta>0} \subset H^1(\Omega \times (-1, 1); \mathcal{A})$ satisfies a uniform energy bound $F_\delta[Q_\delta] < C_0$ then there is a subsequence $\{Q_{\delta_j}\}$ such that $Q_{\delta_j} \rightarrow Q$ as $\delta_j \rightarrow 0$ for some $Q \in \mathcal{H}$.

From now on we use the following representation of $Q \in H$ invoked, for example, in [6] and [3]:

$$Q = \begin{pmatrix} p_1 - \frac{\beta}{2} & p_2 & 0 \\ p_2 & -p_1 - \frac{\beta}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}. \quad (2.14)$$

It is a convenient change of variables in the setting when one eigenvector of the Q -tensor is parallel to the z -axis. For simplicity, we also assume that $\beta = -1/3$ and that a uniaxial tensor minimizing W has eigenvalues $-1/3$, $-1/3$, and $2/3$. Then

$$Q(p_1, p_2) = \begin{pmatrix} \frac{1}{6} + p_1 & p_2 & 0 \\ p_2 & \frac{1}{6} - p_1 & 0 \\ 0 & 0 & -\frac{1}{3} \end{pmatrix}, \quad (2.15)$$

and

$$f_{LdG}(Q) = \left(\operatorname{tr} Q^2 \right)^2 - \frac{4}{3} \operatorname{tr} Q^3 - \frac{2}{3} \operatorname{tr} Q^2 + \frac{8}{27},$$

where the constant $8/27$ was added to ensure that the minimum value of W is equal 0. The potential function can now be written as

$$\tilde{f}_{LdG}(p) := W(Q(p)) = \frac{1}{4} \left(4|p|^2 - 1 \right)^2$$

in terms of $p = (p_1, p_2)$. Dropping the subscript xy in (2.13), we also have that

$$|\nabla Q|^2 = 2|\nabla p|^2,$$

so that the bulk contribution to (2.13) takes the form

$$\int_{\Omega} \left\{ 4|\nabla p|^2 + \frac{1}{2\varepsilon^2} \left(4|p|^2 - 1 \right)^2 \right\} dx. \quad (2.16)$$

With a slight abuse of notation, we set $f_s^{(2)}(p, g) := f_s^{(2)}(Q(p_1, p_2), g)$, where $g : \partial\Omega \rightarrow \mathbb{S}^1$ is fixed. In order to establish the form of $f_s^{(2)}$, we appeal to the Rapini-Papoular form of the surface energy [20] that in the Oseen-Frank director description can be written as

$$\sigma \left((n \cdot g)^2 - \cos^2 \left(\frac{\alpha}{2} \right) \right)^2. \quad (2.17)$$

Here n is the nematic director and $\frac{\alpha}{2}$ is a preferred angle between the director n and the uniaxial data g on the boundary with $\alpha \in (0, \pi)$. We now recall the relationship between the director n and the uniaxial tensor Q . Because we assumed that Q is given by (2.15), the largest eigenvalue minimizing the potential energy is $2/3$. If the director $n = (n_1, n_2, n_3)$ lies in the xy -plane, we have that $n_3 = 0$ and

$$Q = n \otimes n - \frac{1}{3}I,$$

so that

$$n \otimes n = \begin{pmatrix} n_1^2 & n_1 n_2 & 0 \\ n_1 n_2 & n_2^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} + p_1 & p_2 & 0 \\ p_2 & \frac{1}{2} - p_1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (2.18)$$

Then

$$\begin{aligned} (n \cdot g)^2 &= (n \otimes n) \cdot (g \otimes g) = \left(\frac{1}{2} + p_1 \right) g_1^2 + 2p_2 g_1 g_2 + \left(\frac{1}{2} - p_1 \right) g_2^2 \\ &= \frac{1}{2} + \left(g_1^2 - g_2^2 \right) p_1 + 2g_1 g_2 p_2 = \frac{1}{2} + p \cdot \hat{g}, \end{aligned} \quad (2.19)$$

where $\hat{g} = (g_1^2 - g_2^2, 2g_1g_2)$. It follows that we can write (2.17) as

$$f_s^{(2)}(p, \hat{g}) = \sigma \left(p \cdot \hat{g} - \frac{1}{2} \cos \alpha \right)^2. \quad (2.20)$$

This choice is well-motivated physically and clearly favors the desired cone condition for the angle of the director for nematic directors of fixed length, $2|p| = 1$. However, when relaxing this constraint via the Ginzburg-Landau functional this boundary energy effectively does not enforce the angle condition when $2|p| < 1$. Indeed, in order to obtain the desired behavior at boundary defects it is necessary to add a term for which the boundary energy is minimized when $|p| = 1/2$ lies on the cone of aperture α with the axis that coincides with the normal to Γ . With this observation in mind, we replace (2.20) with

$$f_s^{(2)}(p, \hat{g}) = \frac{\sigma}{4} \left[\frac{1}{2} (|2p|^2 - 1)^2 + (2p \cdot \hat{g} - \cos \alpha)^2 \right]. \quad (2.21)$$

Defining $u := 2p$ and $E_\varepsilon^{g, \alpha}[u] := \frac{1}{2} F_0[Q(u/2)]$, dropping the hat in \hat{g} , and denoting $\Upsilon := \sigma/2$ we arrive at the expression (1.1) for the energy $E_\varepsilon^{g, \alpha}$.

Note that the weak anchoring condition is now coercive: using complex notation, the condition (2.20) when $u \in S^1 \subset \mathbb{C}$ says that the angle between $\hat{g} = g^2$ and u is twice that of the angle between the director n and g , which is consistent since the phase of u is doubled compared to that of n .

We also note that the main theorem is stated for $\alpha \in (0, \frac{\pi}{2})$. The case $\alpha \in (\frac{\pi}{2}, \pi)$ follows directly from this case, as will be mentioned in the course of the proof.

3. Upper bounds

In this section we prove two fundamental estimates: a rough upper bound on the energy of minimizers, and *a priori* pointwise bounds for all solutions of the Euler-Lagrange equations,

$$\left. \begin{aligned} -\Delta u + \frac{1}{\varepsilon^2} (|u|^2 - 1)u &= 0, \quad \text{in } \Omega, \\ \frac{\partial u}{\partial \nu} + \Upsilon_\varepsilon \left((|u|^2 - 1)u + [(u, g) - \cos \alpha]g \right) &= 0, \quad \text{on } \Gamma, \end{aligned} \right\} \quad (3.1)$$

where $\Upsilon_\varepsilon = \varepsilon^{-s}$, with $0 < s \leq 1$.

Lemma 3.1. *Let $g = e^{i\gamma} : \Gamma \rightarrow S^1$ be a C^1 smooth map, with*

$$\mathcal{D} = \deg(g; \Gamma) > 0, \text{ and } E_\varepsilon^{g, \alpha} := \min_{H^1(\Omega)} E_\varepsilon^{g, \alpha}.$$

Recall $C_\alpha = (\frac{\alpha}{\pi})^2 + (1 - \frac{\alpha}{\pi})^2$, $\alpha \in (0, \frac{\pi}{2})$,

(i) *If $sC_\alpha \geq \frac{1}{2}$ then*

$$E_\varepsilon^{g, \alpha} \leq \pi \mathcal{D} |\ln \varepsilon| + C_1 \quad (3.2)$$

(ii) *If $sC_\alpha < \frac{1}{2}$, then*

$$E_\varepsilon^{g, \alpha} \leq 2\pi \mathcal{D} s C_\alpha |\ln \varepsilon| + C_1 \quad (3.3)$$

Proof. In case (i) we let v_ε be the energy minimizer of the standard Ginzburg-Landau functional with Dirichlet boundary conditions $u|_\Gamma = g e^{i\alpha}$ (so as to make the boundary anchoring energy vanish.) The bound (3.2) then follows from the work of Bethuel-Brezis-Hélein [4] since $E_\varepsilon^{g, \alpha}$ becomes the Ginzburg-Landau functional.

In case (ii), we will construct an S^1 -valued test function with boundary defects. Note that in that case, the upper bound in (3.3) is smaller than the bound (3.2). The construction follows Kurzke [9] (see also [[1], Lemma 3.1]) although our boundary condition is quite different. This construction is also very helpful in understanding what minimizers should look like.

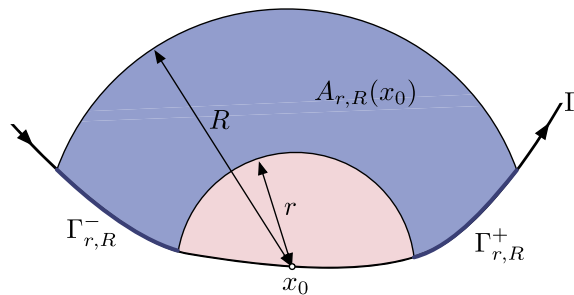


Fig. 1. Near a boundary point $x_0 \in \Gamma$, the disk $\omega_R(x_0)$ and annulus $A_{r,R}$, which separates the boundary $\Gamma \cap A_{r,R}$ into two arcs, $\Gamma_{r,R}^\pm$.

Choose $2\mathcal{D}$ points $q_1, \dots, q_{2\mathcal{D}} \in \Gamma$, well separated, and fix $R > 0$ with $R < \frac{1}{2}|q_i - q_j| \ \forall i \neq j$. We order the points along Γ so that the index of q_i increases as Γ is traced out counterclockwise. For each i we define v_ε^i in $\omega_R(q_i) = B_R(q_i) \cap \Omega$ via polar coordinates (ρ, θ) centered at q_i with θ measured from the oriented unit tangent τ to Γ at q_i . Since Γ is smooth, by reducing R (if necessary) we may ensure that $\omega_R(q_i)$ is a polar rectangle, and nearly a half-disk:

$$\omega_R(q_i) = \{(\rho, \theta) \mid \theta_+(\rho) < \theta < \theta_-(\rho), 0 < \rho < R\}$$

with $\theta_\pm \in C^1$ and $|\theta_+(\rho)| \leq c\rho$, $|\pi - \theta_-(\rho)| \leq c\rho$.

The odd q_{2j-1} will be “light” boojums, with phase decreasing by 2α , while the even q_{2j} will be “heavy” boojums, with phase decreasing by $2\pi - 2\alpha$. Consider the “light” case; the “heavy” case will be essentially the same, except for the coefficient.

With $g = e^{i\gamma}$, define phases for v_ε^i on the two components of $\Gamma \cap B_R(q_i) \setminus \{q_i\}$ around a point q_i (see Fig. 1), parametrized by

$$\Gamma^\pm = \{(\rho, \theta_\pm(\rho)) : 0 < \rho \leq R\},$$

as follows: let

$$h_\pm(\rho) = \gamma(\rho, \theta_\pm(\rho)) \mp \alpha$$

and

$$\psi(\rho, \theta) = h_+(\rho) \frac{\theta - \theta_-(\rho)}{\theta_+(\rho) - \theta_-(\rho)} + h_-(\rho) \frac{\theta - \theta_+(\rho)}{\theta_-(\rho) - \theta_+(\rho)},$$

which linearly interpolates between them. We introduce a cut-off near q_i : $\chi_\varepsilon(\rho) \in C^\infty$,

$$0 \leq \chi_\varepsilon(\rho) \leq 1, \chi_\varepsilon(\rho) = 0 \text{ for } 0 \leq \rho < \varepsilon^s, \chi_\varepsilon(\rho) = 1 \text{ for } \rho \geq 2\varepsilon^s, |\nabla \chi_\varepsilon(\rho)| \leq c\varepsilon^{-s}.$$

Then we define v_ε^i in $\omega_R(q_i)$ with i odd by:

$$v_\varepsilon^i(\rho, \theta) = \exp \{i[\chi_\varepsilon(\rho)\psi(\rho, \theta) + (1 - \chi_\varepsilon(\rho))\gamma(q_i)]\}$$

Note that on $\Gamma^+ \setminus B_{2\varepsilon^s}(q_i)$, $v_\varepsilon^i = g e^{-i\alpha}$ and on $\Gamma^- \setminus B_{2\varepsilon^s}(q_i)$, $v_\varepsilon^i = g e^{i\alpha}$, so that $W(v_\varepsilon^i, g) = 0$ on $\Gamma^\pm \setminus B_{2\varepsilon^s}(q_i)$. In particular,

$$\Upsilon_\varepsilon \int_{\Gamma \cap B_R(q_i)} W(v_\varepsilon^i, g) ds \leq O(1).$$

Also, $|v_\varepsilon^i| = 1$ in $\omega_R(q_i)$, so

$$\varepsilon^{-2} \int_{B_R(q_i)} (|v_\varepsilon^i|^2 - 1)^2 dx = 0.$$

Furthermore, v_ε^i is smooth and ε -independent in $\omega_R(q_i) \setminus \omega_{\varepsilon^s}(q_i)$ with

$$\int_{\omega_R(q_i)} |\partial_\rho v_\varepsilon^i|^2 \leq C \text{ and } \int_{\omega_{\varepsilon^s}(q_i)} |\partial_\theta v_\varepsilon^i|^2 \leq C$$

so the main contribution to the gradient energy is via $|\partial_\theta v_\varepsilon^i|$ in $\omega_R(q_i) \setminus \omega_{\varepsilon^s}(q_i)$:

$$\begin{aligned} \frac{1}{2} \int_{\omega_R(q_i) \setminus \omega_{\varepsilon^s}(q_i)} \frac{1}{\rho^2} |\partial_\theta v_\varepsilon^i|^2 dx &= \frac{1}{2} \int_{\omega_R(q_i) \setminus \omega_{\varepsilon^s}(q_i)} \chi_\varepsilon^2(r) |\partial_\theta \psi(\rho, \theta)|^2 \frac{1}{\rho^2} dx \\ &\leq \frac{1}{2} \int_{\omega_R(q_i) \setminus \omega_{\varepsilon^s}(q_i)} \frac{(h_+(\rho) - h_-(\rho))^2}{(\theta_+(\rho) - \theta_-(\rho))^2} \frac{1}{\rho^2} dx \\ &\leq \frac{1}{2} \int_{\varepsilon^s}^R \frac{(h_+(\rho) - h_-(\rho))^2}{(\theta_+(\rho) - \theta_-(\rho))} \frac{1}{\rho} d\rho \\ &\leq \frac{1}{2} \int_{\varepsilon^s}^R \frac{((2\alpha) + c\rho)^2}{(\pi - c\rho)} \frac{1}{\rho} d\rho \\ &\leq 2\pi \left(\frac{\alpha}{\pi}\right)^2 \ln\left(\frac{R}{\varepsilon^s}\right) + O(1), \end{aligned}$$

for i odd. Thus we have

$$E_\varepsilon(v_\varepsilon^i; \omega_R(q_i)) \leq 2\pi \left(\frac{\alpha}{\pi}\right)^2 s |\ln(\varepsilon)| + C,$$

for odd i . When i is even, we modify h^\pm to

$$\tilde{h}^-(\rho) = \gamma(\rho, \theta_-(\rho)) - \alpha; \quad \tilde{h}^+(\rho) = \gamma(\rho, \theta_+(\rho)) + \alpha - 2\pi,$$

and follow the same estimates to arrive at:

$$E_\varepsilon(v_\varepsilon^i; \omega_R(q_i)) \leq 2\pi \left(\frac{\pi - \alpha}{\pi}\right)^2 s |\ln(\varepsilon)| + C.$$

Now, consider the (ε -independent) domain, $\tilde{\Omega} = \Omega \setminus \bigcup_{i=1}^{2\mathcal{D}} B_R(q_i)$. Define $\tilde{g} : \partial\tilde{\Omega} \rightarrow S^1$ by:

$$\tilde{g} = \begin{cases} g & \text{on } \Gamma \setminus \bigcup_{i=1}^{2\mathcal{D}} B_{2R}(q_i) \\ v_\varepsilon^i & \text{on } \partial B_{2R}(q_i) \cap \Omega. \end{cases}$$

By the construction of v_ε^i , the function \tilde{g} is ε -independent, piecewise C^1 , continuous, and $\deg(\tilde{g}; \partial\tilde{\Omega}) = 0$. Therefore we can find $\tilde{v} \in H_g^1(\tilde{\Omega})$ with

$$E_\varepsilon(\tilde{v}; \tilde{\Omega}) \leq C.$$

Hence, setting

$$v_\varepsilon = \begin{cases} \tilde{v} & \text{in } \tilde{\Omega} \\ v_\varepsilon^i & \text{in } \omega_R(q_i), \end{cases}$$

we have $v_\varepsilon \in H^1(\Omega)$ with

$$E_\varepsilon(v_\varepsilon) \leq 2\pi \mathcal{D}s \left(\left(\frac{\alpha}{\pi}\right)^2 + \left(1 - \frac{\alpha}{\pi}\right)^2 \right) |\ln \varepsilon| + C,$$

which is the desired upper bound (3.3) and this ends the proof of the Lemma. \square

Next we prove the following pointwise upper bounds on solutions to (3.1).

Lemma 3.2. *Let u_ε be any solution of (3.1).*

- (i) *Suppose that $\varepsilon \Upsilon_\varepsilon \leq C$. Then $\|u_\varepsilon\|_\infty \leq 2$ and there exists a constant $C_1 = C_1(\Omega) > 0$ so that $|\nabla u_\varepsilon| \leq C_1/\varepsilon$, for all $x \in \Omega$.*
- (ii) *If we further assume that $\varepsilon \Upsilon_\varepsilon \rightarrow 0$ as $\varepsilon \rightarrow 0$, then $\limsup_{\varepsilon \rightarrow 0} \|u_\varepsilon\|_\infty \leq 1$.*

Proof. Let u_ε solve (3.1), and suppose by contradiction that u_ε is not uniformly bounded, and that there is a point $p_\varepsilon \in \Omega$ such that $|u_\varepsilon(p_\varepsilon)| = \|u_\varepsilon\|_\infty > 2$. Set $V_\varepsilon = |u_\varepsilon|^2$ and (using u , V rather than u_ε , V_ε), we obtain $\nabla V = 2u \cdot \nabla u$ and

$$\frac{1}{2} \Delta V = |\nabla u|^2 + u \cdot \Delta u = |\nabla u|^2 + \frac{1}{\varepsilon^2} V(V - 1).$$

If $p_\varepsilon \in \Omega$, V attains an interior maximum at p_ε with $V(p_\varepsilon) > 1$ so that $\frac{1}{2} \Delta V(p_\varepsilon) > 0$, which is a contradiction.

If instead $p_\varepsilon \in \partial\Omega$, note that

$$\frac{\partial V}{\partial \nu} = 2u \cdot \frac{\partial u}{\partial \nu} = -2\Upsilon_\varepsilon \left[V(V - 1) + [u \cdot g - \cos \alpha](u \cdot g) \right]$$

and hence denoting by $m_\varepsilon := \|u_\varepsilon\|_\infty$ and still assuming that it is not uniformly bounded we obtain:

$$\begin{aligned} \frac{\partial V}{\partial \nu} &\leq -2\Upsilon_\varepsilon \left[m_\varepsilon^2(m_\varepsilon^2 - 1) - |u \cdot g - \cos \alpha| |u \cdot g| \right] \\ &\leq -2\Upsilon_\varepsilon \left[m_\varepsilon^4 - m_\varepsilon^2 - [(m_\varepsilon + |\cos \alpha|)m_\varepsilon] \right] \\ &\leq -2\Upsilon_\varepsilon \left[\frac{1}{2} m_\varepsilon^4 - 2m_\varepsilon^2 \right] \\ &\leq -\Upsilon_\varepsilon \left[m_\varepsilon^4 - 4m_\varepsilon^2 \right] \\ &< 0, \end{aligned}$$

in case $m_\varepsilon > 2$. But if V attains its maximum at $p_\varepsilon \in \partial\Omega$, then $\frac{\partial V}{\partial \nu}(p_\varepsilon) \geq 0$, which is a contradiction. Therefore $m_\varepsilon = \|u_\varepsilon\|_\infty$ is bounded by 2.

Next we show that if $\varepsilon \Upsilon_\varepsilon \rightarrow 0$ as $\varepsilon \rightarrow 0$, then $\limsup_{\varepsilon \rightarrow 0} \|u_\varepsilon\|_\infty \leq 1$. Indeed, assume for a contradiction that (along some subsequence) $m_\varepsilon \rightarrow m_0 > 1$. Note that if $\|u_\varepsilon\|_\infty$ is attained inside Ω , by the above $|u_\varepsilon(x)| \leq 1$, $\forall x \in \bar{\Omega}$. So suppose that $p_\varepsilon \in \partial\Omega$. Without loss of generality, we rotate the domain such that the normal $\nu(p_\varepsilon) = \vec{e}_2$. Blowing up at scale ε around the points p_ε , define for $y \in \Omega_\varepsilon := \varepsilon[\Omega - p_\varepsilon]$ the function $v_\varepsilon(y) = u_\varepsilon(p_\varepsilon + \varepsilon y)$ and let $\tilde{g}(y)$ denote the boundary values g for $y \in \partial\Omega_\varepsilon$. As $\varepsilon \rightarrow 0$, the set Ω_ε becomes the upper half plane \mathbb{R}_+^2 and we have:

$$\begin{aligned} \Delta v_\varepsilon &= \varepsilon^2 \Delta u_\varepsilon = (|v_\varepsilon|^2 - 1)v_\varepsilon, \\ \frac{\partial v_\varepsilon}{\partial \nu} &= \varepsilon \frac{\partial u_\varepsilon}{\partial \nu} = -\Upsilon_\varepsilon \varepsilon \left[(|v_\varepsilon|^2 - 1)v_\varepsilon + [v_\varepsilon \cdot \tilde{g} - \cos \alpha] \tilde{g} \right] \end{aligned}$$

Note that $|v_\varepsilon| \leq m_\varepsilon \leq 2$ by the above, so that in $B_R^+(0)$ we have $v_\varepsilon \rightarrow v_0$ in C_{loc}^2 (along a subsequence.) Therefore, using that $\varepsilon \Upsilon_\varepsilon \rightarrow 0$, we obtain

$$\begin{aligned} \Delta v_0 &= (|v_0|^2 - 1)v_0, \\ \frac{\partial v_0}{\partial \nu} &= 0, \text{ and } |v_0(0)| = m_0 > 1. \end{aligned}$$

As usual, we define $V_0(y) := |v_0(y)|^2$, and we obtain for V_0 :

$$\frac{1}{2} \Delta V_0 = |\nabla v_0|^2 + v_0 \cdot \Delta v_0 \geq \frac{1}{\varepsilon^2} V_0(V_0 - 1) > 0,$$

while having a maximum at $y = 0$ with $\frac{\partial V_0}{\partial v} = 0$: this contradicts the Hopf Lemma. We conclude that $\limsup_{\varepsilon \rightarrow 0} \|u_\varepsilon\|_\infty \leq 1$.

To establish the gradient bound, we argue by contradiction: suppose there exist sequences $\varepsilon_k \rightarrow 0$, $x_k \in \overline{\Omega}$ for which $t_k := |\nabla u_k(x_k)| = \|\nabla u_k\|_\infty$ satisfies $t_k \varepsilon_k \rightarrow \infty$. Blowing up at scale t_k around the points x_k , define $v_k(x) := u_k\left(x_k + \frac{x}{t_k}\right)$. By our choice of scaling, $\|v_k\|_\infty < C$, and v_k solves

$$-\Delta v_k = \frac{1}{(t_k \varepsilon_k)^2} (|v_k|^2 - 1) v_k \rightarrow 0,$$

uniformly on Ω (since $\|u_k\|_\infty = \|v_k\|_\infty < C$, by the first part of the lemma.) If, for some subsequence, $t_k \text{dist}(x_k, \partial\Omega) \rightarrow \infty$, then the domain $t_k[\Omega - x_k]$ of v_k converges to all \mathbb{R}^2 , and $v_k \rightarrow v$ in C_{loc}^k . Moreover, the limit v is a bounded harmonic function on \mathbb{R}^2 , and hence constant: $\nabla v(x) \equiv 0$. However, by construction, $|\nabla v_k(0)| = 1$ for all k , and hence $|\nabla v(0)| = 1$, a contradiction.

On the other hand, if $t_k \text{dist}(x_k, \partial\Omega)$ is uniformly bounded, then the domains $t_k[\Omega - x_k]$ of v_k converge to a half-space \mathbb{R}_+^2 , with boundary condition

$$\frac{\partial v_k}{\partial \nu} = -\frac{\Upsilon_{\varepsilon_k}}{t_k} \left[v_k (|v_k|^2 - 1) - \left[\left(v_k, g \left(x_k + \frac{x}{t_k} \right) \right) - \cos \alpha \right] g \left(x_k + \frac{x}{t_k} \right) \right] \rightarrow 0,$$

since $\frac{\Upsilon_{\varepsilon_k}}{t_k} \rightarrow 0$ and v_k is uniformly bounded by the a priori bound on u_ε proven above. That is, $v_k \rightarrow v$ which is bounded and harmonic in \mathbb{R}_+^2 , and with a Neumann condition $\partial_\nu v = 0$ on the boundary. By the reflection principle and Liouville's theorem we again conclude that v is constant, which leads to the same contradiction as in the previous case. Thus, the desired gradient bound must hold. \square

4. Isolating the defects

We begin by proving an η -compactness (also called η -ellipticity) result (see [18], [16]). We then define vortex balls, of radius of order ε in the interior and of radius of order ε^s on the boundary of the domain, and following Struwe ([18]) we show that they form a uniformly bounded family.

4.1. η -compactness

Basically, if the energy contained in a ball of radius ε^β is too small, there can be no vortex in a slightly smaller ball, $B_{\varepsilon^\gamma}(x_0)$. To this end, we recall that $\Upsilon = \Upsilon(\varepsilon) = \varepsilon^{-s}$ for $s \in (0, 1]$, and fix β, γ such that $\frac{3}{4}s \leq \beta < \gamma < s$. We also let $a \in (0, \frac{1}{2})$ to be chosen later.

Proposition 4.1 (η -compactness). *There exist constants $\eta, C, \varepsilon_0 > 0$ such that for any solution u_ε of (3.1) with $\varepsilon \in (0, \varepsilon_0)$, if $x_0 \in \overline{\Omega}$, $a \in (0, \frac{1}{2})$ and*

$$E_\varepsilon(u_\varepsilon; B_{\varepsilon^\beta}(x_0)) \leq \eta |\ln \varepsilon|, \quad (4.1)$$

then

$$|u_\varepsilon|^2 \geq 1 - \sqrt{2}a \quad \text{in} \quad B_{\varepsilon^\gamma}(x_0), \quad (4.2)$$

$$W(u, g) := \frac{1}{2} (|u|^2 - 1)^2 + [(u, g) - \cos \alpha]^2 \leq a^2 \quad \text{on} \quad \Gamma \cap B_{\varepsilon^\gamma}(x_0), \quad (4.3)$$

$$\frac{1}{4\varepsilon^2} \int_{B_{\varepsilon^\gamma}(x_0)} (|u_\varepsilon|^2 - 1)^2 dx + \frac{\Upsilon}{2} \int_{\Gamma \cap B_{\varepsilon^\gamma}(x_0)} W(u_\varepsilon, g) ds \leq C\eta. \quad (4.4)$$

We note that in case $\Gamma \cap B_{\varepsilon^\beta}(x_0) = \emptyset$, this has been proven in Lemma 2.3 of [18], and hence it suffices to consider $x_0 \in \Gamma \subset \partial\Omega$ when proving Proposition 4.1.

Define $\Gamma_r(x_0) = \partial\Omega \cap B_r(x_0)$, and following Struwe [18], define

$$F(r) = F(r; x_0, u, \varepsilon) = r \left[\int_{\partial B_r(x_0) \cap \Omega} \frac{1}{2} \left\{ |\nabla u|^2 + \frac{1}{2\varepsilon^2} (|u|^2 - 1)^2 \right\} ds + \frac{\Upsilon(\varepsilon)}{2} \sum_{x \in \partial\Gamma_r(x_0)} W(u, g) \right]. \quad (4.5)$$

Note that if $\partial\Gamma_r(x_0) \neq \emptyset$, then for $r > 0$ sufficiently small it consists of two points.

The proof of Proposition 4.1 relies on the following estimate. For any $x_0 \in \overline{\Omega}$ and $R > 0$, we define (as in the proof of Lemma 3.1)

$$\omega_R(x_0) = B_R(x_0) \cap \Omega. \quad (4.6)$$

Then, we first prove:

Lemma 4.2. *There exist $C > 0$ and $r_0 > 0$ such that for $\varepsilon \in (0, 1)$, $x_0 \in \Gamma$, and $r \in (0, r_0)$, we have that*

$$\frac{1}{2\varepsilon^2} \int_{\omega_r(x_0)} (|u_\varepsilon|^2 - 1)^2 dx + \Upsilon \int_{\Gamma_r(x_0)} W(u, g) ds \leq C \left\{ r \int_{\omega_r(x_0)} |\nabla u_\varepsilon|^2 dx + F(r) + r^2 \Upsilon \right\},$$

where $F(r)$ is as in (4.5).

Proof of Lemma 4.2. We denote $u = u_\varepsilon$, $\omega_r = \omega_r(x_0)$, and $\Gamma_r = \Gamma_r(x_0)$ for convenience, as $x_0 \in \Gamma$ and $\varepsilon > 0$ are fixed.

Let $\psi \in C^\infty(\Omega; \mathbb{R}^2)$ be a vector field, to be determined later. Taking the complex scalar product of the equation (3.1) with $\psi \cdot \nabla u$ and integrating over ω_r , we obtain the Pohozaev-type equality,

$$\begin{aligned} \int_{\partial\omega_r} \left\{ -(\partial_v u, \psi \cdot \nabla u) + \frac{1}{2} |\nabla u|^2 (\psi \cdot \nu) + \frac{1}{4\varepsilon^2} (|u|^2 - 1)^2 (\psi \cdot \nu) \right\} ds \\ = \int_{\omega_r} \left\{ \frac{1}{4\varepsilon^2} (|u|^2 - 1)^2 \operatorname{div} \psi + \frac{1}{2} |\nabla u|^2 \operatorname{div} \psi - \sum_{i,j} \partial_i \psi_j (\partial_i u, \partial_j u) \right\} dx. \end{aligned} \quad (4.7)$$

We choose $r_0 > 0$ sufficiently small so that $\Gamma \cap B_r(x_0)$ consists of a single smooth arc, and ω_r is strictly starshaped with respect to some $x_1 \in \omega_r$, for all $0 < r \leq r_0$.

Let \mathcal{N} be a $2r_0$ -neighborhood of Γ . We claim that, by taking r_0 smaller if necessary, there exists a vector field $X \in C^2(\mathcal{N}; \mathbb{R}^2)$ with the following properties (see [9], [11]):

$$X \cdot \nu = 0, \quad \text{for all } x \in \Gamma_r, \quad (4.8)$$

$$|X - (x - x_0)| \leq C|x - x_0|^2, \quad |DX - Id| \leq C|x - x_0|, \quad \text{for all } x \in \omega_r, \quad (4.9)$$

for a constant $C > 0$, for any $x_0 \in \Gamma$. The existence of such a vector field in a disk $B_r(x_0)$ follows from the smoothness of Γ ; to obtain the uniform global estimates (4.8), (4.9) we use the compactness of Γ and a partition of unity. In particular, note that $X = (X \cdot \tau)\tau \simeq (x - x_0)\tau$ lies along the tangent vector on Γ_r .

We now take $\psi = X$ in (4.7) and estimate each term in (4.7), separating the $\partial\omega_r$ terms into the pieces along Γ_r and along $\partial B_r(x_0) \cap \Omega$. First, on Γ_r we have $X \cdot \nu = 0$, and the only contribution to the left hand side of (4.7) is:

$$\begin{aligned} - \int_{\Gamma_r} (\partial_v u, X \cdot \nabla u) ds &= \Upsilon \int_{\Gamma_r} \left\{ (|u|^2 - 1)(u, X \cdot \nabla u) + [(u \cdot g) - \cos \alpha] (g, X \cdot \nabla u) \right\} ds \\ &= \Upsilon \int_{\Gamma_r} \left\{ (|u|^2 - 1) \left(u, \frac{\partial u}{\partial \tau} \right) + [(u \cdot g) - \cos \alpha] \left(g, \frac{\partial u}{\partial \tau} \right) \right\} (X \cdot \tau) ds \\ &= \Upsilon \int_{\Gamma_r} \left[\partial_\tau \left(\frac{1}{2} [(u, g) - \cos \alpha]^2 \right) - [(u, g) - \cos \alpha] (\partial_\tau g, u) \right] ds \end{aligned}$$

$$\begin{aligned}
& + \partial_\tau \left(\frac{1}{4} (|u|^2 - 1)^2 \right) \Big] X \cdot \tau \, ds \\
& = I_1 - I_2 + I_3
\end{aligned}$$

To estimate I_1 , we use integration by part and (4.9) as follows:

$$I_1 = \Upsilon \int_{\Gamma_r} \frac{\partial}{\partial \tau} \left\{ \frac{1}{2} [u \cdot g - \cos \alpha]^2 \right\} X \cdot \tau \, ds \quad (4.10)$$

$$= \frac{\Upsilon}{2} \left\{ [u \cdot g - \cos \alpha]^2 (X \cdot \tau) \Big|_{\partial \Gamma_r} - \int_{\Gamma_r} \left\{ [(u \cdot g) - \cos \alpha]^2 \right\} \partial_\tau (X \cdot \tau) \, ds \right\} \quad (4.11)$$

$$= \frac{\Upsilon}{2} \left\{ r \sum_{\partial \Gamma_r} [(u \cdot g) - \cos \alpha]^2 - \int_{\Gamma_r} \left\{ [(u \cdot g) - \cos \alpha]^2 \right\} dx \right\} + O(\Upsilon r^2), \quad (4.12)$$

using (4.9) in the last line. Indeed, on the endpoints of Γ_r , $|X \cdot \tau \mp r| \leq Cr^2$ and on Γ_r itself, $\partial_\tau (X \cdot \tau) = 1 + O(|x - x_0|)$.

For I_2 , we have the rough estimate:

$$|I_2| \leq \Upsilon |\Gamma_r| \left((\|u\|_\infty + 1)^2 \left\| \frac{\partial g}{\partial \tau} \right\|_\infty \|X \cdot \tau\|_\infty \right) \leq C \Upsilon r^2,$$

using again (4.9). Finally, I_3 is estimated in the same way as I_1 :

$$I_3 = \Upsilon \int_{\Gamma_r} \frac{1}{4} \partial_\tau (|u|^2 - 1)^2 X \cdot \tau \, ds \quad (4.13)$$

$$= \Upsilon \left\{ \frac{1}{4} (|u|^2 - 1)^2 (X \cdot \tau) \Big|_{\partial \Gamma_r} - \frac{1}{4} \int_{\Gamma_r} (|u|^2 - 1)^2 \partial_\tau (X \cdot \tau) \, ds \right\} \quad (4.14)$$

$$= \frac{\Upsilon}{2} \left\{ r \sum_{\partial \Gamma_r} \frac{1}{2} (|u|^2 - 1)^2 - \frac{1}{2} \int_{\Gamma_r} (|u|^2 - 1)^2 \, ds \right\} + O(\Upsilon r^2) \quad (4.15)$$

The remaining terms on the left-hand side of (4.7) may also be estimated in a simple way, using $|X \cdot v|, |X \cdot \tau| \leq Cr$ and (4.8):

$$\left| \int_{\partial \omega_r \cap \Omega} \left\{ -(\partial_v u, X \cdot \nabla u) + \frac{1}{2} |\nabla u|^2 X \cdot v \right\} ds \right| \leq Cr \int_{\partial \omega_r \cap \Omega} |\nabla u|^2 \, ds \quad (4.16)$$

$$\left| \frac{1}{4\varepsilon^2} \int_{\partial \omega_r} (|u|^2 - 1)^2 (X \cdot v) \, ds \right| = \left| \frac{1}{4\varepsilon^2} \int_{\partial B_r \cap \Omega} (|u|^2 - 1)^2 (X \cdot v) \, ds \right| \quad (4.17)$$

$$\leq \frac{Cr}{\varepsilon^2} \int_{\partial B_r \cap \Omega} (|u|^2 - 1)^2 \, ds. \quad (4.18)$$

For the terms on the right side of (4.7), we use (4.9): $|\partial_i X_j - \delta_{ij}| \leq Cr$, and for r_0 chosen smaller if necessary, we may assume $\operatorname{div} X \geq 2 - Cr > 1$ in ω_r . Thus, the right side of (4.7) may be estimated as:

$$\int_{\omega_r} \left\{ \frac{1}{4\varepsilon^2} (|u|^2 - 1)^2 \operatorname{div} X + \frac{1}{2} |\nabla u|^2 \operatorname{div} X - \sum_{i,j} \partial_i X_j (\partial_i u, \partial_j u) \right\} dx \geq \int_{\omega_r} \left\{ \frac{1}{4\varepsilon^2} (|u|^2 - 1)^2 - Cr |\nabla u|^2 \right\} dx. \quad (4.19)$$

Putting the above estimates together, we arrive at the desired bound. \square

We are ready for the

Proof of Proposition 4.1. We follow [18], [11]. If $x_0 \in \Omega \setminus \Gamma$, this is proven in [18], so we restrict our attention to $x_0 \in \Gamma$.

Recalling the definition of F (4.5), we note that since

$$\eta \ln \frac{1}{\varepsilon} \geq E_\varepsilon(u_\varepsilon; \omega_{\varepsilon^\beta} \setminus \omega_{\varepsilon^\gamma}) = \int_{\varepsilon^\gamma}^{\varepsilon^\beta} \frac{F(r)}{r} dr, \quad (4.20)$$

there exists $r_\varepsilon \in (\varepsilon^\gamma, \varepsilon^\beta)$ so that

$$F(r_\varepsilon) \leq \frac{\eta}{\gamma - \beta}.$$

By Lemma 4.2 with $\Gamma_{r_\varepsilon} := \partial\omega_{r_\varepsilon} \cap \Gamma$, we deduce:

$$\begin{aligned} \frac{1}{2\varepsilon^2} \int_{\omega_{r_\varepsilon}(x_0)} (|u|^2 - 1)^2 dx + \Upsilon_\varepsilon \int_{\Gamma_{r_\varepsilon}(x_0)} W(u_\varepsilon, g) ds \\ \leq C \left\{ r_\varepsilon \int_{\omega_{r_\varepsilon}(x_0)} |\nabla u_\varepsilon|^2 dx + F(r_\varepsilon) + r_\varepsilon^2 \Upsilon_\varepsilon \right\} \\ \leq C \left\{ \varepsilon^\beta \eta |\ln \varepsilon| + \frac{\eta}{\gamma - \beta} + \varepsilon^{2\beta} \varepsilon^{-s} \right\} \\ \leq C' \eta, \end{aligned} \quad (4.21)$$

which proves (4.4) since $r_\varepsilon > \varepsilon^\gamma$. Note that no conditions are required on η at this point, and this will prove useful later on (see Corollary 4.3.)

To prove (4.2), assume (for contradiction) that there is a point $x_2 \in B_{\varepsilon^\gamma}(x_0)$ with $|u_\varepsilon(x_2)| < 1 - a$. By Lemma 3.2, $|\nabla u_\varepsilon| \leq C_1/\varepsilon$, and hence there is a constant $C > 0$ such that $|u(x)| < 1 - \frac{a}{2}$, $\forall x \in B_{C\varepsilon}(x_2) \subset B_{\varepsilon^\gamma}(x_0)$. In that case,

$$\begin{aligned} \frac{1}{4\varepsilon^2} \int_{B_{\varepsilon^\gamma}(x_0)} (|u|^2 - 1)^2 dx &\geq \frac{1}{4\varepsilon^2} \int_{B_{C\varepsilon}(x_0)} (|u|^2 - 1)^2 dx \\ &\geq Ca^2. \end{aligned}$$

We then choose $\eta > 0$ small enough so this contradicts (4.4) and hence (4.2) holds for all such η (which is independent of x_0).

To verify (4.3), we return to the Pohozaev identity (4.7). We recall that for $r = r_\varepsilon$ (as in the proof of (4.4)) sufficiently small, the smoothness and compactness of Γ ensure that $\omega_{r_\varepsilon} = B_{r_\varepsilon}(x_0) \cap \Omega$ is strictly starshaped around some $x_1 \in \omega_{r_\varepsilon}$, and we have $(x - x_1) \cdot \nu \geq r_\varepsilon/4$ on $\partial\omega_{r_\varepsilon}$. Taking $\psi = x - x_1$ in (4.7), we obtain:

$$\begin{aligned} \int_{\partial\omega_{r_\varepsilon}} \left\{ (x - x_1) \cdot \nu \left[|\partial_\tau u_\varepsilon|^2 - |\partial_\nu u_\varepsilon|^2 \right] + (x - x_1) \cdot (\nu - \tau) (\partial_\nu u_\varepsilon, \partial_\tau u_\varepsilon) \right\} ds \\ \leq \frac{1}{2\varepsilon^2} \int_{\omega_{r_\varepsilon}} (1 - |u_\varepsilon|^2)^2 dx. \end{aligned} \quad (4.22)$$

To estimate the second term in the left hand side of this inequality we use Cauchy-Schwartz,

$$\left| \int_{\partial\omega_{r_\varepsilon}} (x - x_1) \cdot (v - \tau) (\partial_v u_\varepsilon, \partial_\tau u_\varepsilon) \right| \leq 2r_\varepsilon \int_{\partial\omega_{r_\varepsilon}} \left\{ \frac{1}{32} |\partial_\tau u_\varepsilon|^2 + 8 |\partial_v u_\varepsilon|^2 \right\} ds,$$

and hence

$$\frac{r_\varepsilon}{16} \int_{\partial\omega_{r_\varepsilon}} |\partial_\tau u_\varepsilon|^2 ds \leq Cr_\varepsilon \int_{\partial\omega_{r_\varepsilon}} |\partial_v u_\varepsilon|^2 ds + \frac{1}{2\varepsilon^2} \int_{\omega_{r_\varepsilon}} (1 - |u_\varepsilon|^2)^2 dx$$

which yields:

$$\begin{aligned} \int_{\partial\omega_{r_\varepsilon}} |\partial_\tau u_\varepsilon|^2 ds &\leq C' \int_{\partial\omega_{r_\varepsilon}} |\partial_v u_\varepsilon|^2 ds + \frac{8}{r_\varepsilon \varepsilon^2} \int_{\omega_{r_\varepsilon}} (1 - |u_\varepsilon|^2)^2 dx \\ &\leq C' \Upsilon^2 \int_{\Gamma_{r_\varepsilon}} [(u_\varepsilon, g) - \cos \alpha] g + (|u|^2 - 1) u^2 ds + \frac{8}{r_\varepsilon \varepsilon^2} \int_{\omega_{r_\varepsilon}} (1 - |u_\varepsilon|^2)^2 dx + \frac{C''}{r_\varepsilon} F(r_\varepsilon) \\ &\leq C''' \left[\Upsilon^2 \int_{\Gamma_{r_\varepsilon}} W(u, g) ds + \frac{8}{r_\varepsilon \varepsilon^2} \int_{\omega_{r_\varepsilon}} (1 - |u_\varepsilon|^2)^2 dx + \frac{F(r_\varepsilon)}{r_\varepsilon} \right] \\ &\leq C'''' \eta \{ \varepsilon^{-s} + \varepsilon^{-\gamma} \} \\ &\leq C \varepsilon^{-s}, \end{aligned}$$

using (4.4) in the next to last line. By the Sobolev embedding theorem (on the one-dimensional set Γ_{r_ε}), there exists a constant $C > 0$ independent of x_0 and of ε for which

$$|u_\varepsilon(x) - u_\varepsilon(y)| \leq C \sqrt{|x - y|} \varepsilon^{-s/2} \quad (4.23)$$

holds for all $x, y \in \Gamma_{r_\varepsilon}$.

The conclusion now follows as in Proposition 3.6 of [9]. Assume there exists $x_2 \in \Gamma_{r_\varepsilon}$ for which $W(u, g) > a$. Using (4.23), there would exist a radius $\rho = c\varepsilon^s$, for constant $c > 0$ independent of x_0 , for which $W(u, g) > \frac{a}{2}$ when $x \in \Gamma_{r_\varepsilon} \cap B_\rho(x_2)$. In that case, we would have, by (4.4),

$$C\eta \geq \Upsilon \int_{\Gamma_{r_\varepsilon} \cap B_{c\varepsilon^s}} W(u, g) ds > \Upsilon \frac{a}{2} 2\pi c\varepsilon^s = \pi ac',$$

which would lead to a contradiction for η chosen sufficiently small. By reducing the value of η required for the proof of (4.2) if necessary, we obtain (4.3). Thus there exists $\eta > 0$ for which all three statements are valid and this completes the proof of Proposition 4.1. \square

Corollary 4.3. *Let $(u_\varepsilon)_{\varepsilon>0}$ be a family of solutions with $E_\varepsilon(u_\varepsilon) \leq K |\ln \varepsilon|$ and $\frac{3}{4}s < \gamma < s$. Then, $\forall x_0 \in \bar{\Omega}$,*

$$\frac{1}{2\varepsilon^2} \int_{B_{\varepsilon^\gamma}(x_0)} (|u_\varepsilon|^2 - 1)^2 dx + \Upsilon \int_{\Gamma \cap B_{\varepsilon^\gamma}(x_0)} W(u_\varepsilon, g) ds \leq C(K)$$

Proof. As mentioned in the proof of Proposition 4.1, (4.21) holds for any η as long as $E(u_\varepsilon; B_{\varepsilon^\beta}(x_0)) \leq \eta |\ln \varepsilon|$, which is clearly satisfied with $\eta = K$. Since $B_{\varepsilon^\beta}(x_0) \subset B_{r_\varepsilon}(x_0)$, the conclusion follows. \square

4.2. Defining bad balls

We define the family of sets

$$S_\varepsilon = \left\{ x \in \Omega : |u_\varepsilon(x)|^2 < 1 - \sqrt{2}a \right\}, \quad T_\varepsilon = \left\{ x \in \partial\Omega : W(u_\varepsilon, g) > a^2 \right\}.$$

Following Lemmas 3.1 and 3.2 of [18], we show that the sets $S_\varepsilon, T_\varepsilon$ which include the defects may be contained in a bounded number of vary small balls.

Lemma 4.4. *There exists $N_0 = N_0(a, g, s, \alpha)$, $\kappa > 1$, and points $p_{\varepsilon,1}, \dots, p_{\varepsilon,I_\varepsilon} \in S_\varepsilon$, $y_{\varepsilon,1}, \dots, y_{\varepsilon,J_\varepsilon} \in T_\varepsilon \cap \Gamma$ such that*

- (i) $I_\varepsilon + J_\varepsilon \leq N_0$;
- (ii) $\{B_{\kappa\varepsilon}(p_{\varepsilon,i}), B_{\kappa\varepsilon^s}(y_{\varepsilon,j})\}_{1 \leq i \leq I_\varepsilon, 1 \leq j \leq J_\varepsilon}$ are mutually disjoint; more precisely $|p_{\varepsilon,i} - p_{\varepsilon,j}| > 8\kappa\varepsilon$, $|p_{\varepsilon,i} - y_{\varepsilon,j}| > 8\kappa\varepsilon^s$ and $|y_{\varepsilon,i} - y_{\varepsilon,j}| > 8\kappa\varepsilon^s$
- (iii)

$$S_\varepsilon \subset \bigcup_{i=1}^{I_\varepsilon} B_{\kappa\varepsilon}(p_{\varepsilon,i}) \text{ and } T_\varepsilon \subset \bigcup_{j=1}^{J_\varepsilon} B_{\kappa\varepsilon^s}(y_{\varepsilon,j}). \quad (4.24)$$

Proof. The is essentially the same as in Struwe [18], who considered the case of Dirichlet boundary conditions, for which all of the “bad balls” have the same radius ε , so here we need to make some modification due to our boundary conditions. As the existence of ε -balls covering S_ε is the same as in [18], we only need to treat T_ε .

By the η -compactness Proposition 4.1, if $y \in T_\varepsilon$, it follows that $E_\varepsilon(u_\varepsilon; B_{\varepsilon^\beta}(y)) > \eta|\ln \varepsilon|$. Furthermore, applying the Vitali’s covering Theorem to the collection $(B_{\varepsilon^\beta}(y))_{y \in T_\varepsilon}$, there is a finite choice $y_1, \dots, y_{N_1} \in \overline{T_\varepsilon}$ for which $(B_{\varepsilon^\beta}(y_i))_{i=1, \dots, N_1}$ are disjoint, and $\left[\Omega \cap \bigcup_{y \in T_\varepsilon} B_{\varepsilon^\beta}(y)\right] \subset \left(\bigcup_{i=1}^{N_1} B_{5\varepsilon^\beta}(y_i)\right)$. Therefore it follows:

$$N_1 \eta |\ln \varepsilon| \leq \sum_{i=1}^{N_1} E_\varepsilon(u_\varepsilon; B_{\varepsilon^\beta}(y_i)) \leq E_\varepsilon(u_\varepsilon) \leq K |\ln \varepsilon|, \quad (4.25)$$

which means that $N_1 = N_1(\varepsilon)$ is uniformly bounded from above.

Next, using the same argument as in (4.20), there exists $r_\varepsilon \in (\varepsilon^\gamma, \varepsilon^\beta)$ such that

$$(\gamma - \beta) |\ln \varepsilon| F(r_\varepsilon) \leq E(u_\varepsilon; \omega_{\varepsilon^\beta \setminus \varepsilon^\gamma}(y)) \leq K |\ln \varepsilon|, \text{ i.e. } F(r_\varepsilon) \leq C_1$$

$\forall \varepsilon, y \in T_\varepsilon$, so by Lemma 4.2 we obtain the uniform estimate

$$\begin{aligned} \frac{1}{2\varepsilon^2} \int_{\omega_{r_\varepsilon}(y)} (|u_\varepsilon|^2 - 1)^2 dx + \Upsilon \int_{\Gamma_{r_\varepsilon}(y)} W(u, g) ds &\leq C(F(r_\varepsilon) + r_\varepsilon^2 \Upsilon + O(1)) \\ &\leq C_2, \end{aligned}$$

uniformly in $\varepsilon, y \in T_\varepsilon$.

On the other hand, by the Hölder bound arguments employed in the proof of Proposition 4.1 (see (4.23)), there exists constants c_1, c_2 (independent of ε) such that $\forall y \in T_\varepsilon$,

$$\Upsilon_\varepsilon \int_{B_{c_1 \varepsilon^s}(y)} W(u, g) dx \geq c_2 > 0,$$

independently of $\varepsilon, y \in T_\varepsilon$.

Now following Struwe (see Lemma 3.2 in [18]) and using Vitali’s covering Theorem again, we conclude that there exists a finite collection $y_1, \dots, y_J \in T_\varepsilon$, with J uniformly bounded in ε such that the sets $\{B_{\varepsilon^s}(y_j)\}_{j=1, \dots, J}$ are disjoint and $T_\varepsilon \subset \bigcup_{j=1}^J B_{5\varepsilon^s}(y_j)$. Finally, by the same argument as that of Theorem IV.1 of [4], by enlarging and if necessary fusing together vortex balls which intersect, we may find $\kappa > 1$ and modified centers p_i, y_j for which (ii) holds. \square

5. Classifying the defects

Our goal in this section is to classify defects $x_0 \in \overline{\Omega}$, defined as a center of one of the “bad balls” constructed in Lemma (4.4), and associate a degree to each. For any $x_0 \in \overline{\Omega}$, and $0 < r < R < \infty$, denote the annulus centered at x_0 by

$$A_{r,R}(x_0) = w_R(x_0) \setminus w_r(x_0).$$

We will analyze the structure of u_ε in such annuli around defects.

We begin with a lemma which shows the energy densities are coercive near their minima:

Lemma 5.1. *For any $\alpha \in (0, \frac{\pi}{2})$, we can find a constant $C_\alpha > 0$ and $a_0 = a_0(\alpha)$ such that for $u \in \mathbb{C}$ and $g = e^{i\gamma} \in S^1 \subset \mathbb{C}$ with $W(u, g) < a_0^2$ we may represent $u = f e^{i\psi}$ with*

$$\begin{aligned} |f^2 - 1| &\leq \sqrt{2W(u, g)} < \sqrt{2}a_0 \text{ and} \\ \text{either } |\psi - \gamma - \alpha| &< C_\alpha \sqrt{W(u, g)} \text{ or } |\psi - \gamma + \alpha| < C_\alpha \sqrt{W(u, g)} \end{aligned} \quad (5.1)$$

Note that by choosing a_0 sufficiently small, the intervals

$$\mathcal{I}_\pm := \{\psi : |\psi - \gamma \pm \alpha| < C_\alpha \sqrt{W(u, g)}\} \quad (5.2)$$

will be disjoint. In particular, in places where W is small, we know that u must be close to either $e^{i(\gamma \pm \alpha)}$, but not both.

Proof of the Lemma 5.1. Let $a := \sqrt{W(u, g)} < a_0$, a_0 to be determined.

$$\frac{1}{2}(|u|^2 - 1)^2 \leq a^2 \iff 1 - \sqrt{2}a \leq |u|^2 \leq 1 + \sqrt{2}a$$

It follows that for $a_0 < \frac{1}{4}$, $a \in (0, a_0)$, we may write $u = f e^{i\psi}$ with

$$1 - \sqrt{2}a \leq f^2 \leq 1 + \sqrt{2}a \text{ and } \phi := \psi - \gamma \in [-\pi, \pi].$$

This choice of ϕ is natural since we have in addition,

$$[(u, g) - \cos \alpha]^2 \leq a^2 \iff \cos \alpha - a \leq f \cos \phi \leq \cos \alpha + a.$$

Therefore

$$\frac{\cos \alpha - a}{\sqrt{1 + \sqrt{2}a}} \leq \cos \phi \leq \frac{\cos \alpha + a}{\sqrt{1 - \sqrt{2}a}},$$

and it follows:

$$\cos \phi \leq (\cos \alpha + a)(1 + 4a) < \cos \alpha + C_1 a \quad (5.3)$$

$$\cos \phi \geq (\cos \alpha - a)(1 - a) > \cos \alpha - C_1 a, \quad (5.4)$$

and hence

$$|\cos \phi - \cos \alpha| < C_1 a.$$

Since $\alpha \in (0, \frac{\pi}{2})$, and $\phi \in (-\pi, \pi)$, choosing $a_0 = a_0(\alpha)$ sufficiently small, $\forall a \in [0, a_0]$, we have

$$\{\phi \in (-\pi, \pi) : |\cos \phi - \cos \alpha| < C_1 a\} \subset (-\alpha - C_\alpha a, -\alpha + C_\alpha a) \cup (\alpha - C_\alpha a, \alpha + C_\alpha a).$$

Recalling that $a = \sqrt{W(u, g)}$, this completes the proof. \square

For the remainder of the paper, we fix once and for all a value $a_0 = a_0(\alpha)$ such that the intervals \mathcal{I} in (5.2) where $\psi - \gamma$ is close to either α or $-\alpha$ are disjoint.

We now treat the question of classification of defects, and their associated degrees. If $x_0 \in \Omega$ then the defect is an interior vortex, and its degree $d(x_0) \in \mathbb{Z}$ is defined in the usual way. When $x_0 \in \Gamma = \partial\Omega$ the situation is more interesting and more subtle.

In case $x_0 \in \Gamma$, for R sufficiently small the piece of the boundary $\partial A_{r,R}(x_0) \cap \partial\Omega$ consists as before of exactly two arcs along $\Gamma_R = \Gamma \cap B_R(x_0)$, which we will denote by $\Gamma_{r,R}^\pm$. (See Fig. 1.) We recall from the upper bound construction in Lemma 3.1 that Γ_R^\pm may be parametrized as

$$\Gamma_R^\pm = \{(\rho, \theta_\pm(\rho)) : 0 < \rho \leq R\},$$

for smooth $\theta_\pm(\rho)$, with $\theta_+(\rho) = O(\rho)$ and $\theta_-(\rho) = \pi + O(\rho)$.

We now apply Proposition 4.1 to u_ε to conclude that for any $0 < r < R$ with $A_{r,R}(x_0)$ disjoint from the bad balls covering $S_\varepsilon \cap T_\varepsilon$, we have $|u_\varepsilon|^2 \geq 1 - \sqrt{2}a$ in $A_{r,R}(x_0)$ and, for $x_0 \in \Gamma$, $W(u_\varepsilon, g) \leq a^2$ on Γ_R^\pm . In particular, Lemma 5.1 applies and we obtain the representation

$$u_\varepsilon = f(\rho, \theta) e^{i\psi(\rho, \theta)}, \quad \text{with } |f^2 - 1| < \sqrt{2}a \text{ in } A_{r,R}, \quad (5.5)$$

and the phase ψ on $\Gamma_{r,R}^\pm(x_0)$ is chosen with either $\psi \in \mathcal{I}_-$ or $\psi \in \mathcal{I}_+$, that is,

- (I) $|\psi - \gamma - \alpha| < C_\alpha \sqrt{W(u, g)} < C_\alpha a$ or
- (II) $|\psi - \gamma + \alpha| < C_\alpha \sqrt{W(u, g)} < C_\alpha a$,

By the continuity of $g = e^{i\gamma}$, for R small we can treat $\gamma(x) \simeq \gamma_0 := \gamma(x_0)$ on Γ_R , and in fact the complex phase difference of u along each of Γ_R^\pm is also small (on the order of R) and hence the winding of the phase around a boundary vortex occurs principally around the half-circle $\partial B_R(x_0) \cap \Omega$. Introduce polar coordinates (ρ, θ) centered at x_0 , with θ measured from the unit tangent τ to Γ at x_0 . (See Fig. 1.)

We distinguish three possibilities for each boundary defect $x_0 \in \Gamma$, define the degree, and introduce a new topological index $\tau(x_0) \in \{-1, 0, 1\}$, the “boojum number”.

CLASSIFICATION OF BOUNDARY DEFECTS:

(i) “Light boojums”.

In this case, (I) holds on $\Gamma_{r,R}^-(x_0)$ while (II) holds on $\Gamma_{r,R}^+(x_0)$. This means that the phase decreases by 2α (modulo 2π) along Γ_R . So let $n(x_0) \in \mathbb{Z}$ be the number of multiples of 2π by which the phase increases around x_0 . Note that $n(x_0)$ represents the degree at x_0 . In particular, we may write $u(\rho, \theta) = f(\rho, \theta) \exp(i\psi(\rho, \theta))$ in polar coordinates centered at x_0 , with phase

$$\psi(\rho, \theta) = \gamma_0 - \alpha + 2\frac{\theta}{\pi}(\alpha + n(x_0)\pi) + \phi(\rho, \theta), \quad \theta_+(\rho) < \theta < \theta_-(\rho), \quad (5.6)$$

with ϕ a smooth single-valued function in $A_{r,R}(x_0)$. Note that for light boojums, $(iu_\varepsilon, g) = |u_\varepsilon| \sin(\psi - \gamma)$ changes sign, from positive to negative, moving counter-clockwise across the boundary defect x_0 . We define the boojum number $\tau(x_0) = -1$ for a light boojum.

(ii) “Heavy boojums”.

In this case, (II) holds on $\Gamma_{r,R}^-(x_0)$ while (I) holds on $\Gamma_{r,R}^+(x_0)$. This means that the phase increases by 2α (modulo 2π) along Γ_R . Again, let $n(x_0) \in \mathbb{Z}$ be the number of multiple of 2π by which the phase increases. As above, $n(x_0)$ represents the degree of a heavy boojum, and using polar coordinates centered at $x_0 \in \Gamma$, we may write $u(\rho, \theta) = f(\rho, \theta) \exp(i\psi(\rho, \theta))$, with phase

$$\psi(\rho, \theta) = \gamma_0 + \alpha + 2\frac{\theta}{\pi}(-\alpha + n(x_0)\pi) + \phi(\rho, \theta), \quad \theta_+(\rho) < \theta < \theta_-(\rho), \quad (5.7)$$

with ϕ a smooth single-valued function in $A_{r,R}(x_0)$. As for light boojums, $(iu_\varepsilon, g) = |u_\varepsilon| \sin(\psi - \gamma)$ changes sign across the defect x_0 , but for heavy boojums it goes from negative to positive as we move counter clockwise. The boojum number for a heavy boojum is $\tau(x_0) = +1$.

(iii) “Boundary vortices”.

This occurs when either (I) or (II) holds on both $\Gamma_{r,R}^\pm(x_0)$. In particular, the phase ψ rotates by $2\pi n$ along $\partial B_\rho(x_0) \cap \Omega$, with $n \in \mathbb{Z}$, so in polar coordinates we may write

$$\psi(\rho, \theta) = \gamma_0 \pm \alpha + 2n\theta + \phi(\rho, \theta), \quad \theta_+(\rho) < \theta < \theta_-(\rho), \quad (5.8)$$

for smooth, single-valued $\phi(\rho, \theta)$ in $A_{r,R}(x_0)$. The degree associated with the boundary vortex is $n = n(x_0) \in \mathbb{Z}$, and the boojum number $\tau(x_0) = 0$. Note that the sign of $(iu_\varepsilon, g) = |u_\varepsilon| \sin(\psi - \gamma)$ does not change across a boundary vortex.

Remark 5.2. If we extend the modulus and phase $f_\varepsilon, \psi_\varepsilon$ to all of Γ_R by linearly interpolating in Γ_r from the values in Γ_R^\pm , we may define a nonvanishing extension $\tilde{u}_\varepsilon = \tilde{f}_\varepsilon e^{i\tilde{\psi}_\varepsilon}$ of u_ε to all of Γ_R . Setting $\tilde{u}_\varepsilon = u_\varepsilon$ on $\partial B_R(x_0) \cap \Omega$, we obtain an S^1 -valued map $\frac{\tilde{u}}{|\tilde{u}|} : \partial\omega_R(x_0) \rightarrow S^1$, whose degree measured on $\partial\omega_R(x_0)$ is $n(x_0)$, as defined above.

Remark 5.3. It is here that we see that the case $\alpha \in (\frac{\pi}{2}, \pi)$ is the same as the case $\alpha \in (0, \frac{\pi}{2})$: it only exchanges the role of “heavy” and “light” boojums.

Now that we have defined degrees corresponding to the bad balls constructed in Lemma 4.4, we may verify that they must always sum to the degree $\mathcal{D} = \deg(g; \partial\Omega)$:

Lemma 5.4. Let $\{B_{\kappa\varepsilon}(p_{\varepsilon,i})\}_{1 \leq i \leq I_\varepsilon}$, $\{B_{\kappa\varepsilon^s}(y_{\varepsilon,j})\}_{1 \leq j \leq J_\varepsilon}$ be as in Lemma 4.4, and $d_i = n(p_{\varepsilon,i})$, $n_j = n(y_{\varepsilon,j}) \in \mathbb{Z}$ be their degrees. Then,

$$\deg(g; \partial\Omega) = \mathcal{D} = \sum_{i=1}^{I_\varepsilon} d_i + \sum_{j=1}^{J_\varepsilon} n_j.$$

The proof of Lemma 5.4 involves excising half-disks around the boundary defects, and redefining u_ε on the arcs $\Gamma_R(x_0)$ as in Remark 5.2. The details may be found in part (i) of [1, Lemma 5.3].

6. Energy lower bound for defects

We are ready to prove lower bounds on the energy in annular regions around the defects.

Proposition 6.1. Suppose $E_\varepsilon(u_\varepsilon) \leq K|\ln \varepsilon|$ with constant K independent of ε . Assume $x_0 \in \Gamma = \partial\Omega$, $R > r > \varepsilon^s$, and that $|u|^2 \geq 1 - \sqrt{2}a$ on the annulus $A_{r,R}(x_0)$ and $W(u, g) \leq a^2$ on $\Gamma_{r,R}^\pm$. If x_0 has degree $n(x_0)$ and boojum number $\tau(x_0) \in \{-1, 0, 1\}$. Then, there exists a constant C (depending on α, a and $\partial\Omega$), such that:

$$\frac{1}{2} \int_{A_{r,R}} |\nabla u_\varepsilon|^2 dx \geq 2\pi \left(n(x_0) - \tau(x_0) \frac{\alpha}{\pi} \right)^2 \ln \left(\frac{R}{r} \right) - C. \quad (6.1)$$

It is well-known that for interior vortices $x_0 \in \Omega$, the energy lower bound is given by

$$\frac{1}{2} \int_{A_{r,R}} |\nabla u_\varepsilon|^2 dx \geq \pi (n(x_0))^2 \ln \left(\frac{R}{r} \right) - C.$$

Proof of Proposition 6.1. For simplicity, we drop the ε subscripts, and write $n := n(x_0)$ and $\tau = \tau(x_0)$. We may unify the polar coordinate representations (5.6), (5.7), and (5.8) using boojum number, and write $u(\rho, \theta) = f(\rho, \theta) e^{i\psi(\rho, \theta)}$ in $A_{r,R}(x_0)$ with

$$\psi(\rho, \theta) = \gamma_0 + 2n\theta + \tau\alpha \left(1 - \frac{2\theta}{\pi} \right) + \phi(\rho, \theta). \quad \theta_+(\rho) < \theta < \theta_-(\rho). \quad (6.2)$$

Thus, we have:

$$\begin{aligned}
|\nabla u_\varepsilon|^2 &\geq f^2 |\nabla \psi|^2 \geq f^2 \left| 2 \left(n - \tau \frac{\alpha}{\pi} \right) \nabla \theta + \nabla \phi \right|^2 \\
&= f^2 \left[4 \left(n - \tau \frac{\alpha}{\pi} \right)^2 |\nabla \theta|^2 + 4 \left(n - \tau \frac{\alpha}{\pi} \right) \nabla \theta \cdot \nabla \phi + |\nabla \phi|^2 \right] \\
&= 4 \left(n - \tau \frac{\alpha}{\pi} \right)^2 \frac{1}{\rho^2} + \mathcal{E},
\end{aligned} \tag{6.3}$$

with remainder term,

$$\mathcal{E} := (f^2 - 1) 4 \left(n - \tau \frac{\alpha}{\pi} \right)^2 \frac{1}{\rho^2} + 4 f^2 \left(n - \tau \frac{\alpha}{\pi} \right) \frac{1}{\rho^2} \frac{\partial \phi}{\partial \theta} + f^2 |\nabla \phi|^2.$$

We claim that $\int_{A_{r,R}(x_0)} \mathcal{E} dx \geq C$, with constant C independent of ε as long as $r > \varepsilon^s$. Assuming the claim for the moment, we obtain the desired lower bound, since then,

$$\begin{aligned}
\frac{1}{2} \int_{A_{r,R}} |\nabla u_\varepsilon|^2 dx &\geq 2 \left(n - \tau \frac{\alpha}{\pi} \right)^2 \int_{A_{r,R}} \frac{1}{\rho^2} dx + C \\
&= 2 \left(n - \tau \frac{\alpha}{\pi} \right)^2 \int_r^R \int_{\theta^-(\rho)}^{\theta^+(\rho)} \frac{1}{\rho} d\theta d\rho + C \\
&= 2 \left(n - \tau \frac{\alpha}{\pi} \right)^2 \int_r^R \frac{1}{\rho} [\theta^-(\rho) - \theta^+(\rho)] d\rho + C \\
&= 2\pi \left(n - \tau \frac{\alpha}{\pi} \right)^2 \int_r^R \frac{1}{\rho} d\rho + C \\
&= 2\pi \left(n - \tau \frac{\alpha}{\pi} \right)^2 \ln \left(\frac{R}{r} \right) + C.
\end{aligned}$$

It remains to verify the claim. We will start by showing that the first term in \mathcal{E} has small integral. Using the upper bound on the energy from Lemma 3.1, and recalling (see Section 4) $r > \varepsilon^s$ with $\frac{3}{4}s < \gamma < s$, we have:

$$\left| \int_{A_{r,R}} (1 - f^2) \frac{1}{\rho^2} dx \right| \leq \left[\left(\int_{B_R} (1 - f^2)^2 dx \right) \left(\int_{A_{r,R}} \frac{1}{\rho^4} dx \right) \right]^{\frac{1}{2}} \tag{6.4}$$

$$\leq \left[C \varepsilon^2 |\ln \varepsilon| \left(\frac{1}{r^2} - \frac{1}{R^2} \right) \right]^{\frac{1}{2}} \rightarrow 0 \tag{6.5}$$

as $\varepsilon \rightarrow 0$.

Next we show that we can bound the second term in \mathcal{E} by the (positive) third term. We write,

$$\int_{A_{r,R}} f^2 \frac{1}{\rho^2} \frac{\partial \phi}{\partial \theta} dx = \int_{A_{r,R}} \frac{\partial \phi}{\partial \theta} \frac{1}{\rho^2} dx + \int_{A_{r,R}} \frac{f^2 - 1}{\rho^2} \frac{\partial \phi}{\partial \theta} dx \tag{6.6}$$

and estimate each term separately. For the first term on the right hand side, we write:

$$\int_{A_{r,R}} \frac{\partial \phi}{\partial \theta} \frac{1}{\rho^2} dx = \int_r^R \int_{\theta^-(\rho)}^{\theta^+(\rho)} \frac{\partial \phi}{\partial \theta} \frac{1}{\rho} d\theta d\rho$$

$$= \int_r^R [\phi(\rho, \theta^-(\rho)) - \phi(\rho, \theta^+(\rho))] \frac{d\rho}{\rho}$$

and therefore

$$\left| \int_{A_{r,R}} \frac{\partial \phi}{\partial \theta} \frac{1}{\rho^2} dx \right| \leq C \left(\int_{\Gamma_{r,R}^+(x_0)} |\phi| \frac{d\rho}{\rho} + \int_{\Gamma_{r,R}^-(x_0)} |\phi| \frac{d\rho}{\rho} \right).$$

To continue we require the estimates in Lemma 5.1. Note that the intervals \mathcal{I}_\pm for the phase ψ may be defined modulo 2π , and the fact that $n = n(x_0)$ is the degree of the defect implies that $\psi(x) - 2\pi n \in \mathcal{I}_-$ or \mathcal{I}_+ for all $x \in \Gamma_{r,R}^\pm$. For concreteness, let's assume $\psi - 2\pi n \in \mathcal{I}_-$ on $\Gamma_{r,R}^-$; all other cases may be handled in the same way. From Lemma 5.1 (with the above observation) we may then conclude that on $\Gamma_{r,R}^-(x_0)$ it holds:

$$\begin{aligned} C_\alpha \sqrt{W(u, \rho)} &> |\psi - \gamma - \alpha - 2n\pi| \\ &= |\gamma_0 - \alpha + 2\left(\frac{\alpha}{\pi} + n\right)\theta^-(\rho) + \phi(\rho, \theta) - \gamma - \alpha - 2n\pi| \\ &= |(\gamma_0 - \gamma) + 2\alpha \left(\frac{\theta^-(\rho)}{\pi} - 1\right) + 2n(\theta^-(\rho) - \pi) + \phi(\rho, \theta)| \\ &\geq |\phi(\rho, \theta)| - |\gamma_0 - \gamma| - \frac{2\alpha}{\pi} |\theta^-(\rho) - \pi| - 2n |\theta^-(\rho) - \pi| \\ &\geq |\phi| - C\rho. \end{aligned}$$

Therefore on $\Gamma_{r,R}^-(x_0)$

$$|\phi| \leq C_\alpha \sqrt{W(u, g)} + O(\rho),$$

and similarly on $\Gamma_{r,R}^+(x_0)$.

In consequence we have

$$\int_{\Gamma_{r,R}^+(x_0) \cup \Gamma_{r,R}^-(x_0)} |\phi| \frac{d\rho}{\rho} \leq \int_{\Gamma_{r,R}^+(x_0) \cup \Gamma_{r,R}^-(x_0)} C_\alpha \frac{1}{\rho} \sqrt{W(u, g)} d\rho + O(1) \quad (6.7)$$

We split $\Gamma_{r,R}^\pm(x_0)$ in two parts:

$$\Gamma_{r,R}^\pm(x_0) = \Gamma_{r,\varepsilon\gamma}^\pm(x_0) \cup \Gamma_{\varepsilon\gamma,R}^\pm(x_0),$$

and using the Corollary 4.3 we estimate:

$$\begin{aligned} &\int_{\Gamma_{r,\varepsilon\gamma}^+(x_0) \cup \Gamma_{r,\varepsilon\gamma}^-(x_0)} \frac{1}{\rho} \sqrt{W(u, g)} d\rho \\ &\leq \left[\left(\int_{\Gamma_{r,\varepsilon\gamma}^+(x_0) \cup \Gamma_{r,\varepsilon\gamma}^-(x_0)} W(u, g) d\rho \right) \left(\int_{\Gamma_{r,\varepsilon\gamma}^+(x_0) \cup \Gamma_{r,\varepsilon\gamma}^-(x_0)} \frac{d\rho}{\rho^2} \right) \right]^{\frac{1}{2}} \\ &\leq \frac{C}{r^{\frac{1}{2}} \Upsilon} = o(1), \end{aligned}$$

since $r > \varepsilon^s = \Upsilon^{-1}$. Furthermore, by the global upper bound on the energy $E_\varepsilon(u_\varepsilon) \leq K |\ln \varepsilon|$,

$$\begin{aligned}
& \int_{\Gamma_{\varepsilon^\gamma, R}^+(x_0) \cup \Gamma_{\varepsilon^\gamma, R}^-(x_0)} \frac{1}{\rho} \sqrt{W(u, g)} d\rho \\
& \leq \left[\left(\int_{\Gamma_{\varepsilon^\gamma, R}^+(x_0) \cup \Gamma_{\varepsilon^\gamma, R}^-(x_0)} W(u, g) d\rho \right) \left(\int_{\Gamma_{\varepsilon^\gamma, R}^+(x_0) \cup \Gamma_{\varepsilon^\gamma, R}^-(x_0)} \frac{d\rho}{\rho^2} \right) \right]^{\frac{1}{2}} \\
& \leq C \Upsilon^{-1} |\ln \varepsilon| \varepsilon^{-\gamma} \rightarrow 0,
\end{aligned}$$

since $s - \gamma > 0$.

We are left with estimating the second term in (6.6):

$$\begin{aligned}
\left| \int_{A_{r, R}} \frac{f^2 - 1}{\rho^2} \frac{\partial \phi}{\partial \theta} dx \right| & \leq \frac{1}{\varepsilon^s} \int_{A_{r, R}} |f^2 - 1| \left| \frac{1}{\rho} \frac{\partial \phi}{\partial \theta} \right| dx \\
& \leq \varepsilon^{-s} \left[\int_{A_{r, R}} |f^2 - 1|^2 \int_{A_{r, R}} |\nabla \phi|^2 \right]^{\frac{1}{2}} \\
& \leq \varepsilon^{-s} \left[K \varepsilon^2 |\ln \varepsilon| \int_{A_{r, R}} |\nabla \phi|^2 \right]^{\frac{1}{2}} \\
& \leq C \varepsilon^{1-s} \sqrt{|\ln \varepsilon|} \left[\int_{A_{r, R}} |\nabla \phi|^2 \right]^{\frac{1}{2}} \\
& = o(1) \left(\int_{A_{r, R}} |\nabla \phi|^2 \right)^{\frac{1}{2}} + o(1)
\end{aligned} \tag{6.8}$$

Finally, the last term in \mathcal{E} is bounded below,

$$\int_{A_{r, R}} f^2 |\nabla \phi|^2 dx \geq (1 - \sqrt{2}a)^2 \int_{A_{r, R}} |\nabla \phi|^2 dx,$$

and hence this positive term controls (6.8). Putting all of these estimates together, we obtained the desired lower bound on the residual term, $\int_{A_{r, R}} \mathcal{E} dx \geq C$, and the desired lower bound is established. \square

Remark 6.2. We note that it is in deriving the estimate (6.7), on the energy contribution of the “excess phase” ϕ to the energy of a boundary defect, where we need to introduce the boundary penalization of $(|u|^2 - 1)^2$ in $W(u, g)$. (See (2.20) and the following remarks there.) In particular, while we know that $|u_\varepsilon|^2 \geq 1 - \sqrt{2}a > 0$ away from the bad balls, this is not a strong enough estimate to control the error term in (6.7) without introducing additional logarithmically growing terms.

Next we compare the energies of boundary boojums and boundary vortices. First, we remark that, since the phase $\psi \simeq \gamma \pm \alpha$ away from the bad balls, and $0 < \alpha < \frac{\pi}{2}$, light and heavy boojums must be paired and in fact must alternate as we trace out $\Gamma = \partial\Omega$. In addition, given the lower bound (6.1) for annuli, we observe that the lower bound for the energy of a “ground state” boojum pair, with $(n, \tau) = (0, -1), (1, 1)$, is smaller than that of a boundary vortex since

$$C_\alpha := \left(\frac{\alpha}{\pi} \right)^2 + \left(1 - \frac{\alpha}{\pi} \right)^2 < 1.$$

This suggests that boojum pairs will always be energetically preferred over boundary vortices. We will indeed show this in the course of proving the main theorem, but the following fundamental lemma is suggestive of this fact (and will be instrumental in proving it).

In the following lemma we will denote by n_j^0 the degree of a boundary vortex, and by n_i^+ the degree of a heavy boojum while n_i^- will be that of a light boojum:

Lemma 6.3. Assume $\exists N^v, N^b \in \{0, 1, 2, \dots\}$ and integers $\{n_j^0\}_{j=1, \dots, N^v}, \{n_i^+, n_i^-\}_{i=1, \dots, N^b}$ with $\sum_{i=1}^{N^b} (n_i^+ + n_i^-) + \sum_{j=1}^{N^v} n_j^0 = D$. Then

$$\sum_{j=1}^{N^v} (n_j^0)^2 + \sum_{i=1}^{N^b} \left[(n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 \right] \geq |D| C_\alpha. \quad (6.9)$$

Furthermore, in case that $D > 0$, we have equality if and only if

$$n_j^0 = 0 \forall j, \quad n_i^+ = 1 \forall i, \quad \text{and} \quad n_i^- = 0, i = 1, \dots, D = N^b,$$

while if $D < 0$, we have equality if and only if

$$n_j^0 = 0 \forall j, \quad n_i^+ = 0 \forall i, \quad \text{and} \quad n_i^- = -1, i = 1, \dots, D = N^b$$

Remark 6.4. We note that the minimum value is therefore obtain by N^b boojum pairs of light and heavy boojums and with no boundary vortex.

Remark 6.5. In proving Lemma 6.3 it is advantageous to list the different types of defects (light and heavy boojums and boundary vortices) separately, but for later purposes it will be more convenient to make a single list of the defects $y_{\varepsilon, \ell}$, using the integer degree n_ℓ and boojum number $\tau_\ell \in \{0, -1, +1\}$ to distinguish their topological type. In the latter case, the lower bound expressed in equation (6.9) is reformulated as:

$$\sum_{\ell=1}^{N^v + N^b} (n_\ell - \tau_\ell \frac{\alpha}{\pi})^2 \geq |D| C_\alpha. \quad (6.10)$$

Recall that $\tau = 0$ for a boundary vortex, $\tau = \pm 1$ for a heavy, respectively light, boojum and that $N^v + N^b$ is the total number of boundary defects.

Proof. Assume $D > 0$. We use induction on $D \in \mathbb{N}$ and assume that the lower bound is false, i.e. that the inequality (6.9) is reversed; for $D = 1$ we then have:

$$\sum_{j=1}^{N^v} (n_j^0)^2 + \sum_{i=1}^{N^b} \left[(n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 \right] \leq C_\alpha.$$

As we have a sum of positive terms, this means:

$$\sum_{j=1}^{N^v} (n_j^0)^2 \leq C_\alpha < 1 \implies n_j^0 = 0 \forall j.$$

Further,

$$\sum_{i=1}^{N^b} \left[(n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 \right] \leq C_\alpha,$$

which means that for each i we have

$$\left[(n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 \right] \leq C_\alpha = (\frac{\alpha}{\pi})^2 + (1 - \frac{\alpha}{\pi})^2 < 1,$$

and hence either

$$(n_i^-, n_i^+) = (0, 1) \text{ or } (0, 0) \text{ or } (-1, 0).$$

Since $D = 1 > 0$, for at least one i_0 we have

$$(n_{i_0}^-, n_{i_0}^+) = (0, 1), \text{ and } (n_{i_0}^- + \frac{\alpha}{\pi})^2 + (n_{i_0}^+ - \frac{\alpha}{\pi})^2 = C_\alpha,$$

so

$$\sum_{i \neq i_0} \left[(n_i^+ + \frac{\alpha}{\pi})^2 + (n_i^- - \frac{\alpha}{\pi})^2 \right] \leq 0 \implies N^b = 1, i_0 = 1, (n_1^-, n_1^+) = (0, 1).$$

This corresponds to the case of equality in (6.9) with $D = 1$, and hence we conclude that (6.9) must hold in the case $D = 1$.

Next, consider the case $D > 1$ and assume

$$\sum_{j=1}^{N^v} (n_j^0)^2 + \sum_{i=1}^{N^b} \left[(n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 \right] \leq D C_\alpha, \quad (6.11)$$

holds with D replaced by $D - m$, $m = 1, 2, \dots, D - 1$, with equality if and only if $n_j^0 = 0 \forall j$, $n_i^- = 0 \forall i$, and $n_i^+ = 1, i = 1, \dots, D - m = N^b$, and we will prove that this still holds for D , leading to the conclusion of the Lemma in the case that $D > 0$.

Since $D > 0$, there must be a positively charged defect somewhere. If $\exists n_j^0 \geq 1$, we eliminate that boundary vortex to obtain a new configuration. Indeed, assuming without loss of generality that $j = 1$, we have a configuration

$$\left(\{n_j^0\}_{j=2, \dots, N^v}, \{n_i^-, n_i^+\}_{i=1, \dots, N^b} \right),$$

with degree $D - n_1^0 \leq D - 1$, and

$$\begin{aligned} \sum_{j=2}^{N^v} (n_j^0)^2 + \sum_{i=1}^{N^b} \left[(n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 \right] &\leq D C_\alpha - (n_1^0)^2 \\ &= (D - n_1^0) C_\alpha + n_1^0 C_\alpha - (n_1^0)^2 \\ &< (D - n_1^0) C_\alpha, \end{aligned} \quad (6.12)$$

since $n_1^0 \geq 1$ by assumption.

By induction hypothesis, we conclude that

$$n_j^0 = 0 \forall j = 2, 3, \dots, N^v, N^b = D - n_1^0, n_i^- = 0 \forall i, n_i^+ = 1 \forall i = 1, \dots, D - n_1^0.$$

This means that the left hand side in (6.12) becomes:

$$\sum_{j=2}^{N^v} (n_j^0)^2 + \sum_{i=1}^{N^b} \left[(n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 \right] = (D - n_1^0) C_\alpha,$$

which is a contradiction, so this case cannot occur.

Thus, it must be that $\exists i$, which without loss of generality we will take to be 1, with $n_1^- + n_1^+ \geq 1$. Moreover, since for $x < y$,

$$(x + \frac{\alpha}{\pi})^2 + (y - \frac{\alpha}{\pi})^2 < (y + \frac{\alpha}{\pi})^2 + (x - \frac{\alpha}{\pi})^2,$$

we may assume that $n_1^+ \geq n_1^-, n_1^+ \geq 1$ since otherwise we would switch n_1^+ and n_1^- and obtain a smaller value in (6.11).

Note that

$$\begin{aligned} (n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 &= (n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - 1 + (1 - \frac{\alpha}{\pi}))^2 \\ &\geq (n_i^+ + \frac{\alpha^2}{\pi^2}) + (n_i^- - 1 + (1 - \frac{\alpha}{\pi})^2) = n_i^- + n_i^+ - 1 + C_\alpha \end{aligned} \quad (6.13)$$

so eliminating this boojum pair to create a new configuration with degree $\tilde{D} = D - (n_i^- + n_i^+) < D$, we have from (6.11)

$$\begin{aligned} \sum_{j=1}^{N^v} (n_j^0)^2 + \sum_{i=2}^{N^b} \left[(n_i^- + \frac{\alpha}{\pi})^2 + (n_i^+ - \frac{\alpha}{\pi})^2 \right] &\leq C_\alpha D - [n_1^- + n_1^+ - 1 + C_\alpha] \\ &= \{C_\alpha(D-1) - [n_1^- + n_1^+ - 1]\} \\ &\leq C_\alpha[(D-1) - (n_1^- + n_1^+ - 1)] \\ &= \tilde{D}C_\alpha \end{aligned}$$

with equality if and only if $n_1^- = 0, n_1^+ = 1$. By the induction hypothesis, $\tilde{D} < D$, and

$$n_j^0 = 0 \forall j, N^b = \tilde{D} + n_1^- + n_1^+ = D, n_i^- = 0, n_i^+ = 1, i = 1, \dots, D.$$

This completes the proof for $D > 0$.

When $D < 0$, we note that this reduces to the positive case if we replace $n_j^0 \rightarrow -n_j^0, n_j^+ \rightarrow -n_j^-,$ and $n_j^- \rightarrow -n_j^+,$ that is, negative degree heavy boojums are counted the same way as positive degree light boojums, and vice-versa. The case $D = 0$ is trivially true. \square

7. Proof of the Main Theorem

Returning to the bad balls constructed in Lemma 4.4, we may pass to a subsequence $\varepsilon_n \rightarrow 0$ for which there exist points $\xi_k \in \Omega, k = 1, \dots, N^v, \zeta_k \in \Gamma, k = 1, \dots, N^b,$ for which

$$\begin{aligned} y_{\varepsilon_n, j} &\longrightarrow \zeta_k \quad \text{for some } k \in \{1, \dots, N^b\}, \text{ and} \\ p_{\varepsilon_n, i} &\longrightarrow \xi_k \text{ for some } k \in \{1, \dots, N^v\}, \text{ or } p_{\varepsilon_n, i} \longrightarrow \zeta_k \text{ for some } k \in \{1, \dots, N^b\}. \end{aligned} \quad (7.1)$$

That is, certain interior vortices y_i for u_ε might accumulate at a boundary point $\zeta_k \in \Gamma$. Our task is to provide a global lower bound on the energy to match the upper bounds from Lemma 3.1. To do this we adapt techniques of vortex ball analysis introduced by Jerrard [8] and Sandier [17], but we must treat the various types of defect (boojums, boundary vortices, interior vortices, and interior vortices approaching the boundary) with care, as each leads to a different contribution to the energy.

For $\sigma > 0$, define

$$\mathcal{B}_\sigma := \left(\bigcup_{k=1}^{N^v} B_\sigma(\xi_k) \right) \cup \left(\bigcup_{k=1}^{N^b} B_{\sigma^\varepsilon}(\zeta_k) \right), \quad \text{and} \quad \Omega_\sigma := \Omega \setminus \mathcal{B}_\sigma. \quad (7.2)$$

Lemma 7.1. *Let $1 > \sigma > 0$ be fixed. Then there exists $C = C(g, \alpha, \Omega)$ such that:*

$$E_\varepsilon(u_\varepsilon; \mathcal{B}_\sigma) \geq 2\pi s C_\alpha |\mathcal{D}| \ln\left(\frac{\sigma}{\varepsilon}\right) + C, \quad \text{if } s C_\alpha \leq \frac{1}{2},$$

and

$$E_\varepsilon(u_\varepsilon; \mathcal{B}_\sigma) \geq \pi |\mathcal{D}| \ln\left(\frac{\sigma}{\varepsilon}\right) + C, \quad \text{if } s C_\alpha > \frac{1}{2},$$

Combined with Lemma 3.1 we may then conclude that the energy is bounded above away from any neighborhood of the defects:

Corollary 7.2. *For any $\sigma > 0$, there exists C such that:*

$$E_\varepsilon(u_\varepsilon; \Omega_\sigma) \leq \begin{cases} 2\pi s C_\alpha |\mathcal{D}| |\ln \sigma| + C, & \text{if } s C_\alpha \leq \frac{1}{2}, \\ \pi |\mathcal{D}| |\ln \sigma| + C, & \text{if } s C_\alpha > \frac{1}{2}. \end{cases}$$

Proof of Lemma 7.1. We let $1 > \sigma > 0$ be given, but such that

$$\sigma^s < 4 \min \left\{ |\xi_i - \xi_j|, |\zeta_i - \zeta_j|, \text{dist}(\xi_i, \Gamma) \mid i \neq j, i = 1, \dots, N^v, j = 1, \dots, N^b \right\},$$

so that the balls $B_\sigma(\xi_i), B_\sigma(\zeta_j)$ be well separated in $\overline{\Omega}$. We take $\varepsilon \rightarrow 0$ along the subsequence employed in (7.1) above. By taking a further subsequence we may assume that each of the centers of the bad balls constructed in Lemma 4.4 lies within σ of its limiting ξ_i or ζ_j . We assume $\varepsilon \rightarrow 0$ along this subsequence, but without explicit notation by subscripts.

First, we separate out the “bad balls” defined in Lemma 4.4 whose centers converge to interior points $\xi_j \in \Omega$ (see (7.1) above). Along the subsequence, the total degree due to these, D^{int} is constant, and applying the result of Sandier or Jerrard in a slightly smaller domain $\Omega' \Subset \Omega$, we have the lower bound for the energy in this collection of interior balls,

$$E_\varepsilon \left(u_\varepsilon; \bigcup_{k=1}^{N^v} B_\sigma(\xi_k) \right) \geq \pi |D^{int}| \ln \left(\frac{\sigma}{\varepsilon} \right) + c, \quad (7.3)$$

for any fixed $\sigma > 0$.

For the bad balls which accumulate on the boundary we employ the same procedure introduced in [17] to obtain lower bounds for the classical Ginzburg-Landau functional with Dirichlet boundary condition, adapted to deal with boundary defects. We construct families of balls, $\mathcal{B}(t)$, $t \geq 1$, containing the bad balls of Lemma 4.4, and growing in time. Each ball $B^i(t) \in \mathcal{B}(t)$ carries a degree, a radius $R_i(t)$, and a “seed size” $r_i(t)$, which in some sense remembers the scale of the original ball ($O(\varepsilon)$ or $O(\varepsilon^s)$.) The lower bound is derived through a two-step evolution. The first step is “expansion”: to continuously grow the balls’ radii, and use Proposition 6.1 to estimate the energy in the annuli contained between the expanded balls and the original bad balls, in terms of the logarithm of the ratio of the radii. When two or more balls come into contact, the second “merger” step combines balls together, and uses Lemma 6.3 to bound the energy in the resulting larger balls from below. These two steps are repeated until the radii of the growing balls exceeds σ .

To do this we need to further separate the remaining balls into two classes, those whose centers lie on the boundary versus interior balls converging to the boundary. Assume that $s C_\alpha \leq \frac{1}{2}$; the modifications required for the opposite case will be described at the end of the proof.

Step 0: Initialization. Set the initial time $t_0 = 1$ (for convenience), and begin the process with the remaining bad balls as defined in Lemma 4.4, numbered in a single list, $B^i(t_0)$, $i = 1, \dots, N_0$. Define two index sets $\mathcal{I}_b, \mathcal{I}'$ as follows:

- For $i \in \mathcal{I}_b$, $B^i(t_0)$ are centered on the boundary Γ . Boundary balls have initial radii $r_i(t_0) = \kappa \varepsilon^s$, and carry both a degree n_i and a Boojum number τ_i . We let $D^0 := \sum_{i \in \mathcal{I}_b} n_i$, the total degree of defect balls centered on $\partial\Omega$.
- For $i \in \mathcal{I}'$, $B^i(t_0)$ lie in the interior (but accumulate on the boundary as $\varepsilon \rightarrow 0$.) These balls have degree d_i and initial radii $r_i(t_0) = \kappa \varepsilon$. The total degree of defect balls approaching $\partial\Omega$ will be denoted D' .

We note that by Lemma 5.4 we must have $D^{int} + D^0 + D' = \mathcal{D}$, the total degree associated to the boundary function g . We also define

$$D^b := D^0 + D' = \mathcal{D} - D^{int},$$

and note that D^b is also constant in ε .

The values $r_i(t_0)$ are initially chosen to be the actual radii of vortex balls, but following Sandier [17] we think of them as a “seed size”, which will change in the process of merging the expanding balls but retain the order of magnitude of the original radii.

Step 1: Initial expansion. We grow the radii of each ball continuously in time t , maintaining a uniform ratio of the radius of each ball to its initial radius. We do this in a different way depending on the two classes of bad balls near the boundary. We recall that the initial time $t_0 = 1$. If $B_1(t_0)$ is centered on the boundary Γ and $B_2(t_0)$ is an interior ball converging to the boundary, we require that their radii $R_1(t)$, $R_2(t)$ satisfy:

$$\frac{R_1(t)}{r_1(t_0)} = \frac{t}{t_0} = \left(\frac{R_2(t)}{r_2(t_0)} \right)^s. \quad (7.4)$$

By (ii) of Lemma 4.4 we can increase t , expanding each ball for some positive time $t > t_0 = 1$, in which the balls will remain disjoint. During this expansion phase the seed sizes $r_i(t) = r_i(t_0)$ remain constant. Call $t_1 > t_0 = 1$ the first time at which two or more expanding balls touch. Applying Proposition 6.1 to each ball at time $1 = t_0 \leq t \leq t_1$, we obtain a lower bound in each annulus, of outer radius $R_i(t)$ and inner radius $r_i(t_0)$ around each center:

$$\begin{aligned} E_\varepsilon \left(u_\varepsilon ; \bigcup_{i=1}^{N_0} B^i(t) \right) &\geq E_\varepsilon \left(u_\varepsilon ; \bigcup_{i=1}^{N_0} (B^i(t) \setminus B^i(t_0)) \right) \\ &\geq \sum_{i \in \mathcal{I}_b} 2\pi \left(n_i - \tau_i \frac{\alpha}{\pi} \right)^2 \ln \frac{R_i(t)}{r_i(t_0)} + \sum_{i \in \mathcal{I}'} \pi d_i^2 \ln \frac{R_i(t)}{r_i(t_0)} + c_1 \\ &= \left\{ \sum_{i \in \mathcal{I}_b} 2\pi \left(n_i - \tau_i \frac{\alpha}{\pi} \right)^2 + \sum_{i \in \mathcal{I}'} \frac{\pi}{s} d_i^2 \right\} \ln \frac{t}{t_0} + c_1 \end{aligned} \quad (7.5)$$

Using Lemma 6.3, (see also (6.10)) we then obtain a lower bound on the energy in the expanded balls near $\partial\Omega$,

$$\begin{aligned} E_\varepsilon \left(u_\varepsilon ; \bigcup_{i=1}^{N_0} B^i(t) \right) &\geq \left[2\pi C_\alpha |D^0| + \frac{\pi}{s} |D'| \right] \ln \frac{t}{t_0} + c_1 \\ &\geq \pi \mu |D^b| \ln \frac{t}{t_0} + c_1, \end{aligned} \quad (7.6)$$

for $1 = t_0 < t \leq t_1$, where we recall $D^b = D^0 + D'$ and denote

$$\mu = \min \left\{ 2C_\alpha, \frac{1}{s} \right\}. \quad (7.7)$$

Step 2: Merging. At time t_1 , some of the expanding balls will come into contact with each other, in the sense that their closures will intersect. The merging process is based on the observation:

$$\text{if } \frac{R_1}{r_1} = t = \frac{R_2}{r_2} \text{ then } \frac{R_1 + R_2}{r_1 + r_2} = t. \quad (7.8)$$

Thus, we can combine balls whose closures touch into new balls by summing the radii, and the lower bound will be preserved if we adjust the “seed size”, which remembers the radii of the initial balls, accordingly. That is, the new denominator $\tilde{r} = r_1 + r_2$ will no longer be the initial radius but will be a quantity of the same order of magnitude.

If the closures of two or more interior balls $B^1(t_1), \dots, B^k(t_1)$ touch, (but remain disjoint from boundary balls), they are enclosed within a new interior ball, $\tilde{B}^j(t_1)$, of radius $\tilde{R}_j(t_1) := R_1(t_1) + \dots + R_k(t_1)$. The degree of this new ball will be $\tilde{d}_j = \sum_{i=1}^k d_i$, and we will choose a new “seed size” $\tilde{r}_j(t_1) := r_1(t_0) + \dots + r_k(t_0) = O(\varepsilon)$. In this way, we are maintaining the ratio,

$$\left[\frac{\tilde{R}_j(t_1)}{\tilde{r}_j(t_1)} \right]^s = \left[\frac{R_i(t_1)}{r_i(t_0)} \right]^s = \frac{t_1}{t_0}, \quad i = 1, \dots, k.$$

The energy contained in the new ball at $t = t_1$ may be bounded below,

$$\begin{aligned}
E_\varepsilon(u_\varepsilon; \tilde{B}^j(t_1)) &\geq \sum_{i=1}^k E_\varepsilon(u_\varepsilon; B^i(t_1)) \\
&\geq \sum_{i=1}^k \pi d_i^2 \ln \left[\frac{t_1}{t_0} \right]^{\frac{1}{s}} + O(1) \\
&\geq \frac{\pi}{s} |\tilde{d}_j| \ln \frac{t_1}{t_0} + O(1).
\end{aligned} \tag{7.9}$$

The case of two or more boundary balls $B^1(t_1), \dots, B^k(t_1)$ merging is only slightly more complicated. As above, the new merged ball $\tilde{B}^j(t_1)$ will have radius $\tilde{R}_j(t_1) = \sum_{i=1}^k R_i(t_1)$, and new “seed size” $\tilde{r}_j(t_1) := r_1(t_0) + \dots + r_k(t_0) = O(\varepsilon^s)$. We recall that light and heavy boojums must alternate along Γ , and thus if we enclose two or more boundary balls in a larger $\tilde{B}^j(t_1)$, the boojum number of the merged ball $\tilde{\tau}_j = \sum_{i=1}^k \tau_i \in \{-1, 0, 1\}$. Likewise, the degree also sums, $\tilde{n}_j = \sum_{i=1}^k n_i \in \mathbb{Z}$. Thus, the new boundary ball’s energy may be bounded below by:

$$\begin{aligned}
E_\varepsilon(u_\varepsilon; \tilde{B}^j(t_1)) &\geq \sum_{i=1}^k E_\varepsilon(u_\varepsilon; B^i(t_1)) \\
&\geq \sum_{i=1}^k 2\pi \left(n_i - \tau_i \frac{\alpha}{\pi} \right)^2 \ln \left[\frac{t_1}{t_0} \right] + O(1).
\end{aligned} \tag{7.10}$$

The most delicate case is when interior defect balls collide with boundary balls. (If interior balls contact $\partial\Omega$ itself, we can think of this as the merger of interior balls with an empty boundary ball, of radius, degree, and boojum number all zero.) Assume k boundary balls and ℓ interior balls (with radii $R_i(t_1)$ and seed size $r_i(t_0)$) meet at $t = t_1$. We create a new boundary ball $\tilde{B}^j(t_1)$ with radius and new seed size,

$$\tilde{R}_j(t_1) = \sum_{i=1}^k R_i(t_1) + \sum_{i=k+1}^{k+\ell} [R_i(t_1)]^s, \quad \tilde{r}_j(t_1) = \sum_{i=1}^k r_i(t_0) + \sum_{i=k+1}^{k+\ell} [r_i(t_0)]^s = O(\varepsilon^s).$$

As $0 < s < 1$, $\tilde{R}_j(t_1)$ is larger than the sum of the radii of the old balls, and so $\tilde{B}^j(t_1)$ encloses each of the merging balls inside. Employing the key observation (7.8), we obtain the same lower bound on the energy in the new boundary ball (7.10) as in the previous case.

Putting each case together, we have created a new family of defect balls $\{\tilde{B}^j(t_1)\}_{j=1, \dots, N_1}$, whose union contains the expanded balls $\bigcup_{i=1}^{N_0} B^i(t_1)$. By the merging process, the closure of these balls is disjoint. We divide the balls into two classes via the index sets $\tilde{\mathcal{I}}_b$ and $\tilde{\mathcal{I}}'$ (separating the family into balls centered on the boundary versus those in the interior but approaching the boundary), and denote by

$$\tilde{D}^0 = \sum_{j \in \tilde{\mathcal{I}}_b} \tilde{n}_j \quad \text{and} \quad \tilde{D}' = \sum_{j \in \tilde{\mathcal{I}}'} \tilde{d}_j,$$

the total degrees. Then, applying Proposition 6.3 we have a lower bound:

$$\begin{aligned}
E_\varepsilon \left(u_\varepsilon; \bigcup_{j=1}^{N_1} \tilde{B}^j(t_1) \right) &\geq \left[\sum_{j \in \tilde{\mathcal{I}}_b} 2\pi \left(n_i - \tau_i \frac{\alpha}{\pi} \right)^2 + \sum_{j \in \tilde{\mathcal{I}}'} \frac{\pi}{s} |\tilde{d}_j| \right] \ln \frac{t_1}{t_0} + O(1) \\
&\geq \left[2\pi C_\alpha |\tilde{D}^0| + \frac{\pi}{s} |\tilde{D}'| \right] \ln \frac{t_1}{t_0} + O(1) \\
&\geq \pi \mu |D^b| \ln \frac{t_1}{t_0} + O(1),
\end{aligned} \tag{7.11}$$

in terms of the new merged defect balls. (We note that, while \tilde{D}^0, \tilde{D}' may be different from D^0, D' because of merging, $D^b = D^0 + D' = \tilde{D}^0 + \tilde{D}'$.)

Step 3: Repeat as necessary. Restart the expansion process in Step 1, but starting now with the merged balls $\{\tilde{B}^j(t_1)\}_{j=1, \dots, N_1}$, whose closures are disjoint. Dropping the tildas, we expand the balls according to (7.4) but for

$t \geq t_1$, with the new seed sizes $r_j(t_1)$. Again, expansion may continue until two or more expanded balls touch, at some $t_2 > t_1$. Applying Proposition 6.1 in each annular region $B^j(t_2) \setminus \overline{B^j(t_1)}$, we obtain a lower bound analogous to (7.5)

$$\begin{aligned} E_\varepsilon \left(u_\varepsilon; \bigcup_{i=1}^{N_1} [B^j(t) \setminus B^j(t_1)] \right) &\geq \sum_{i \in \mathcal{I}_b} 2\pi \left(n_j - \tau_j \frac{\alpha}{\pi} \right)^2 \ln \frac{R_j(t)}{r_j(t_1)} + \sum_{j \in \mathcal{I}'} \pi d_j^2 \ln \frac{R_j(t)}{r_j(t_1)} + c_1 \\ &= \left\{ \sum_{j \in \mathcal{I}_b} 2\pi \left(n_j - \tau_j \frac{\alpha}{\pi} \right)^2 + \sum_{i \in \mathcal{I}'} \frac{\pi}{s} d_j^2 \right\} \ln \frac{t}{t_1} + O(1) \\ &\geq \left[2\pi C_\alpha |D^0| + \frac{\pi}{s} |D'| \right] \ln \frac{t}{t_1} + O(1) \\ &\geq \pi \mu |D^b| \ln \frac{t}{t_1} + O(1), \end{aligned}$$

with μ defined in (7.7). Combining this with (7.11) we have improved our lower bound to:

$$\begin{aligned} E_\varepsilon \left(u_\varepsilon; \bigcup_{i=1}^{N_1} B^j(t) \right) &\geq E_\varepsilon \left(u_\varepsilon; \bigcup_{i=1}^{N_1} [B^j(t) \setminus B^j(t_1)] \right) + E_\varepsilon \left(u_\varepsilon; \bigcup_{i=1}^{N_1} B^j(t_1) \right) \\ &\geq \pi \mu |D^b| \ln \frac{t}{t_0} + O(1), \end{aligned}$$

for all $t \in (t_1, t_2)$.

This process must terminate after a bounded finite number of steps, as by Lemma 4.4 the number of bad balls is uniformly bounded in ε . After all the mergers are finished, there are only N^b boundary balls remaining, each centered on Γ , converging to the points $\zeta_k \in \Gamma$, and the expansion step may continue without interruption until the sum of the radii $\sum_{j=1}^{N^b} R_j(t_*) = \sigma^s/2$. Since the seed size $r_j(t) = O(\varepsilon^s)$ for boundary centered balls, we obtain (for all sufficiently small ε in the subsequence),

$$\begin{aligned} E_\varepsilon \left(u_\varepsilon; \bigcup_{j=1}^{N^b} B_{\sigma^s}(\zeta_j) \right) &\geq E_\varepsilon \left(u_\varepsilon; \bigcup_{i=1}^{N^b} B^j(t_*) \right) \\ &\geq \pi \mu |D^b| \ln \frac{t_*}{t_0} + O(1) \\ &\geq \pi \mu |D^b| \ln \frac{\sigma^s}{\varepsilon^s} + O(1) \\ &= s\pi \mu |D^b| \ln \frac{\sigma}{\varepsilon} + O(1) \end{aligned}$$

For a lower bound on the energy contained in all of the balls, we include the lower bound (7.3) on the energy of defect balls contained in the interior of Ω . Thus, we have

$$E_\varepsilon(u_\varepsilon; \mathcal{B}_\sigma) \geq \pi \left[\mu s |D^b| + |D^{int}| \right] \ln \left(\frac{\sigma}{\varepsilon} \right) + C,$$

where \mathcal{B}_σ is defined in (7.2). In case $\mu = 1/s \leq 2C_\alpha$, since $\mathcal{D} = |D^b| + |D^{int}| \leq |D^b| + |D^{int}|$, we obtain the desired lower bound and the proof of the lemma is complete. In case $\mu = 2C_\alpha < 1/s$, we have $1 > 2sC_\alpha$ and a similar argument leads to the desired lower bound,

$$\begin{aligned} E_\varepsilon(u_\varepsilon; \mathcal{B}_\sigma) &\geq \pi \left[2sC_\alpha |D^b| + |D^{int}| \right] \ln \left(\frac{\sigma}{\varepsilon} \right) + C \\ &\geq 2\pi sC_\alpha |\mathcal{D}| \ln \frac{\sigma}{\varepsilon} + c_2. \quad \square \end{aligned}$$

Remark 7.3. We note that when defining the collection of bad balls \mathcal{B}_σ we may delete any balls (interior or boundary) for which the degree $\deg(u_\varepsilon; \partial B_\varepsilon(\xi)) = 0$ (or $\deg(u_\varepsilon; \partial B_{\varepsilon^s}(\xi)) = 0$ for boundary balls.) Doing so does not change the lower bound on the energy contained in the bad set \mathcal{B}_σ , and thus any bad balls with net degree zero form part of the “regular” set where u_ε converges.

Proof of Theorem 1.1. From Corollary 7.2 we can choose a subsequence u_ε of minimizers which is bounded in $H^1(\Omega \setminus \mathcal{B}_\sigma; \mathbb{C})$, for any small $\sigma > 0$, and for which the corresponding bad balls (from Lemma 4.4) converge to the defect sites $\xi_i \in \Omega$ or $\zeta_j \in \Gamma$. By the upper bound in Corollary 7.2 (extracting another subsequence, if necessary), $u_\varepsilon \rightharpoonup u_*$ in H_{loc}^1 away from the defects $\xi_i \in \Omega$, $\zeta_j \in \Gamma$, with $|u_*| = 1$. As in [18] the limiting u_* is an \mathbb{S}^1 -valued harmonic map with defects on the finite point set $\Sigma := \{\xi_i, \zeta_j \mid i = 1, \dots, N^v, j = 1, \dots, N^b\}$. Following [4,16] the convergence may be improved to $H_{loc}^1(\Omega \setminus \Sigma)$ and $C_{loc}^{1,\beta}(\bar{\Omega} \setminus \Sigma)$. In particular, passing to the limit in (3.1) on $\Gamma \setminus \{\zeta_j\}_{j=1, \dots, N^b}$, we may conclude that $W(u_*, g) = 0$ away from the boundary defects. That is, $u_* = ge^{\pm i\alpha}$ on the boundary arcs determined by the defects on Γ . We may also conclude that the degrees d_i (corresponding to interior limiting defects ξ_i) and n_j (corresponding to boundary limiting vortices ζ_j , with boojum number τ_j) are preserved in the limit.

We now fix

$$R \leq \frac{1}{4} \min \left\{ |\xi_i - \xi_j|, |\zeta_i - \zeta_j|, \text{dist}(\xi_i, \Gamma) \mid i \neq j, i = 1, \dots, N^v, j = 1, \dots, N^b \right\},$$

so that the balls of radius R around each defect are pairwise disjoint. For any $\sigma > 0$ with $\sigma^s < R$, we apply Proposition 6.1 to u_ε in each annular region $A_{\sigma,R}(\xi_i)$, $A_{\sigma^s,R}(\zeta_j)$, to obtain a lower bound,

$$\begin{aligned} E_\varepsilon(u_\varepsilon; \Omega_\sigma) &\geq E_\varepsilon \left(u_\varepsilon; \Omega \setminus \left[\bigcup_i A_{\sigma,R}(\xi_i) \cup \bigcup_j A_{\sigma^s,R}(\zeta_j) \right] \right) \\ &\geq \left[\pi \sum_i d_i^2 + 2\pi s \sum_j \left(n_j - \tau_j \frac{\alpha}{\pi} \right)^2 \right] \ln \frac{R}{\sigma} + O(1). \end{aligned}$$

From the upper bound in Corollary 7.2 and Lemma 6.3 we then have:

$$\begin{aligned} \pi \mu s \mathcal{D} |\ln \sigma| &\geq E_\varepsilon(u_\varepsilon; \Omega_\sigma) \\ &\geq \left[\pi \sum_i d_i^2 + 2\pi s \sum_j \left(n_j - \tau_j \frac{\alpha}{\pi} \right)^2 \right] \ln \frac{R}{\sigma} + O(1) \\ &\geq \left[\pi \sum_i |d_i| + 2\pi C_\alpha s |D^b| \right] \ln \frac{R}{\sigma} + O(1) \\ &\geq \left[\pi |D^{int}| + 2\pi C_\alpha s |D^b| \right] \ln \frac{R}{\sigma} + O(1), \end{aligned}$$

with equality if and only if $d_i = \text{sgn } D^{int}$, and $n_j = 0$ for $\tau_j = 0, 1$ while $n_j = 1$ for $\tau_j = -1$. As this inequality is true for all $\sigma > 0$, we must have

$$s\mu |\mathcal{D}| \geq \sum_i |d_i| + 2C_\alpha s |D^b| \geq s\mu \left(|D^{int}| + |D^b| \right) \geq s\mu |\mathcal{D}|, \quad (7.12)$$

and thus each term is equal.

If we assume $\mu = 2C_\alpha < 1/s$ we must then conclude that $d_i = 0 \ \forall i$, and $\mathcal{D} = D^b$, so all of the topologically nontrivial defects occur on the boundary, with degrees $n_j = 0$ for $\tau_j = 0, 1$ while $n_j = 1$ for $\tau_j = -1$. Consequently, there are exactly $2\mathcal{D}$ defects, alternating between light and heavy boojums. On the other hand, if $\mu = 1/s < 2C_\alpha$ then the equality of each term in (7.12) forces $D^b = 0$, and hence $\mathcal{D} = D^{int}$ and $d_i = 1$ for all i . In this case there are exactly \mathcal{D} interior defects. When $2C_\alpha s = 1$ each defect (boundary or interior) has the same energy cost at highest order, and the question of characterizing the defects is more subtle. \square

8. Renormalized energies

After proving Theorem 1.1, which details the nature of defects under weak anchoring to oblique angle condition at the boundary, it is natural to ask whether we may determine the location of boojums in the $\varepsilon \rightarrow 0$ limit. This

involves verifying (as in [4]) that the defect locations minimize a Renormalized Energy, determined by a more precise asymptotic expansion of the energy which identifies the order-one term. Rather than carry out the necessary estimates as in [4], we argue formally in this section in order to give the form of the Renormalized Energy and come to some heuristic conclusion in special geometries relevant to physical cases.

As the case $2sC_\alpha > 1$ is essentially the same as the Dirichlet case studied in [4], we restrict our attention to the more novel situation $2sC_\alpha < 1$ in which minimizers exhibit boojum pairs, which (as in the statement of Theorem 1.1), we denote by y_j, \tilde{y}_j , $j = 1, \dots, \mathcal{D}$, with y_j a light, and \tilde{y}_j a heavy, boojum. We recall that (along a subsequence) $u_\varepsilon \rightarrow u_* = \exp(i\varphi_*)$, in $C_{loc}^{1,\beta}(\bar{\Omega} \setminus \{y_1, \tilde{y}_1, \dots, y_{\mathcal{D}}, \tilde{y}_{\mathcal{D}}\})$. The limit u_* is an \mathbb{S}^1 -valued harmonic map in Ω with defects on the given boundary points. In addition, $W(u_*, g) = 0$ on $\Gamma \setminus \{y_1, \tilde{y}_1, \dots, y_{\mathcal{D}}, \tilde{y}_{\mathcal{D}}\}$, and thus on Γ , $u_* = g \exp(\pm i\alpha)$, with jumps of -2α or $-(2\pi - 2\alpha)$ at the light and heavy boojums, y_j, \tilde{y}_j respectively. These must alternate along Γ , and the heavy boojum carries a degree $n_j = 1$ for each $j = 1, \dots, \mathcal{D}$. As described in [4,16], the energy of minimizers is then expanded as:

$$E_\varepsilon(u_\varepsilon) = \mathcal{D}(\pi s C_\alpha |\ln \varepsilon| + Q_b) + W(y_1, \tilde{y}_1, \dots, y_{\mathcal{D}}, \tilde{y}_{\mathcal{D}}) + o(1), \quad (8.1)$$

where Q_b is a constant, representing the energy of boojum cores at the length scale ε^s . This defines the Renormalized Energy, $W : \Gamma^{2\mathcal{D}} \rightarrow \mathbb{R}$, where $\Gamma^{2\mathcal{D}}$ is the set of all $2\mathcal{D}$ points on Γ . To connect W to the limit $u_* = \exp(i\varphi_*)$ of the minimizers u_ε , we define the conjugate harmonic function to the phase φ_* : $\Phi(x) = \Phi(x; \{y_j, \tilde{y}_j\})$ with $\nabla \Phi = -\nabla^\perp \varphi_*$. The conjugate solves

$$\left. \begin{aligned} \Delta \Phi &= 0, \quad \text{in } \Omega, \\ \frac{\partial \Phi}{\partial \nu} &= g \wedge g_\tau - \sum_{j=1}^{\mathcal{D}} \left[2\alpha \delta_{y_j}(x) + 2(\pi - \alpha) \delta_{\tilde{y}_j}(x) \right], \quad \text{on } \Gamma, \end{aligned} \right\} \quad (8.2)$$

the boundary condition reflecting the jump in the harmonic phase φ_* at light and heavy boojums. Then, it may be shown [4] that the Renormalized Energy is given by

$$W(y_1, \tilde{y}_1, \dots, y_{\mathcal{D}}, \tilde{y}_{\mathcal{D}}) := \lim_{\rho \rightarrow 0} \left(\frac{1}{2} \int_{\Omega \setminus \mathcal{B}_\rho} |\nabla \Phi(x; \{y_j, \tilde{y}_j\})|^2 dx - \pi s C_\alpha \mathcal{D} \ln \frac{1}{\rho} \right), \quad (8.3)$$

where $\mathcal{B}_\rho = \bigcup_{j=1}^{\mathcal{D}} [B_\rho(y_j) \cup B_\rho(\tilde{y}_j)]$.

In the special case where $\Omega = B_1$, the unit disk, with equivariant $g = g(\theta) = e^{i\mathcal{D}\theta}$ of degree $\mathcal{D} > 0$, the Renormalized Energy may be expressed simply. In that case, $g \wedge g_\tau = \mathcal{D}$ is constant, so Φ is a linear combination of Green's functions $G(x, p)$ with pole $p \in \Gamma$:

$$-\Delta_x G(x, p) = 0, \quad \text{in } \Omega, \quad \frac{\partial G}{\partial \nu_x}(x, p) = 1 - 2\pi \delta_p(x), \quad \text{for } x \in \Gamma = \partial B_1,$$

whose solution is $G(x, p) = 2 \ln |x - p|$. Then, we have:

$$\Phi(x; \{y_j, \tilde{y}_j\}) = \sum_{j=1}^{\mathcal{D}} \left[\frac{\alpha}{\pi} G(x, y_j) + \left(1 - \frac{\alpha}{\pi}\right) G(x, \tilde{y}_j) \right].$$

Substituting into (8.3) and integrating by parts (see [4, I.4] for interior vortices and [1, Section 6] for boundary defects), we obtain an explicit formula for the Renormalized Energy,

$$\begin{aligned} W(y_1, \tilde{y}_1, \dots, y_{\mathcal{D}}, \tilde{y}_{\mathcal{D}}) &= \sum_{\substack{i,j=1 \\ i \neq j}}^{\mathcal{D}} \left[\frac{\alpha}{\pi} G(y_i, y_j) + \left(1 - \frac{\alpha}{\pi}\right) G(\tilde{y}_i, \tilde{y}_j) \right] - \sum_{i,j=1}^{\mathcal{D}} G(y_i, \tilde{y}_j) \\ &= -2 \sum_{\substack{i,j=1 \\ i \neq j}}^{\mathcal{D}} \left[\frac{\alpha}{\pi} \ln |y_i - y_j| + \left(1 - \frac{\alpha}{\pi}\right) \ln |\tilde{y}_i - \tilde{y}_j| \right] - 2 \sum_{i,j=1}^{\mathcal{D}} \ln |y_i - \tilde{y}_j|. \end{aligned}$$

In the case $\mathcal{D} = 1$ there is only one boojum pair and $W(y_1, \tilde{y}_1) = -4 \ln |y_1 - \tilde{y}_1|$, so it is clear that the light and heavy boojums must be antipodally placed on the circle Γ . For the Landau-de Gennes case $\mathcal{D} = 2$, different weights appear in the sum,

$$W(y_1, \tilde{y}_1, y_2, \tilde{y}_2) = -4 \left[\frac{\alpha}{\pi} \ln |y_1 - y_2| + \left(1 - \frac{\alpha}{\pi}\right) \ln |\tilde{y}_1 - \tilde{y}_2| \right] \\ - 2 \ln [|y_1 - \tilde{y}_1| |y_1 - \tilde{y}_2| |y_2 - \tilde{y}_1| |y_2 - \tilde{y}_2|].$$

9. Numerical examples

In this section we present several examples of configurations with vortices that can be observed in numerically computed critical points of the energy (1.1). These are obtained by simulating gradient flow for $E_\varepsilon^{g,\alpha}$ using the finite elements software package COMSOL [22].

Note that we do not claim that solutions that we obtain are minimizers of $E_\varepsilon^{g,\alpha}$ or prove that these solutions converge to critical points of the limiting energy. Rather, we use numerical simulations as a useful tool that demonstrates that the behavior of computed solutions is similar to what is predicted by rigorous analysis discussed in the previous sections.

In each of the examples below, we consider a circular domain Ω of radius 1 centered at the origin and set $\varepsilon = 0.02$. We assume $\alpha = \frac{\pi}{3}$ so that $C_\alpha = \frac{5}{9}$ and consider two cases: $s = 1$ and $s = 0.72$ corresponding to a situation described in part (a) and (b) of Theorem 1.1, respectively.

9.1. Boundary data of degree one

Here we suppose that $g(x) = \frac{x}{|x|}$ on $\partial\Omega$ so that $\deg g = 1$.

First, let $s = 1$. According to Theorem 1.1, the minimizers of $E_\varepsilon^{g,\alpha}$ must converge to an \mathbb{S}^1 -valued harmonic map with a single vortex in the interior of the domain Ω . The numerically computed critical point of $E_\varepsilon^{g,\alpha}$ exhibits this feature as is shown in Fig. 2. Note that the absence of boundary singularities corresponds to u being continuous on the boundary then u must essentially coincide everywhere on $\partial\Omega$ with $e^{i\pi/3}g$ (or $e^{-i\pi/3}g$) in order to minimize the surface energy.

Recall that in Section 2 we established the relationship between u and the nematic director n . We can now use (2.18) to find the distribution of the director in Ω . This distribution is depicted in Fig. 3 and is characterized by the presence of a single disclination of degree $1/2$ at the origin.

Now, let $s = 0.72$. Since $0.72 < 0.9 = \frac{1}{2C_\alpha}$, from Theorem 1.1 we expect that a numerically computed critical point of $E_\varepsilon^{g,\alpha}$ should have one light and one heavy boojum on $\partial\Omega$. This is indeed the case for a critical point in Fig. 4. The light boojum corresponds to the shallower depression of $|u|$ on the boundary in the top left inset in Fig. 4 and it is placed antipodally from the heavy boojum. Further, as the vector field is forced to switch its orientation with respect to g on $\partial\Omega$ at boundary singularities, the bottom inset in Fig. 4 demonstrates that u “jumps” between $e^{-i\pi/3}g$ and $e^{i\pi/3}g$ as one traverses $\partial\Omega$.

The distribution of the nematic director n when $s = 0.72$ is shown in Fig. 5.

9.2. Boundary data of degree two

Here we let $g(x) = (x_1^2 - x_2^2, 2x_1x_2)/|x|^2$ on $\partial\Omega$ so that $\deg g = 2$.

As expected, for $s = 1$, the numerically computed critical point of $E_\varepsilon^{g,\alpha}$ has two interior, degree one singularities as is shown in Fig. 6. The same is true for the nematic director (Fig. 7) that now has two degree $1/2$ singularities in the interior of Ω .

For $s = 0.72$, a numerically computed critical point of $E_\varepsilon^{g,\alpha}$ has two light and two heavy boojums on $\partial\Omega$ as demonstrated in Fig. 8. The boojums types are interleaved as one traverses the boundary and the boojums are equidistant from each other.

The distribution of the nematic director n when $s = 0.72$ is shown in Fig. 9. The director has four boundary singularities, two light and two heavy boojums.

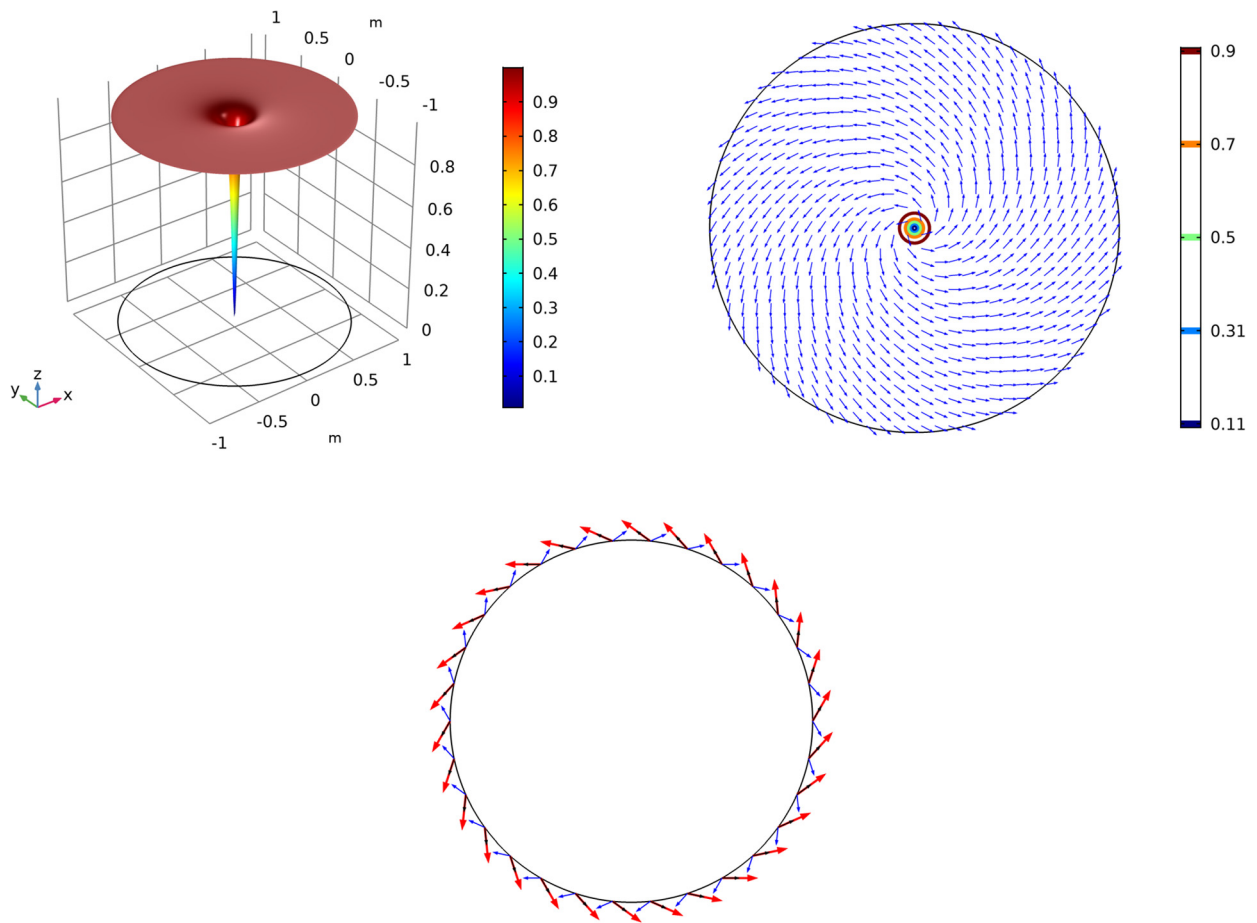


Fig. 2. A critical point of $E_\varepsilon^{g,\alpha}$ for $g(x) = \frac{x}{|x|}$, $\alpha = \frac{\pi}{3}$, and $s = 1$. Top left: The plot of $|u|$; Top right: The vector field u . Contour lines of $|u|$ are depicted to indicate the location of the singularity; Bottom: The restriction of the vector field u to $\partial\Omega$. Here u is shown in red, $e^{-i\pi/3}g$ and $e^{i\pi/3}g$ are shown in blue and black, respectively. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

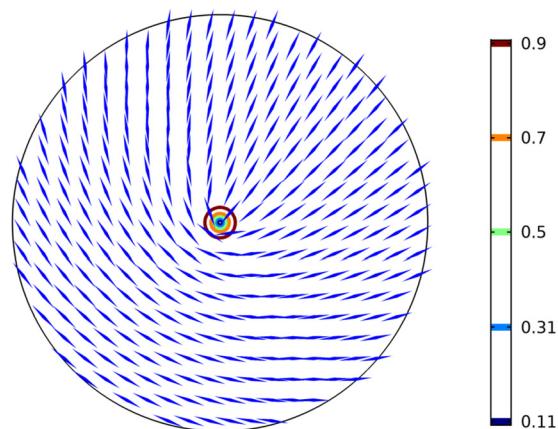


Fig. 3. The director field n for $g(x) = \frac{x}{|x|}$, $\alpha = \frac{\pi}{3}$, and $s = 1$. Contour lines of $|u|$ are shown to indicate the location of the singularity.

The original motivation for this study stems from experimental results of Volovik and Lavrentovich [14], for the case of a (three-dimensional) nematic ball. Although our treatment in this paper is restricted to a two-dimensional,

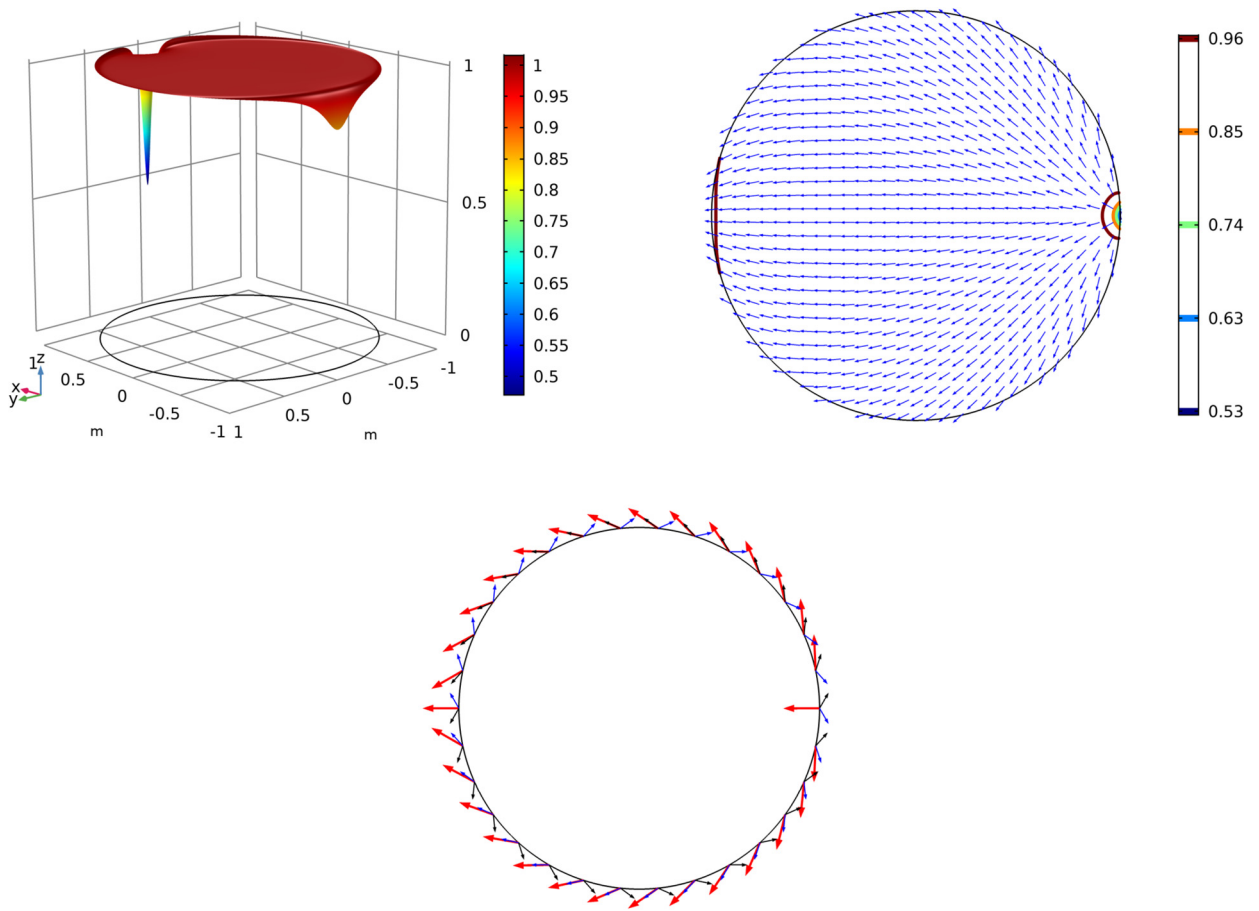


Fig. 4. A critical point of $E_\epsilon^{g,\alpha}$ for $g(x) = \frac{x}{|x|}$, $\alpha = \frac{\pi}{3}$, and $s = 0.72$. Top left: The plot of $|u|$; Top right: The vector field u . Contour lines of $|u|$ are depicted to indicate the locations of the singularities; Bottom: The restriction of the vector field u to $\partial\Omega$. Here u is shown in red, $e^{-i\pi/3}g$ and $e^{i\pi/3}g$ are shown in blue and black, respectively.

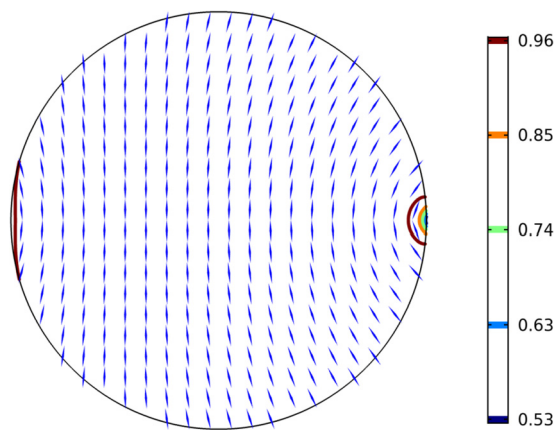


Fig. 5. The director field n for $g(x) = \frac{x}{|x|}$, $\alpha = \frac{\pi}{3}$, and $s = 0.72$. Contour lines of $|u|$ are shown to indicate the locations of the singularities.

thin film geometry, we may still observe the resemblance of the configuration in Fig. 9 with that in Fig. 7b in [14], which shows two polar point defects and an equatorial disclination ring on the surface of a spherical particle. Because the 3D configuration in [14] is invariant with respect to both the axial and mirror symmetries in each cross-section

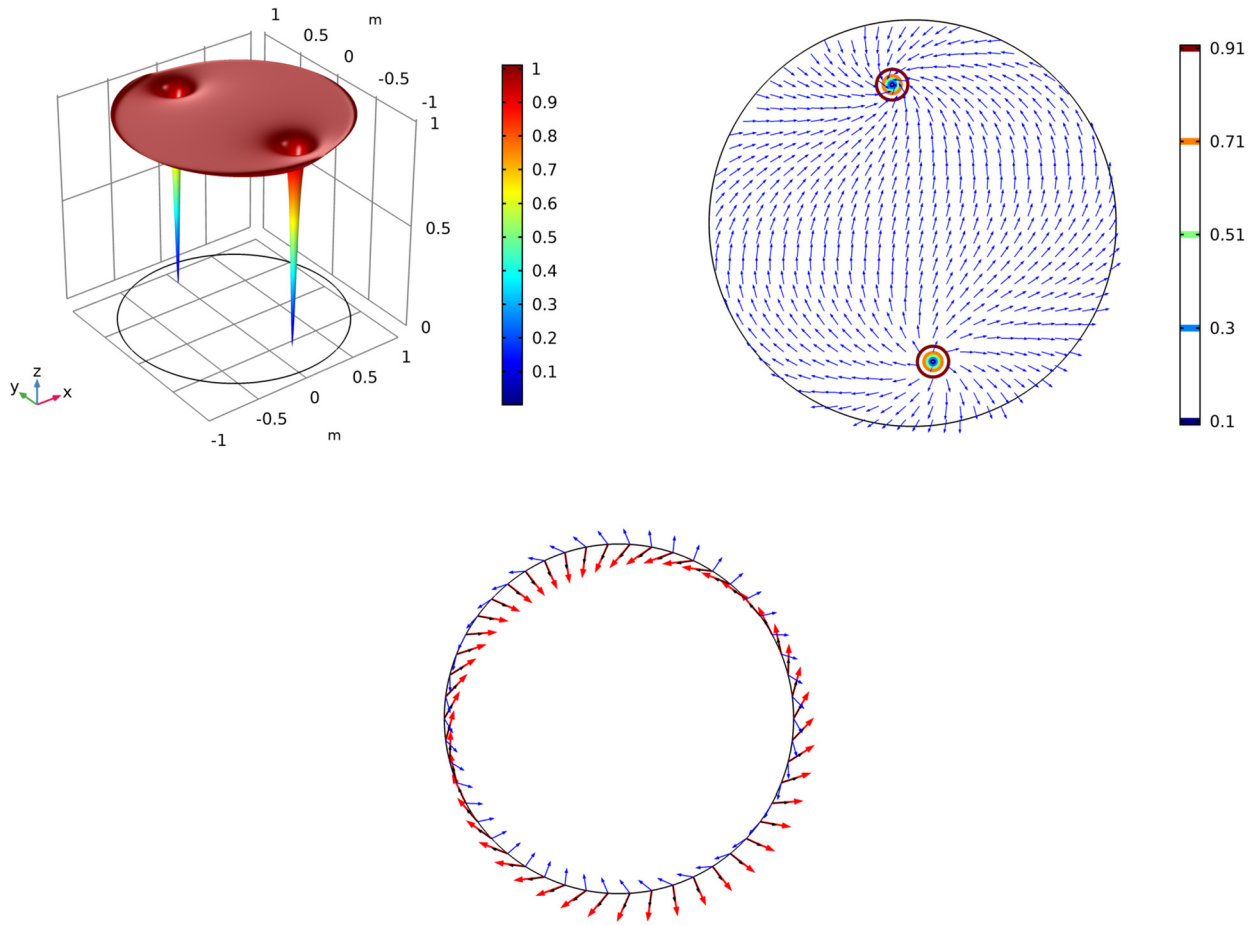


Fig. 6. A critical point of $E_\varepsilon^{g,\alpha}$ for $g(x) = (x_1^2 - x_2^2, 2x_1x_2)/|x|^2$, $\alpha = \frac{\pi}{3}$, and $s = 1$. Top left: The plot of $|u|$; Top right: The vector field u . Contour lines of $|u|$ are depicted to indicate the location of the singularity; Bottom: The restriction of the vector field u to $\partial\Omega$. Here u is shown in red, $e^{-i\pi/3}g$ and $e^{i\pi/3}g$ are shown in blue and black, respectively.

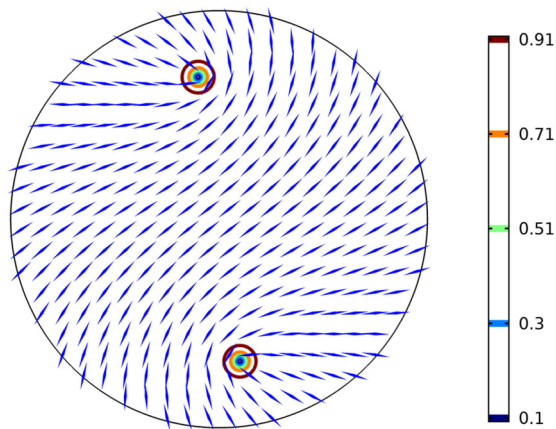


Fig. 7. The director field n for $g(x) = (x_1^2 - x_2^2, 2x_1x_2)/|x|^2$, $\alpha = \frac{\pi}{3}$, and $s = 1$. Contour lines of $|u|$ are shown to indicate the location of the singularity.

of the particle that contains the axis of symmetry, it displays four surface point singularities separated by 90 degrees angles. Topologically this is the same situation as in Fig. 9: there are two heavy boojums that are the traces of the

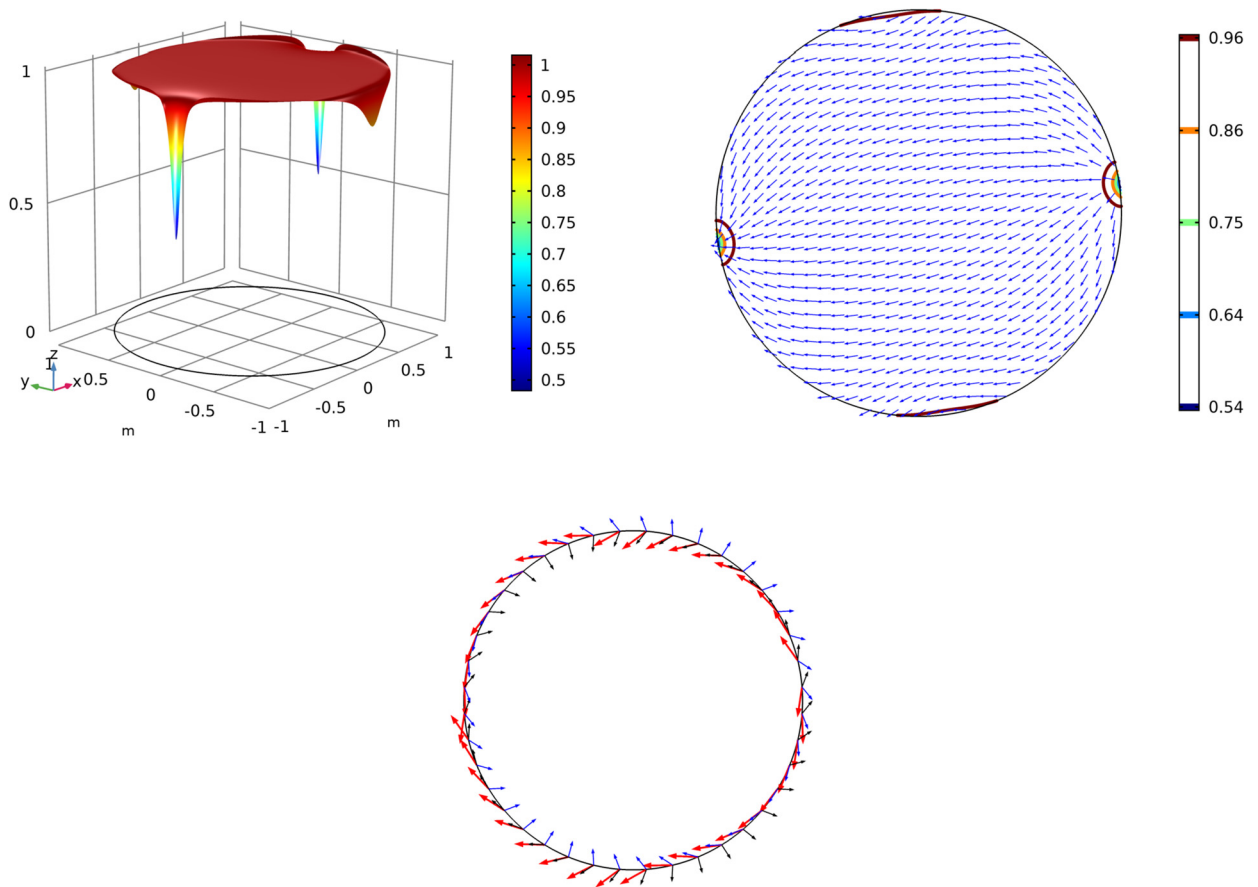


Fig. 8. A critical point of $E_\varepsilon^{g,\alpha}$ for $g(x) = (x_1^2 - x_2^2, 2x_1x_2)/|x|^2$, $\alpha = \frac{\pi}{3}$, and $s = 0.72$. Top left: The plot of $|u|$; Top right: The vector field u . Contour lines of $|u|$ are depicted to indicate the locations of the singularities; Bottom: The restriction of the vector field u to $\partial\Omega$. Here u is shown in red, $e^{-i\pi/3}g$ and $e^{i\pi/3}g$ are shown in blue and black, respectively.

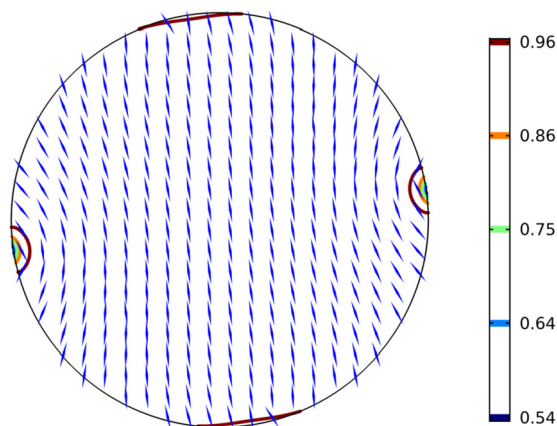


Fig. 9. The director field n for $g(x) = (x_1^2 - x_2^2, 2x_1x_2)/|x|^2$, $\alpha = \frac{\pi}{3}$, and $s = 0.72$. Contour lines of $|u|$ are shown to indicate the locations of the singularities.

singularities at the poles, and two light boojums corresponding to the intersection between the circular cross-section and the equatorial disclination ring. Here both the equatorial ring and the light boojums serve the same purpose of unwinding the extra phase gained at the poles due to the heavy boojums.

Furthermore, the experimental work in [14] also indicates that when the angle of inclination between the director and the normal on the surface of the particle is close to 90 degrees, it might be reasonable to seek minimizers of the 3D problem in the class of functions that possess both axial and inversion symmetries. This is the approach that we undertook recently in a separate work [2], and we conjecture that these techniques can be extended to the present problem in 3D.

Declaration of competing interest

There are no personal or financial issues in this work.

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