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VORTICES IN TWO-DIMENSIONAL NEMATICS*

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Abstract. We study a two-dimensional model describing spatial variations of orientational ordering in nematic liquid crystals. In particular, we show that the spatially extended Onsager-Maier-Saupe free energy may be decomposed into Landau-de Gennes-type and relative entropy-type contributions. We then prove that in the high concentration limit the states of the system display characteristic vortex-like patterns and derive an asymptotic expansion for the free energy of the system.

Key words. Liquid crystals, nematics, spatial patterns, vortices.

AMS subject classifications. 82B21, 82B26, 82D30.

1. Introduction

The major phenomenological theories describing spatial variations of orientational order in nematic liquid crystals are due to Oseen and Frank [18, 12], Ericksen [8], and de Gennes [4]. The central object in these theories is a free energy functional whose critical points correspond to equilibrium states of the liquid crystalline system. In the Oseen-Frank theory the free energy is a functional of a director field of locally-preferred orientations of liquid crystalline molecules, whereas in the de Gennes (Landau-de Gennes) theory it is a functional of a tensor order parameter field. The Ericksen model is based on a director field whose magnitude may vary reflecting the strength of nematic ordering. A microscopic derivation of free energy for nematic liquid crystals was first suggested by Onsager [17]. In Onsager's framework the free energy is a functional of probability density of orientations (of liquid crystalline molecules) derived via some cluster or virial expansion. The Onsager theory, however, is insensitive to spatial variations of orientation distribution, i.e., the latter is obtained via sampling over all molecules in the system rather than via local, "mesoscopic," sampling. Even though modern density-functional theories [22, 21] address this issue, some of their essential quantities (e.g., the direct pair-correlation function) cannot be readily computed from microscopic principles, so some phenomenological approximations must still be made to obtain any specific results.

In [11] we suggested a class of models where, as in the density-functional method, the state of the system is described by a spatially-dependent orientation probability density. However, instead of following the microscopic approach to full extent, we proposed using a Landau-de Gennes-type phenomenological elastic contribution to penalize the spatial variations. The principal reason for employing this particular methodology is recent improvement of analytical techniques addressing (spatially-homogeneous) Onsager-type theories. For example, a complete classification of all critical points in various models of this type has been recently established, see e.g., [3, 10, 9, 14, 23]. Combining these ideas with a Dirichlet energy estimate for $\mathbb{S}^1$-maps due to Sandier [20] allows us to achieve a complete rigorous understanding of patterns arising in the suggested model. We first prove that the spatially extended Onsager-Maier-Saupe free energy may be decomposed into a Landau-de Gennes-type and a

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relative entropy-type contributions; in essence this shows that the order-parameter is the correct *macroscopic* variable for this system. Next, we prove that in the high concentration limit the states of the system display characteristic vortex-like patterns. Finally, we sketch a derivation of an asymptotic expansion of the energy reducing the problem of finding equilibrium patterns to variational problem for energy of an ensemble of finitely many particles (vortices).

The paper is organized as follows. In the remaining part of the introduction we review the model presented in [11] specializing to the two-dimensional case and give an informal overview of the principal results obtained in this work. In section 2 we formulate our main results in a systematic rigorous manner and then prove them in section 3. The Appendix contains various auxiliary results and technical details needed for the proofs.

1.1. The two-dimensional spatially-extended Onsager-Maier-Saupe model. In our model the orientation parameter of liquid-crystalline rods is a number in $\mathbb{T}=\mathbb{R}/2\pi$, i.e., it parametrizes a unit circle. The actual orientation (of a symmetric rod-like particle) is really a point on a projective line (a circle with identified diamterically opposed points), however, we follow the traditional approach accepted in physics literature which is also more transparent mathematically (see figure 1.3 and the end of section 1.2 for additional discussion). The spatial domain Ω is two-dimensional and is a subset of the complex plane $\mathbb{C}$: we treat the spatial degree of freedom as a complex scalar rather than a two-dimensional vector. The state of the system is characterized by the space-dependent orientation probability density of liquid-crystalline rods $\varrho(\varphi,\boldsymbol{z})$, $\varphi\in\mathbb{T}$, $\boldsymbol{z}\in\Omega\subset\mathbb{C}$ (at each $\boldsymbol{z}\in\Omega$, $\varrho(\varphi,\boldsymbol{z})$ integrates to unity over φ).

The free energy of the system $\mathcal{E}(\varrho,\Omega)$ is a functional of orientation probability density $\varrho(\varphi,\boldsymbol{z})$ and may be represented as an integral over the spatial domain Ω of two contributions:

$$\mathcal{E}^\gamma(\varrho,\Omega)=\int_\Omega\Big[\mathcal{F}_{\mathrm{o}}^\gamma(\varrho)+\mathcal{F}_{\mathrm{e}}(\varrho)\Big]\,\mathrm{d}\boldsymbol{z}. \tag{1.1}$$

The *orientational free energy density* $\mathcal{F}_{\mathrm{o}}$ is an Onsager-type functional with Maier-Saupe interaction [15] (i.e., a two-dimensional version of it):

$$\mathcal{F}_{\mathrm{o}}^\gamma(\varrho)=\int_0^{2\pi}\varrho(\varphi,\boldsymbol{z})\ln\big[2\pi\varrho(\varphi,\boldsymbol{z})\big]\,\mathrm{d}\varphi \tag{1.2}$$

$$-\frac{\gamma}{2}\iint_0^{2\pi}\cos2(\varphi-\varphi')\,\varrho(\varphi,\boldsymbol{z})\varrho(\varphi',\boldsymbol{z})\,\mathrm{d}\varphi\mathrm{d}\varphi'+C_\gamma, \tag{1.3}$$

where the constant C_γ is chosen to have $\mathcal{F}_{\mathrm{o}}(\varrho)\geq0$ (see Appendix B for details). The factor of 2π in the first term in (1.2) emphasizes that this term is the relative entropy with respect to the uniform density on the circle. Note that neither the constant C_γ nor this factor affect the critical points of the functionals in (1.1) and (1.2) and are introduced for mathematical convenience. The positive parameter γ is referred to as *concentration* and is explicitly indicated as we are particularly interested in the limit when $\gamma\to\infty$. Note that even though we call this limit the limit of high concentration, physically it is more appropriate to call it the long rods limit: it corresponds to systems where the ratio of length of nematic particles to their thickness is large.

The *elastic free energy density* is a quadratic functional of the *order-paramter* field equivalent to that of the Landau-de Gennes theory:

$$\mathcal{F}_{\mathrm{e}}(\varrho)=\frac{\kappa}{2}\,|\nabla\boldsymbol{n}(\boldsymbol{z})|^2. \tag{1.4}$$

Here $\boldsymbol{n}(\boldsymbol{z})$ is the order parameter field related to the orientation probablity density function ϱ via

$$\boldsymbol{n}(\boldsymbol{z}) = \int_0^{2\pi} \mathrm{e}^{2\mathrm{i}\varphi}\, \varrho(\varphi,\boldsymbol{z})\mathrm{d}\varphi. \tag{1.5}$$

The positive parameter κ in equation (1.4) is called the *elastic modulus*. Observe that the *director* field in the sense of Ericksen or Oseen and Frank behaves roughly like $\sqrt{\boldsymbol{n}}$, i.e., the 2π-increment of the phase (rotation) of the order-parameter corresponds to the π-rotation of the director. At the same time $\boldsymbol{n}$ contains exactly the same information as the Landau-de Gennes tensor order parameter.

The boundary effects may be accounted for by augmenting the free energy (1.1) with boundary terms modeling interaction of liquid-crystalline molecules with the container or other surface effects. This can be done, e.g., by means of the following boundary energy:

$$\mathcal{E}_{\mathrm{bnd}}(\varrho,\partial\Omega) = -\oint_{\partial\Omega} \boldsymbol{n}(\boldsymbol{z})\cdot\boldsymbol{U}(\boldsymbol{z})\,\mathrm{d}\ell(\boldsymbol{z}), \tag{1.6}$$

where $\boldsymbol{U}(\boldsymbol{z})$ is a boundary potential which provides the preferred orientation of the director field on the boundary and $\ell(\boldsymbol{z})$ is the measure of the boundary length (one-dimensional Hausdorff measure). Such boundary energy corresponds to imposing Neumann boundary conditions (for the Euler-Lagrange equation) on the order-parameter field: $\kappa\partial_\nu\boldsymbol{n}(\boldsymbol{z}) = \boldsymbol{U}(\boldsymbol{z})$ for $\boldsymbol{z}\in\partial\Omega$ (hereafter ∂_ν denotes normal derivative with the respect to the boundary $\partial\Omega$). In this paper, however, we use a simplified approach and prescribe the boundary values for $\boldsymbol{n}(\boldsymbol{z})$ directly, imposing Dirichlet boundary conditions. Physically, such boundary conditions are quite natural and correspond to situations when it is possible to control orientation of nematic particles on the boundary. Note that imposing boundary conditions on $\varrho(\varphi,\boldsymbol{z})$ will generally lead to an ill-posed problem. The reason is that the Euler-Lagrange equation for the functional $\mathcal{E}^\gamma(\varrho,\Omega)$ reduces to an equation for $\boldsymbol{n}(\boldsymbol{z})$ alone, from which the density of orientations is recovered uniquely. Because of this, unless the boundary conditions only involve $\boldsymbol{n}(\boldsymbol{z})$, there is no guarantee that such a density will match them.

1.2. Informal statement of the results. This paper contains two principal results. The first concerns decomposition of the energy $\mathcal{E}^\gamma(\varrho,\Omega)$ and the structure of its critical points. The second is an asymptotic result regarding the structure of states with appropriately bounded energy in the $\gamma\to\infty$ limit. In what follows we use a few special functions, e.g., the modified Bessel functions $\mathrm{I}_\nu(\cdot)$, the function $\mathrm{A}(\cdot)$, etc. Some of their properties essential for our presentation may be found in Appendix B. We also use bold face font for complex-valued quantities and regular font for their absolute values, e.g., $n=|\boldsymbol{n}|$.

Equilibrium states of the system correspond to the critical points of the total free energy (1.1). As it is informally shown in [10] and presented here as a part of Theorem 2.1, all critical points of the free energy (1.1) are given by

$$\varrho(\varphi,\boldsymbol{z}) = \frac{\exp\big\{\mathrm{A}\big(n(\boldsymbol{z})\big)\cos\big(2\varphi-\arg\boldsymbol{n}(\boldsymbol{z})\big)\big\}}{2\pi\,\mathrm{I}_0\big(\mathrm{A}(n)\big)}. \tag{1.7}$$

Here the field $\boldsymbol{n}(\boldsymbol{z})$ is itself a critical point of the reduced energy

$$E^\gamma(\boldsymbol{n},\Omega) = \int_\Omega \Big[\frac{\kappa}{2}\big|\nabla\boldsymbol{n}(\boldsymbol{z})\big|^2 + W^\gamma\big(n(\boldsymbol{z})\big)\Big]\,\mathrm{d}\boldsymbol{z} \tag{1.8}$$

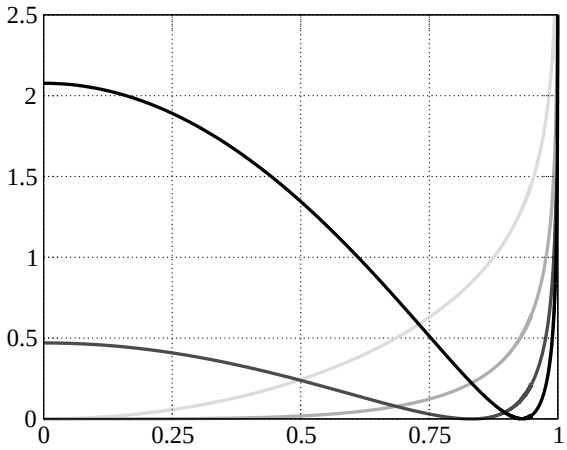

FIG. 1.1. *Graphs of the potential $W^\gamma(n)$ given by equation (1.9). The values of γ, represented from light to dark, are 0.2, 2, 4, 6. The values $\gamma \le 2$ correspond to isotropic state: $W^\gamma(n)$ has a minimum at $n=0$; the values $\gamma > 2$ correspond to nematic state: $W^\gamma(n)$ has a minimum at $n=n^\gamma_{\mathrm{eq}}>0$. Note that as $\gamma\to\infty$, $n^\gamma_{\mathrm{eq}}\to 1$ in a very fast manner (in particular this implies that a distinctly nematic state may be observed at fairly low concentrations).*

with the potential W^γ given by

$$W^\gamma(n) = n\,\mathrm{A}(n) - \frac{\gamma n^2}{2} - \ln \mathrm{I}_0\big(\mathrm{A}(n)\big) + C_\gamma. \tag{1.9}$$

A few graphs of $W^\gamma(n)$ are presented on figure 1.1. One can immediately recognize similarity between the energy $E^\gamma(\boldsymbol{n},\Omega)$ and the (zero magnetic field) Ginzburg-Landau energy for super-conductivity in which the potential is a fourth-order polynomial of the order parameter [13]. Note that the two-dimensional Landau-de Gennes theory of liquid crystals is mathematically equivalent to the Ginzburg-Landau theory. In our model the potential $W^\gamma(n)$ is more complicated, however, it has a similar structure. In some sense, the potential (1.9), unlike the Ginzburg-Landau potential, is derived from the underlying microscopic model rather than postulated from phenomenological principles.

The role of the energy $E^\gamma(\boldsymbol{n},\Omega)$ goes beyond just the critical points: we also prove that the total energy $\mathcal{E}^\gamma(\varrho,\Omega)$ may be decomposed into the sum

$$\mathcal{E}^\gamma(\varrho,\Omega) = E^\gamma(\boldsymbol{n},\Omega) + \int_\Omega \mathcal{S}(\varrho|\hat\varrho)\,\mathrm{d}\boldsymbol{z}, \tag{1.10}$$

where the order parameter field $\boldsymbol{n}$ is related to ϱ via formula (1.5), $\hat\varrho$ is related to $\boldsymbol{n}$ via (1.7), and $\mathcal{S}(\varrho|\hat\varrho)$ is the relative entropy of ϱ with respect to $\hat\varrho$. The field $\hat\varrho$ has a straightforward interpretation: it is the optimal probability density field in the class of all fields with the same order-parameter $\boldsymbol{n}(\boldsymbol{z})$ as ϱ, see figure 1.2 for illustration. This decomposition is also quite natural from the physical point of view, in essence it reflects the fact that the order-parameter field $\boldsymbol{n}(\boldsymbol{z})$ provides a complete *thermodynamic* (or *macroscopic*) description of the system while its *microscopic* state is characterized by the density field of orientations $\varrho(\varphi,\boldsymbol{z})$. Whenever some given orientation density $\varrho(\varphi,\boldsymbol{z})$ may be represented as in (1.7) for some order-parameter

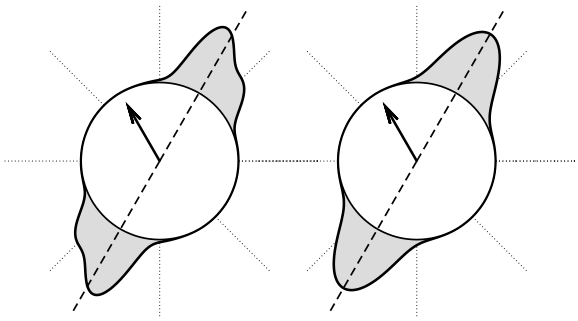

FIG. 1.2. *Schematic representations of the orientation densities $\varrho(\varphi)$ (left) and $\hat{\varrho}(\varphi)$ (right) in polar coordinates; actually plotted are the graphs of $1+\varrho(\varphi)$. The density $\hat{\varrho}$ is produced by the order parameter $\boldsymbol{n}$ corresponding to ϱ (depicted as an arrow) via formula (1.7) and is the "locally-equilibrated" version of ϱ. The dashed line corresponds to the actual director and points along $1/2\arg\boldsymbol{n}$.*

field $\boldsymbol{n}(\boldsymbol{z})$ we say that ϱ is in *local equilibrium*, in this case $\mathcal{S}(\varrho|\hat{\varrho})=0$. From this point of view the field $\hat{\rho}$ is the "locally-equilibrated" version of ϱ; in our theory the particular functional form (1.7) plays a role similar to the role of Maxwell-Boltzmann distribution in gas dynamics.

The high concentration limit is obtained by sending $\gamma\to\infty$. As γ becomes large, the system prefers to be in the nematic state with $|\boldsymbol{n}(\boldsymbol{z})|\approx n_{\mathrm{eq}}^{\gamma}$, where n_{eq}^{γ} is the minimizer of the potential $W^{\gamma}(n)$ (note that $n_{\mathrm{eq}}^{\gamma}\to 1$ as $\gamma\to\infty$). However, if the boundary data for $\boldsymbol{n}(\boldsymbol{z})$ has a nonzero degree (winding number) d, the field $\boldsymbol{n}(\boldsymbol{z})$ has to "melt" in some region, i.e., take values with $|\boldsymbol{n}(\boldsymbol{z})|\approx 0$. This allows its orientation to rotate without incurring a huge energy penalty. In Theorem 2.2 we prove that for the states with appropriately controlled energy, the *tempered* states (see Definition 2.2 in section 2), this melting region is comprised of $|d|$ distinct patches localized near some points $\boldsymbol{z}_j$. The size of each patch is roughly $1/\sqrt{\gamma}$, so as $\gamma\to\infty$ the patches shrink to point singularities: vortices. As this happens the order parameter field converges to

$$\boldsymbol{u}_*(\boldsymbol{z}) = \mathrm{e}^{\mathrm{i}\phi(\boldsymbol{z})}\prod_{j=1}^{|d|}\left[\frac{\boldsymbol{z}-\boldsymbol{z}_j}{|\boldsymbol{z}-\boldsymbol{z}_j|}\right]^{\operatorname{sgn} d} \tag{1.11}$$

with some sufficiently regular function $\phi(\boldsymbol{z})$, while the orientation density field $\varrho(\varphi,\boldsymbol{z})$ converges to $\alpha(\boldsymbol{z})\delta\big(\varphi-\psi(\boldsymbol{z})\big)+\big(1-\alpha(\boldsymbol{z})\big)\delta(\varphi-\psi(\boldsymbol{z})-\pi)$, with $\alpha(\boldsymbol{z})\in[0,1]$, $\psi(\boldsymbol{z})=\frac{1}{2}\arg\boldsymbol{u}_*(\boldsymbol{z})\ (\mathrm{mod}\ 2\pi)$. The factor $\alpha(\boldsymbol{z})$ here is a mathematical artifact which appears because we parametrize the orientations (which really are points on a projective line) by a number in $\mathbb{T}$, i.e., φ and $\varphi+\pi$ correspond to the same point on a projective line, i.e., are indistinguishable physically. When pulled back to the projective line such ϱ becomes a point mass concentrated at a single location. Another consequence of such a parametrization is the effective doubling of the degrees of singularities. For example, single vortices (degree one) of the limiting order-parameter field $\boldsymbol{u}_*(\boldsymbol{z})$ treated as a vector field correspond to *"twisters"* (degree one half) of the nematic director field, which is essentially $\sqrt{\boldsymbol{u}_*(\boldsymbol{z})}$; double vortices of $\boldsymbol{u}_*$ correspond to single vortices of the director field; etc., see figure 1.3 for illustration. With this in mind we should note that formula (1.11) implies that all admissible singularities of the tempered

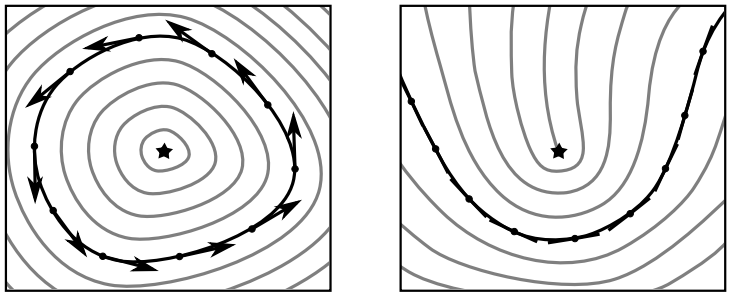

FIG. 1.3. *Matching singularities in vector (left) and director (right) fields* $\boldsymbol{u}_*(\boldsymbol{z})$ *and* $\sqrt{\boldsymbol{u}_*(\boldsymbol{z})}$. *Lines represent integral curves of the fields in the neighborhood of a defect (star). A simple vortex (degree one) in the Ginzburg-Landau-type theory corresponds to a* twister *(degree one half) in nematics.*

nematic states are actually twisters in the physically observable patterns. We may also comment that such vector-director correspondence is quite useful for description of various patterns arising in systems which are not directly related to nematics, see e. g., [16, 6, 7].

Let us emphasize once more that these tempered states are not necessarily critical points: the temperedness condition merely limits the energy in the asymptotic limit, i.e., these results provide description of all states with appropriately controlled energy as $\gamma \to \infty$. Finally, we also sketch a derivation of a lower bound on the energy of the system which shows that after subtracting the relative entropy and the (logarithmically) diverging contribution from the vortices, the remaining free energy is a function which only depends on the vortex locations and boundary conditions. Moreover, this lower bound is achieved exactly on probability density fields which are generated by $\boldsymbol{n}(\boldsymbol{z})$ as in (1.7) with $\boldsymbol{n}(\boldsymbol{z})$ minimizing the energy $E^\gamma(\boldsymbol{n},\Omega)$ in the class of functions with prescribed vortex locations.

2. Main results

Before we formulate our principal results, let us fix some notational conventions. We use bold face font for complex-valued quantities and regular font for their absolute values, e.g., $n = |\boldsymbol{n}|$. Given a curve Γ in $\mathbb{C}$, we denote the winding number (degree) of a complex-valued function $\boldsymbol{w}(\boldsymbol{z})$ with respect to Γ by $\deg(\boldsymbol{w},\Gamma)$. If $\boldsymbol{z}_0$ is a point in $\mathbb{C}$, we denote the winding number of $\boldsymbol{w}$ with respect to a sufficiently small circle around $\boldsymbol{z}_0$ by $\deg(\boldsymbol{w},\boldsymbol{z}_0)$. In what follows we need a few special functions, e.g., the modified Bessel functions $\mathrm{I}_\nu(\cdot)$, the function $\mathrm{A}(\cdot)$, etc. Their definitions and properties may be found in Appendix B.

Throughout this paper we assume that our spatial domain $\Omega \subset \mathbb{C}$ is an open, bounded, and simply connected subset of complex plane with smooth (C^1) boundary $\partial\Omega$.

Our first result concerns decomposition of the energy $\mathcal{E}^\gamma(\varrho,\Omega)$ given by formula (1.1) and the structure of its critical points.

THEOREM 2.1 (Energy decomposition and critical points). *Consider a density field* $\varrho(\varphi,\boldsymbol{z})$. *The following statements hold:*

1. *The energy $\mathcal{E}^\gamma(\varrho,\Omega)$ may be represented as*

$$\mathcal{E}^\gamma(\varrho,\Omega) = E^\gamma(\boldsymbol{n}[\varrho],\Omega) + \int_\Omega \mathcal{S}(\varrho|\hat{\varrho})\,\mathrm{d}\boldsymbol{z}, \tag{2.1}$$

where $\boldsymbol{n}[\varrho]$ is the order-parameter field generated from ϱ:

$$\boldsymbol{n}[\varrho](\boldsymbol{z}) = \int_0^{2\pi} \mathrm{e}^{2\mathrm{i}\varphi}\,\varrho(\varphi,\boldsymbol{z})\,\mathrm{d}\varphi, \tag{2.2}$$

$\hat{\varrho}$ is the mollification of ϱ, i.e., $\hat{\varrho}=\varrho[\boldsymbol{n}[\varrho]]$ where

$$\varrho[\boldsymbol{n}](\varphi,\boldsymbol{z}) = \frac{\exp\{\mathrm{A}\big(n(\boldsymbol{z})\big)\cos\big(2\varphi-\arg\boldsymbol{n}(\boldsymbol{z})\big)\}}{2\pi\mathrm{I}_0\big(\mathrm{A}(n)\big)}, \tag{2.3}$$

and $\mathcal{S}(\varrho|\hat{\varrho})$ is the relative entropy functional,

$$\mathcal{S}(\varrho|\hat{\varrho}) = \int_0^{2\pi} \ln\frac{\varrho(\varphi)}{\hat{\varrho}(\varphi)}\,\varrho(\varphi)\,\mathrm{d}\varphi. \tag{2.4}$$

2. *Critical points of the energy functionals $\mathcal{E}^\gamma(\varrho,\Omega)$ and $E^\gamma(\boldsymbol{n},\Omega)$ are in one-to-one correspondence, i.e., whenever a field $\boldsymbol{n}(\boldsymbol{z})$ is a critical point of $E^\gamma(\boldsymbol{n},\Omega)$, the induced orientation density field $\varrho[\boldsymbol{n}](\varphi,\boldsymbol{z})$ is a critical point of $\mathcal{E}^\gamma(\varrho,\Omega)$, and all critical points of $\mathcal{E}^\gamma(\varrho,\Omega)$ may be obtained this way. Moreover, the corresponding critical points have the same stability properties, i.e., $\boldsymbol{n}(\boldsymbol{z})$ is a minimizer of $E^\gamma(\boldsymbol{n},\Omega)$ if and only if $\varrho[\boldsymbol{n}](\varphi,\boldsymbol{z})$ is a minimizer of $\mathcal{E}^\gamma(\varrho,\Omega)$.*

Remark 2.1. Given any field $\boldsymbol{n}(\boldsymbol{z})$, $\boldsymbol{n}[\varrho[\boldsymbol{n}]]=\boldsymbol{n}$, i.e., by direct computation we can verify that

$$\boldsymbol{n}[\varrho[\boldsymbol{n}]] = \big[2\pi\mathrm{I}_0\big(\mathrm{A}(n)\big)\big]^{-1}\int_0^{2\pi} \mathrm{e}^{2\mathrm{i}\varphi}\exp\big\{\mathrm{A}(n)\cos(2\varphi-\arg\boldsymbol{n})\big\}\,\mathrm{d}\varphi = \boldsymbol{n}. \tag{2.5}$$

The similar statement that given any $\varrho(\varphi,\boldsymbol{z})$, $\varrho[\boldsymbol{n}[\varrho]]=\varrho$ is generally not true since an arbitrary $\varrho(\varphi,\boldsymbol{z})$ does not have the particular form (2.3). However, since $\mathcal{S}(\varrho|\hat{\varrho})=0$ if and only if $\varrho=\hat{\varrho}$, the first assertion of Theorem 2.1 implies that $\varrho[\boldsymbol{n}[\varrho]]=\varrho$ $\boldsymbol{z}$-a.e. if and only if $\mathcal{E}^\gamma(\varrho,\Omega)=E^\gamma(\boldsymbol{n}[\varrho],\Omega)$. In particular, $\varrho[\boldsymbol{n}[\varrho]]=\varrho$ for all critical points of $\mathcal{E}^\gamma(\varrho,\Omega)$.

Our second result describes the structure of families of orientation density fields $\varrho^\gamma(\varphi,\boldsymbol{z})$ and the corresponding order parameter fields $\boldsymbol{n}^\gamma(\boldsymbol{z})$ whose energy is controlled in the limit as $\gamma\to\infty$. We need a few definitions.

Definition 2.1 (Well-prepared boundary data). *Fix a map $\boldsymbol{u}:\partial\Omega\to\mathbb{S}^1=\{\boldsymbol{z}\in\mathbb{C}:|\boldsymbol{z}|=1\}$ with degree (winding number) d on $\partial\Omega$. A family of boundary values $\boldsymbol{n}^\gamma|_{\partial\Omega}$ is* well-prepared *if*

$$\boldsymbol{n}^\gamma(\boldsymbol{z}) = n_{\mathrm{eq}}^\gamma\,\boldsymbol{u}(\boldsymbol{z}) \quad \textit{for} \quad \boldsymbol{z}\in\partial\Omega, \tag{2.6}$$

where n_{eq}^γ is the minimizer of the potential $W^\gamma(n)$.

Definition 2.2 (Tempered fields). *A family of order-parameter fields $\boldsymbol{n}^\gamma(\boldsymbol{z})$ is* tempered, *if $\boldsymbol{n}^\gamma|_{\partial\Omega}$ is well-prepared (in the sense of Definition 2.1) and $\boldsymbol{n}^\gamma$ satisfies the energy bound*

$$E^\gamma(\boldsymbol{n}^\gamma,\Omega) \le \pi\kappa|d|\ln\sqrt{\gamma}+C, \tag{2.7}$$

where $d=\deg(\boldsymbol{u},\partial\Omega)$ *and* C *is a constant independent of* γ. *A family of orientation probability densities* $\varrho^\gamma(\varphi,\boldsymbol{z})$ *is* tempered *if it produces tempered order-parameter field* $\boldsymbol{n}[\varrho]$.

THEOREM 2.2 (Convergence of tempered fields). *Let* $\varrho^\gamma(\varphi,\boldsymbol{z})$ *be a tempered family of orientation probability densities and* $\boldsymbol{n}^\gamma(\boldsymbol{z})=\boldsymbol{n}[\varrho^\gamma](\boldsymbol{z})$ *be the corresponding family of order-parameter fields. Then there exists an unbounded increasing sequence* $\{\gamma_k\}$, $|d|$ *distinct points* $\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|}\in\Omega$, *and a function* ϕ *with* $\nabla\phi\in L^2(\Omega)$ *generating an* $\mathbb{S}^1$*-map*

$$\boldsymbol{u}_*(\boldsymbol{z})=\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{z})}\prod_{j=1}^{d}\frac{\boldsymbol{z}-\boldsymbol{z}_j}{|\boldsymbol{z}-\boldsymbol{z}_j|}\quad \textit{for}\quad d>0,\qquad \boldsymbol{u}_*(\boldsymbol{z})=\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{z})}\prod_{j=1}^{|d|}\frac{\bar{\boldsymbol{z}}-\bar{\boldsymbol{z}}_j}{|\boldsymbol{z}-\boldsymbol{z}_j|}\quad \textit{for}\quad d<0, \tag{2.8}$$

such that as $k\to\infty$,

1. $\boldsymbol{n}^{\gamma_k}\rightharpoonup\boldsymbol{u}_*$ *in* $H^1_{\mathrm{loc}}\big(\bar\Omega\setminus\{\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|}\}\big)$,
2. $\varrho^{\gamma_k}(\varphi,\boldsymbol{z})\to\alpha(\boldsymbol{z})\delta\big(\varphi-\psi(\boldsymbol{z})\big)+\big(1-\alpha(\boldsymbol{z})\big)\delta(\varphi-\psi(\boldsymbol{z})-\pi)$ $\boldsymbol{z}$*-a.e., with* $\psi(\boldsymbol{z})=\frac{1}{2}\arg\boldsymbol{u}_*(\boldsymbol{z})\ (\mathrm{mod}\ 2\pi)$, *and some* $\alpha:\Omega\to[0,1]$.

REMARK 2.2. The $\mathbb{S}^1$-field $\boldsymbol{u}_*(\boldsymbol{z})$ is the so-called *multi-vortex* field: the products in (2.8) explicitly reveal the singularities while the *phase* $\phi(\boldsymbol{z})$ is a regular single-valued function. The field $\boldsymbol{u}_*$ may be regarded as an extension of the field $\boldsymbol{u}$ prescribed on the boundary $\partial\Omega$ into Ω.

REMARK 2.3. The factor $\alpha(\boldsymbol{z})$ in the second assertion is some measurable function which is irrelevant physically and appears because we parametrize the orientations which are points on a projective line by a number in $\mathbb{T}$, i.e., physically, φ and $\varphi+\pi$ correspond to the same orientation.

REMARK 2.4 (Asymptotic expansion of the energy). One can establish the following lower bound on the energy $E^\gamma(\boldsymbol{n},\Omega)$:

$$\liminf_{k\to\infty}\Big[E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\Omega)-\pi\kappa|d|\ln\sqrt{\gamma}-|d|E_0-\kappa\tilde E(\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|},\phi)\Big]\ge 0, \tag{2.9}$$

where E_0 is a constant independent of γ, and $\tilde E$ is the renormalized multi-vortex energy given by

$$\begin{aligned}\tilde E(\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|},\phi)&=\frac{1}{2}\int_\Omega|\nabla\phi(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z}-\pi\sum_{i,j=1,\ i\ne j}^{|d|}\ln|\boldsymbol{z}_i-\boldsymbol{z}_j| \\ &-\sum_{j=1}^{|d|}\oint_{\partial\Omega}\ln|\boldsymbol{z}-\boldsymbol{z}_j|\,\partial_\tau\arg\boldsymbol{u}(\boldsymbol{z})\,\mathrm{d}\ell(\boldsymbol{z})-\frac{1}{2}\sum_{i,j=1}^{|d|}\oint_{\partial\Omega}\ln|\boldsymbol{z}-\boldsymbol{z}_j|\,\partial_\nu\ln|\boldsymbol{z}-\boldsymbol{z}_i|\,\mathrm{d}\ell(\boldsymbol{z}).\end{aligned} \tag{2.10}$$

Here $\boldsymbol{u}:\partial\Omega\to\mathbb{S}^1$ appears in the boundary data for $\boldsymbol{n}^\gamma$ according to Definition 2.1, and ∂_τ denotes derivative in the direction tangential to $\partial\Omega$. Up to the constant E_0, the renormalized energy $\tilde E(\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|},\phi)$ is exactly the same energy that appears in the Ginzburg-Landau theory [2]. The constant E_0 arises from the so-called optimal profile problem: it is the $\mathcal{O}(1)$ contribution from the vicinity of a vortex and its precise value depends on specifics of the potential $W^\gamma(n)$. It is possible to construct a recovery sequence for which equality in (2.9) is obtained exactly. We sketch a derivation of this result in section 3.2.3 but do not present a complete proof due to space constraints and its essential similarity to existing results in the Ginzburg-Landau theory [2, 19].

3. Proofs and auxiliary results

Now we prove the theorems stated in the previous section. The proof of Theorem 2.1 is relatively straightforward and only uses the properties of relative entropy and the potential $W^\gamma(n)$. The proof of Theorem 2.2 uses an estimate of Dirichlet energy $\mathcal{D}(\boldsymbol{u})$ of an $\mathbb{S}^1$-map $\boldsymbol{u}(\boldsymbol{z})$ due to Sandier [20] which is presented here in Theorem A.1, Appendix A.

3.1. Proof of the energy decomposition theorem. Let $\hat{\varrho}$ be related to ϱ as in the statement of Theorem 2.1. We observe the following simple fact:
$(*)$ Given an arbitrary $\boldsymbol{n}_0$, $\varrho=\varrho[\boldsymbol{n}_0]$ defined via (2.3) is a minimizer of $\mathcal{S}\big(\varrho|\hat{\varrho}\big)$.
Indeed, by direct calculation we can verify that if $\varrho=\varrho[\boldsymbol{n}_0]$ for some $\boldsymbol{n}_0$, then $\hat{\varrho}=\varrho[\boldsymbol{n}[\varrho]]=\varrho$, and thus $\mathcal{S}(\varrho|\hat{\varrho})=0$. However, $\mathcal{S}(\varrho|\varrho_0)\geq 0$ for all ϱ, ϱ_0, i.e., $\varrho=\varrho[\boldsymbol{n}_0]$ is a minimizer of $\mathcal{S}(\varrho|\hat{\varrho})$.

Proof. (Theorem 2.1) Observing that

$$\iint_0^{2\pi}\cos 2(\varphi-\varphi')\,\varrho(\varphi)\varrho(\varphi')\,\mathrm{d}\varphi\mathrm{d}\varphi'=n^2, \tag{3.1}$$

and using that

$$\int_0^{2\pi}\ln\big[2\pi\varrho(\varphi)\big]\,\mathrm{d}\varphi=\int_0^{2\pi}\ln\big[2\pi\varrho[\boldsymbol{n}](\varphi)\big]\,\mathrm{d}\varphi+\mathcal{S}\big(\varrho|\varrho[\boldsymbol{n}]\big), \tag{3.2}$$

we can represent the energy $\mathcal{E}^\gamma(\varrho,\Omega)$ as

$$\mathcal{E}^\gamma(\varrho,\Omega)=\int_\Omega\left[\frac{\kappa}{2}|\nabla\boldsymbol{n}|^2+\int_0^{2\pi}\varrho(\varphi)\ln\big[2\pi\varrho[\boldsymbol{n}](\varphi)\big]\,\mathrm{d}\varphi-\frac{\gamma n^2}{2}+C_\gamma\right]\mathrm{d}\boldsymbol{z}\\ +\int_\Omega\mathcal{S}\big(\varrho|\varrho[\boldsymbol{n}]\big)\,\mathrm{d}\boldsymbol{z}. \tag{3.3}$$

Via straightforward calculation we find that

$$\int_0^{2\pi}\varrho(\varphi)\ln\big[2\pi\varrho[\boldsymbol{n}](\varphi)\big]\,\mathrm{d}\varphi=\mathrm{A}(n)\int_0^{2\pi}\cos(2\varphi-\arg\boldsymbol{n})\varrho(\varphi)\,\mathrm{d}\varphi-\ln\mathrm{I}_0(\mathrm{A}(n))\\ =n\,\mathrm{A}(n)-\ln\mathrm{I}_0(\mathrm{A}(n)). \tag{3.4}$$

Substituting this expression into equation (3.3) and comparing with formula (1.9) for the potential $W^\gamma(n)$ we verify the first assertion of the theorem.

To verify the second asserion first let $\boldsymbol{n}_0(\boldsymbol{z})$ be a critical point of $E^\gamma(\boldsymbol{n},\Omega)$, so that the variation $\mathbf{D}E^\gamma(\boldsymbol{n}_0,\Omega)=0$. Since by $(*)$, $\varrho=\varrho[\boldsymbol{n}_0]$ is a critical point of $\mathcal{S}\big(\varrho|\hat{\varrho}\big)$, its variation vanishes and so does the variation $\mathbf{D}\mathcal{E}^\gamma(\varrho[\boldsymbol{n}_0],\Omega)$, i.e., $\varrho=\varrho[\boldsymbol{n}_0]$ is a critical point of $\mathcal{E}^\gamma(\varrho,\Omega)$. Now let ϱ_0 be a critical point of $\mathcal{E}^\gamma(\varrho,\Omega)$, i.e., variation of the energy $\mathcal{E}^\gamma(\varrho,\Omega)$ vanishes. Varying ϱ_0 so that the order parameter remains fixed and equal to $\boldsymbol{n}_0=\boldsymbol{n}[\varrho_0]$ and taking into account that E^γ only depends on $\boldsymbol{n}[\varrho]$, we get that $\delta\mathcal{E}^\gamma(\varrho)=\delta\mathcal{S}(\varrho|\varrho[\boldsymbol{n}_0])=0$. The corresponding Euler-Lagrange equation implies that $\varrho_0=\varrho[\boldsymbol{n}_0]$. This fact however can be deduced without the use of Euler-Lagrange equation: since $\mathcal{S}(\varrho|\varrho[\boldsymbol{n}_0])$ is a convex functional of ϱ and the constraint that $\boldsymbol{n}[\varrho]=\boldsymbol{n}_0$ is linear, the constrained variational problem has a unique critical point (minimum), which clearly is $\varrho[\boldsymbol{n}_0]$. From $(*)$ we then get that ϱ_0 is a critical point of $\mathcal{S}(\varrho|\hat{\varrho})$ by itself (and without any constraints) and thus $\mathbf{D}E^\gamma(\boldsymbol{n}[\varrho_0],\Omega)=0$.

Finally, we prove that the corresponding critical points of $E^\gamma(\boldsymbol{n},\Omega)$ and $\mathcal{E}^\gamma(\varrho,\Omega)$ have the same stability properties. Indeed, let $\boldsymbol{n}_0(\boldsymbol{z})$ be a minimizer of $E^\gamma(\boldsymbol{n},\Omega)$. Since all critical points of $\mathcal{S}(\varrho|\hat{\varrho})$ are minimizers, $\varrho[\boldsymbol{n}_0]$ is a minimizer of $\mathcal{E}^\gamma(\varrho,\Omega)$. Now assume that $\boldsymbol{n}_0(\boldsymbol{z})$ is a saddle point, i.e., there exists a continuous curve $\boldsymbol{n}_t$, $t\geq 0$ such that $E^\gamma(\boldsymbol{n}_t,\Omega)$ is decreasing. However since $\mathcal{S}(\varrho[\boldsymbol{n}_t]|\hat{\varrho}[\boldsymbol{n}_t])=0$, $\mathcal{E}^\gamma(\varrho[\boldsymbol{n}_t],\Omega)$ is also decreasing, i.e., $\varrho[\boldsymbol{n}_0]$ is also a saddle point. ∎

3.2. Proof of the convergence theorem.

Outline of the proof. The first step is obtaining a rough lower bound on the energy $E^\gamma(\boldsymbol{n}^\gamma,\Omega)$ of a tempered family of order-parameter fields $\boldsymbol{n}^\gamma(\boldsymbol{z})$; this result is formulated in Lemma 3.1. This lower bound, as shown in Lemma 3.2, implies existence of a subsequence $\{\boldsymbol{n}^{\gamma_k}\}$ converging weakly to some $\mathbb{S}^1$-map $\boldsymbol{u}_*(\boldsymbol{z})$ with at most $|d|$ singularities (vortices), where d is the degree of the boundary data. In order to show that the map $\boldsymbol{u}_*$ has exactly $|d|$ singularities we use the fact that a vortex of degree d_j contributes $\sim\pi d_j^2\kappa\ln\sqrt{\gamma}$ into the energy (Lemma A.3) which is only compatible with the upper bound (2.7) if all $d_j=\operatorname{sgn}d$. Lemma A.2 states that any such function $\boldsymbol{u}_*$ may be represented as in formula (2.8). Finally we translate convergence of the order-parameter fields $\{\boldsymbol{n}^{\gamma_k}\}$ into convergence of orientation probability densities $\{\varrho^{\gamma_k}\}$ using the fact that as $|\boldsymbol{n}^{\gamma_k}|\to 1$, ϱ^{γ_k} which generates it necessarily converges to some atomic measure.

In what follows we use the following conventions: given an order-parameter field $\boldsymbol{n}(\boldsymbol{z})$ we denote $n=|\boldsymbol{n}|$, $\boldsymbol{u}=\boldsymbol{n}/n$, $\omega_t=\{\boldsymbol{z}\in\Omega: n(\boldsymbol{z})<t\}$, $\Omega_t=\{\boldsymbol{z}\in\Omega: n(\boldsymbol{z})>t\}$. For a set $\mathcal{A}\subset\mathbb{C}$ we denote its one-dimensional Hausdorff measure by $\ell(\mathcal{A})$; $|\mathcal{A}|$ denotes its *diameter* which is defined as the infimum of the sum $D_1+\cdots+D_k$ over all finite coverings of $\mathcal{A}$ by open disks with dimaters D_j. Finally, unless specified explicitly, C denotes a generic positive constant independent of γ.

3.2.1. Rough lower bound.

LEMMA 3.1 (Rough lower bound). *Let $\boldsymbol{n}^\gamma$ have well-prepared boundary values (see Definition 2.1). Then*

$$E^\gamma(\boldsymbol{n}^\gamma,\Omega)\geq\pi|d|\kappa\ln\sqrt{\gamma}-C. \tag{3.5}$$

Moreover, if $\boldsymbol{n}^\gamma$ is tempered (see Definition 2.2) then

$$\pi|d|\kappa\ln\sqrt{\gamma}-C\leq\frac{\kappa}{2}\int_\Omega|n^\gamma\nabla\boldsymbol{u}^\gamma|^2\,\mathrm{d}\boldsymbol{z}\leq\pi|d|\kappa\ln\sqrt{\gamma}+C, \tag{3.6}$$

where we denoted $n^\gamma=|\boldsymbol{n}^\gamma|$, $\boldsymbol{u}^\gamma=\boldsymbol{n}^\gamma/|\boldsymbol{n}^\gamma|$.

REMARK 3.1. The second assertion of this lemma implies that in the limit as $\gamma\to\infty$, the phase of $\boldsymbol{n}^\gamma$ provides the principal contribution into the energy while the contribution from the absolute value n^γ remains bounded:

$$\int_\Omega\Big[\frac{\kappa}{2}|\nabla n^\gamma|^2+W^\gamma(n^\gamma)\Big]\,\mathrm{d}\boldsymbol{z}\leq C. \tag{3.7}$$

The proof of this Lemma is essentially an adaptation of the proof of Theorem 2 in [20]. The major difference appears in the estimates on the potential part of the energy, $W^\gamma(n)$ which is slightly more technical since the dependence on the parameter γ is not as explicit as in the Ginzburg-Landau potential $W^\gamma_{\mathrm{GL}}(n)=\gamma(1-n^2)^2$. In order to

avoid cluttering the formulas we omit the superscript γ whenever this does not cause confusion.

Proof. Recollect the coarea formula:

$$\int_{\omega_t} f(\boldsymbol{z})|\nabla n(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} = \int_0^t \left[\int_{\partial\omega_s} f(\boldsymbol{z})\,\mathrm{d}\ell(\boldsymbol{z})\right]\mathrm{d}s. \tag{3.8}$$

We start by representing the total energy $E^\gamma(\boldsymbol{n},\Omega)$ as

$$E^\gamma(\boldsymbol{n},\Omega) = \int_\Omega \left[\frac{\kappa}{2}|\nabla n(\boldsymbol{z})|^2 + W^\gamma\big(n(\boldsymbol{z})\big)\right]\mathrm{d}\boldsymbol{z} + \frac{\kappa}{2}\int_\Omega n^2(\boldsymbol{z})|\nabla\boldsymbol{u}(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z}. \tag{3.9}$$

Using Cauchy-Schwarz inequality and the coarea formula, we get the following lower bound of the first term in equation (3.9):

$$\begin{aligned}\int_\Omega \left[\frac{\kappa}{2}|\nabla n(\boldsymbol{z})|^2 + W^\gamma\big(n(\boldsymbol{z})\big)\right]\mathrm{d}\boldsymbol{z} &\geq \int_\Omega \sqrt{2\kappa W^\gamma\big(n(\boldsymbol{z})\big)}\,|\nabla n(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} \\ &\geq \int_0^{n_{\mathrm{eq}}}\int_{\partial\omega_t}\sqrt{2\kappa W^\gamma(t)}\,\mathrm{d}\ell(\boldsymbol{z})\,\mathrm{d}t = \int_0^{n_{\mathrm{eq}}}\sqrt{2\kappa W^\gamma(t)}\,\ell(\partial\omega_t)\,\mathrm{d}t.\end{aligned} \tag{3.10}$$

Here we used the fact that $n = n_{\mathrm{eq}}$ on $\partial\Omega$ and hence for all $0 < t < n_{\mathrm{eq}}$ we have $\partial\omega_t \setminus \partial\Omega = \partial\omega_t$. Since $\ell(\partial\omega_t) \geq |\omega_t|$ for all $\eta \leq n_{\mathrm{eq}}$ we have

$$\int_\Omega \left[\frac{\kappa}{2}|\nabla n(\boldsymbol{z})|^2 + W^\gamma\big(n(\boldsymbol{z})\big)\right]\mathrm{d}\boldsymbol{z} \geq \int_0^\eta \sqrt{2\kappa W^\gamma(t)}\,|\omega_t|\,\mathrm{d}t. \tag{3.11}$$

The parameter η is left undefined at this point and will be assigned a suitable value at the right time to simplify some technical calculations. The second term in (3.9) may be rewritten using the coarea formula and integration by parts as

$$\begin{aligned}\frac{\kappa}{2}\int_\Omega n^2(\boldsymbol{z})|\nabla\boldsymbol{u}(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z} &\geq \frac{\kappa}{2}\int_0^{n_{\mathrm{eq}}} t^2\int_{\partial\Omega_t}|\nabla\boldsymbol{u}(\boldsymbol{z})|^2/|\nabla n(\boldsymbol{z})|\,\mathrm{d}\ell(\boldsymbol{z})\,\mathrm{d}t \\ &= -\frac{\kappa}{2}\int_0^{n_{\mathrm{eq}}} t^2\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t}|\nabla\boldsymbol{u}(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z}\,\mathrm{d}t \geq \kappa\int_0^{n_{\mathrm{eq}}} t\int_{\Omega_t}|\nabla\boldsymbol{u}(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z}\,\mathrm{d}t.\end{aligned} \tag{3.12}$$

Using Theorem A.1 (Sandier [20]) we estimate

$$\int_{\Omega_t}|\nabla\boldsymbol{u}(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z} \geq -2\pi|d|\ln|\omega_t| - C, \tag{3.13}$$

and combining (3.11) and (3.12) find that

$$E^\gamma(\boldsymbol{n},\Omega) \geq \int_0^\eta \left[\sqrt{2\kappa W^\gamma(t)}\,|\omega_t| - 2\pi|d|\kappa t\ln|\omega_t|\right]\mathrm{d}t - C. \tag{3.14}$$

We see that the only unknown function on the right-hand side is $|\omega_t|$. In order to find a lower bound we are going to optimize with respect to $|\omega_t|$. We consider

$$\mathcal{J}_\lambda(\phi) = \int_0^\eta \left[\lambda\sqrt{2\kappa W^\gamma(t)}\,\phi(t) - 2\pi|d|\kappa t\ln\phi(t)\right]\mathrm{d}t, \tag{3.15}$$

where $\lambda>0$ is a parameter. Clearly, $E^\gamma(\boldsymbol{n},\Omega)\geq\inf_\phi \mathcal{J}_1(\phi)-C$. Minimizing $\mathcal{J}_\lambda(\phi)$ with respect to $\phi(t)$, we find the optimal function $\phi(t)=\pi|d|t/\lambda\sqrt{2\kappa/W^\gamma(t)}$ and the estimate

$$\inf_\phi \mathcal{J}_\lambda(\phi)\geq\pi|d|\kappa\int_0^\eta t\ln W^\gamma(t)\,\mathrm{d}t-C. \tag{3.16}$$

Now we observe that $W^\gamma(t)\geq C_\gamma-\gamma t^2/2$, where n_{eq} is the nonzero solution of $\gamma t=\mathrm{A}(t)$, see Appendix B. We choose η so that $C_\gamma-\gamma\eta^2/2=1$ and note that such η satisfies $\eta<n_{\mathrm{eq}}$. Therefore we have

$$\inf_\phi \mathcal{J}_\lambda(\phi)\geq\pi|d|\kappa\int_0^\eta t\ln(C_\gamma-\gamma t^2/2)\,\mathrm{d}t-C=\frac{\pi|d|\kappa}{\gamma}\left(C_\gamma\ln C_\gamma-C_\gamma+1\right)-C. \tag{3.17}$$

Using Fact B.3 (see Appendix B) we know that as $\gamma\to\infty$, $C_\gamma=\gamma/2+\mathcal{O}(\ln\gamma)$, and finally estimate

$$\inf_\phi \mathcal{J}_\lambda(\phi)\geq\pi|d|\kappa\ln\sqrt{\gamma}-C. \tag{3.18}$$

Notice the crucial fact that the principal contribution here does not depend on λ (the choice of λ only affects the constant C). Setting $\lambda=1$ we recover the first claim.

Now assume that $\boldsymbol{n}^\gamma$ is tempered, i.e., satisfies the upper bound

$$\begin{aligned}E^\gamma(\boldsymbol{n}^\gamma,\Omega)&=\int_\Omega\Big[\frac{\kappa}{2}|\nabla n(\boldsymbol{z})|^2+W^\gamma\big(n(\boldsymbol{z})\big)\Big]\,\mathrm{d}\boldsymbol{z}+\frac{\kappa}{2}\int_\Omega n^2(\boldsymbol{z})|\nabla\boldsymbol{u}(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z}\\&\leq\pi|d|\kappa\ln\sqrt{\gamma}+C.\end{aligned} \tag{3.19}$$

From the lower-bound on $\mathcal{J}_{1/2}(\phi)$ we obtain

$$\frac{1}{2}\int_\Omega\Big[\frac{\kappa}{2}|\nabla n(\boldsymbol{z})|^2+W^\gamma\big(n(\boldsymbol{z})\big)\Big]\,\mathrm{d}\boldsymbol{z}+\frac{\kappa}{2}\int_\Omega n^2(\boldsymbol{z})|\nabla\boldsymbol{u}(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z}\geq\pi|d|\kappa\ln\sqrt{\gamma}-C. \tag{3.20}$$

Subtracting these inequalities we immediately obtain that

$$\int_\Omega\Big[\frac{\kappa}{2}|\nabla n(\boldsymbol{z})|^2+W^\gamma\big(n(\boldsymbol{z})\big)\Big]\,\mathrm{d}\boldsymbol{z}\leq C, \tag{3.21}$$

which, in turn, implies the second claim. ∎

3.2.2. Convergence.

LEMMA 3.2 (Convergence). *Let $\boldsymbol{n}^\gamma$ be tempered (see Definition 2.2); then there exists an unbounded increasing sequence $\{\gamma_k\}$, exactly $|d|$ distinct points $\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|}\in\bar\Omega$, and an $\mathbb{S}^1$-map $\boldsymbol{u}_*\in H^1_{\mathrm{loc}}(\bar\Omega\setminus\{\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|}\})$ such that for all j $\deg(\boldsymbol{u}_*,\boldsymbol{z}_j)=\operatorname{sgn}d$, and*

$$\boldsymbol{n}^{\gamma_k}\rightharpoonup\boldsymbol{u}_*\quad\textit{weakly}\quad\textit{in}\quad H^1_{\mathrm{loc}}(\bar\Omega\setminus\{\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|}\}). \tag{3.22}$$

Proof. From the Remark 3.1 following Lemma 3.1 we know that the "radial and nonlinear" contributions into the energy are of $\mathcal{O}(1)$ as $\gamma\to\infty$, which implies using formula (3.11) that

$$\int_0^{n^\gamma_{\mathrm{eq}}}\sqrt{2\kappa W^\gamma(t)}\,|\omega_t|\,\mathrm{d}t\leq C. \tag{3.23}$$

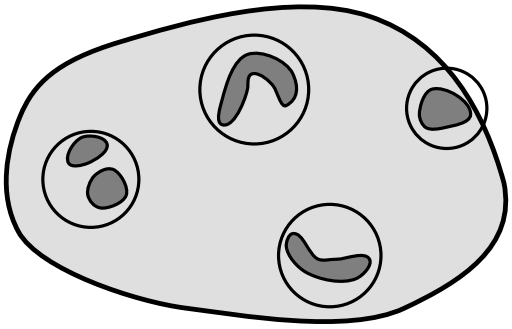

FIG. 3.1. *Illustration of the domain Ω. Light grey: $\Omega_\eta = \{\boldsymbol{z}\in\Omega : n(\boldsymbol{z}) > \eta\}$; dark grey: $\omega_\eta = \{\boldsymbol{z}\in\Omega : n(\boldsymbol{z}) < \eta\}$. The whole set ω_η may be covered by non-intersecting disks B_j, $j=1,\dots,m\le|d|$, whose radii do not exceed $r\sim C/\sqrt{\gamma}$. At the same time, according to (3.32), the energy in $\Omega\setminus\cup_j B_j$ remains bounded as $\gamma\to\infty$, i.e., all singularities are localized within the disks B_j.*

Using this estimate with (3.18) we obtain

$$-2\pi|d|\kappa\int_0^{n_{\rm eq}^\gamma} t\ln|\omega_t|\,\mathrm{d}t \ge \pi|d|\kappa\ln\sqrt{\gamma} - C. \tag{3.24}$$

From (3.12) and temperedness condition on $\{\boldsymbol{n}^\gamma\}$ we obtain that

$$\int_0^{n_{\rm eq}^\gamma} t\int_{\Omega_t}|\nabla\boldsymbol{u}^\gamma(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z} \le \pi|d|\ln\sqrt{\gamma} + C. \tag{3.25}$$

These two inequalities imply the following bound

$$\int_0^{n_{\rm eq}^\gamma} t\left(\int_{\Omega_t}|\nabla\boldsymbol{u}^\gamma(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z} + 2\pi|d|\ln|\omega_t|\right)\mathrm{d}t \le C. \tag{3.26}$$

Now we can use lower bound inequality (3.13) and obtain

$$\int_0^{n_{\rm eq}^\gamma}\left|t\int_{\Omega_t}|\nabla\boldsymbol{u}^\gamma(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z} + 2t\pi|d|\ln|\omega_t|\right|\mathrm{d}t \le C. \tag{3.27}$$

Pick arbitrary $0<\eta_1<\eta_2<1$, and consider γ large enough so that $n_{\rm eq}^\gamma > \eta_2$. Since the integral expression in (3.27) is positive, we may integrate over $[\eta_1,\eta_2]$ with the inequality intact. By the mean value theorem there exists some $\eta\in[\eta_1,\eta_2]$ for which

$$\left|\int_{\Omega_\eta}|\nabla\boldsymbol{u}^\gamma(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z} + 2\pi|d|\ln|\omega_\eta|\right| \le C. \tag{3.28}$$

Thus for this η we have

$$\mathcal{D}(\boldsymbol{u}^\gamma,\Omega_\eta) \le -\pi|d|\ln|\omega_\eta| + C. \tag{3.29}$$

Similarly, consider the inequality (3.23). Using that $|\omega_t|$ is an increasing function of t and Fact B.4 from Appendix B, we get that $|\omega_\eta| < C/\sqrt{\gamma}$ (note that this is true for any fixed $0<\eta<1$).

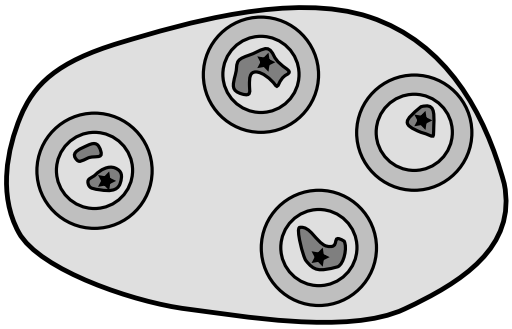

FIG. 3.2. *Decomposition of the domain Ω employed in proving that $m=|d|$. Locations of the vortices $\boldsymbol{z}_j$ are marked with star symbols; dark grey corresponds to the set $\omega_M=\{\boldsymbol{z}\in\Omega : n(\boldsymbol{z})<M\}$; annuli A_j are depicted using medium grey color.*

Using Theorem A.1 we know that for any r such that $C/\sqrt{\gamma}<r<C$, we may cover ω_η with m disjoint disks B_j, $j=1,\dots,m\le|d|$, with radii at most r, so that

$$\mathcal{D}(\boldsymbol{u}^\gamma,\Omega\cap(\cup_{j=1}^m B_j)\setminus\omega_\eta)\ge\pi|d|\ln\frac{r}{|\omega_\eta|}-C, \tag{3.30}$$

see figure 3.1 for illustration. Note that ω_η is covered by $\cup_j B_j$ and thus $\Omega\setminus\cup_j B_j=\Omega_\eta\setminus(\cup_j B_j\setminus\omega_\eta)$. Therefore subtracting the last two formulas we obtain

$$\mathcal{D}(\boldsymbol{u}^\gamma,\Omega\setminus\cup_{j=1}^m B_j)\le-\pi|d|\ln r+C. \tag{3.31}$$

Taking into account the remark after Lemma 3.1 we immediately deduce the following fact:
(∗) For arbitrary $\eta\in(0,1)$ and R satisfying $C/\sqrt{\gamma}<R<C$, we may cover ω_η with m disjoint disks B_j, $j=1,\dots,m\le|d|$, whose radii r_j do not exceed R, so that

$$E^\gamma(\boldsymbol{n}^\gamma,\Omega\setminus\cup_{j=1}^m B_j)\le-\pi|d|\kappa\ln R+C. \tag{3.32}$$

Fix some $\eta\in(1/2,1)$, and some sequence of positive numbers $\{R_l\}$ which tends to zero as $l\to\infty$. For each R_l consider the family $\boldsymbol{z}_{l,j}^\gamma$ of centers of such covering disks as in (∗). Since $\bar\Omega$ is compact, for any fixed l there exists an unbounded increasing sequence $\{\gamma_{l,p}\}$ such that $\boldsymbol{z}_{l,j}^{\gamma_{l,p}}\to\boldsymbol{z}_{l,j}\in\bar\Omega$ as $p\to\infty$. By the same compactness argument, as $l\to\infty$, there exists a subsequence such that (up to relabeling) $\boldsymbol{z}_{l,j}\to\boldsymbol{z}_j\in\bar\Omega$. Thus by a diagonalization argument there exist subsequences $\{l_k\}$, $\{p_k\}$, such that $\boldsymbol{z}_{l_k,j}^{\gamma_{l_k,p_k}}\to\boldsymbol{z}_j$ as $k\to\infty$. For notational convenience we denote the sequence $\{\gamma_{l_k,p_k}\}$ by $\{\gamma_k\}$. Applying (∗) to the corresponding sequence of order parameter fields $\{\boldsymbol{n}^{\gamma_k}\}$ we get that their energy is bounded outside arbitrarily small disks $B_R(\boldsymbol{z}_j)$. Thus the norms of $\boldsymbol{n}^{\gamma_k}(\boldsymbol{z})$ are bounded in $H^1\big(\bar\Omega\setminus\cup B_R(\boldsymbol{z}_j)\big)$ for all $R>0$, i.e., there exists a subsequence converging weakly in $H^1_{\rm loc}(\bar\Omega\setminus\{\boldsymbol{z}_1,\dots,\boldsymbol{z}_m\})$ to some field $\boldsymbol{u}_*$. The fact that $|\boldsymbol{u}_*(\boldsymbol{z})|=1$ $\boldsymbol{z}$-a.e. follows from the estimate on the nonlinear part of the energy (see Remark 3.1 following Lemma 3.1).

Now we prove that $m=|d|$ exactly. Let us split Ω into three subdomains: $\Omega=\omega\cup\mathcal{A}\cup\mathcal{B}$, where $\omega=\cup_j B_{R_1}(\boldsymbol{z}_j)$, $\mathcal{A}=\cup_j A_j$, $A_j=B_{R_2}(\boldsymbol{z}_j)\setminus B_{R_1}(\boldsymbol{z}_j)$, $\mathcal{B}=\Omega\setminus\cup_j B_{R_2}(\boldsymbol{z}_j)$; see figure 3.2. We keep R_2 sufficiently small but fixed, while from (∗) we know that for any $M<1$ we may choose R_1 so that $C_1/\sqrt{\gamma}\le R_1\le C_2/\sqrt{\gamma}$ and $\boldsymbol{n}^{\gamma_k}\ge M$ in

$\Omega\setminus_j \cup B_{R_1}(\boldsymbol{z}_j)$. Consider a sequence $\{\boldsymbol{n}^{\gamma_k}\}$ converging to $\boldsymbol{u}_*$. We have, discarding the contribution from ω,

$$E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\Omega) \geq E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\mathcal{A}) + E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\mathcal{B}) \geq E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\mathcal{A}) + C, \tag{3.33}$$

since in $\mathcal{B}$, $E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\mathcal{B}) \to \mathcal{D}(\boldsymbol{u}_*,\mathcal{B})$. Within each annulus A_j,

$$E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},A_j) \geq \frac{\kappa}{2}\mathcal{D}(\boldsymbol{n}^{\gamma_k},A_j) \geq \frac{\kappa}{2}M^2\mathcal{D}(\boldsymbol{u}^{\gamma_k},A_j), \tag{3.34}$$

and thus employing Lemma A.1, we obtain

$$E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},A_j) \geq \pi d_j^2 \kappa M^2 \ln\frac{R_2}{R_1} \geq \pi d_j^2 \kappa M^2 \ln\sqrt{\gamma} - C. \tag{3.35}$$

Summing up the contributions from all A_j, we obtain

$$E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\Omega) \geq \pi\kappa M^2 \ln\sqrt{\gamma}\sum_{j=1}^{m} d_j^2 - C \geq \frac{M^2|d|}{m}\,\pi\kappa|d|\ln\sqrt{\gamma} - C. \tag{3.36}$$

If $m<|d|$, we can chose $M\in(\sqrt{m/|d|},1)$ so that $M^2|d|/m>1$ and obtain a lower bound on the energy $\mathcal{E}^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\Omega)$ contradicting our assumption that $\boldsymbol{n}^{\gamma}$ is tempered. Thus $m=|d|$. ∎

Proof. [Theorem 2.2.] By Lemma 3.2 there exists an unbounded increasing sequence $\{\gamma_k\}$ such that the sequence of order-parameter fields $\{\boldsymbol{n}^{\gamma_k}=\boldsymbol{n}[\varrho^{\gamma_k}]\}$ converges weakly in $H^1_{\mathrm{loc}}(\bar\Omega\setminus\{\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|}\})$ to some $\mathbb{S}^1$-map $\boldsymbol{u}_*(\boldsymbol{z})$ with $\deg(\boldsymbol{u}_*,\boldsymbol{z}_j)=\operatorname{sgn} d$ for all $j=1,\dots,|d|$. By Lemma A.2, $\boldsymbol{u}_*(\boldsymbol{z})$ may be represented as in (2.8). This concludes the proof of Assertion 1.

We have

$$\left|\boldsymbol{n}^{\gamma_k}(\boldsymbol{z})\right|^2 = 1 - 2\iint_0^{2\pi}\sin^2(\varphi-\psi)\,\varrho^{\gamma_k}(\varphi)\varrho^{\gamma_k}(\psi)\,\mathrm{d}\varphi\,\mathrm{d}\psi. \tag{3.37}$$

Since the space of measures with finite mass over $\mathbb{T}\times\Omega$ is compact, ϱ^{γ_k} converges (up to some sub-sequence) to some finite measure $\mu(\varphi,\boldsymbol{z})$. Since $|\boldsymbol{n}^{\gamma_k}(\boldsymbol{z})|\to 1$ $\boldsymbol{z}$-a.e., we obtain

$$\iint_0^{2\pi}\sin^2(\varphi-\psi)\,\mathrm{d}\mu(\varphi)\,\mathrm{d}\mu(\psi) = 0 \quad \boldsymbol{z}\text{-a.e.}, \tag{3.38}$$

which implies that there exist some functions $\alpha:\Omega\to[0,1]$ and $\psi:\Omega\to\mathbb{R}$ such that the measure $\mu(\varphi,\boldsymbol{z})=\alpha(\boldsymbol{z})\delta\big(\varphi-\psi(\boldsymbol{z})\big)+\big(1-\alpha(\boldsymbol{z})\big)\delta(\varphi-\psi(\boldsymbol{z})-\pi)$ $\boldsymbol{z}$-a.e. Since we also have

$$\boldsymbol{u}_*(\boldsymbol{z}) = \int_0^{2\pi}\mathrm{e}^{2\mathrm{i}\varphi}\,\mathrm{d}\mu(\varphi) = \mathrm{e}^{2\mathrm{i}\psi(\boldsymbol{z})} \quad \boldsymbol{z}\text{-a.e.}, \tag{3.39}$$

we verify Assertion 2. ∎

3.2.3. Expansion of the energy. Finally, we sketch an argument which yields expansion (2.9) in Remark 2.4 following the theorem. Denote $\omega_r=\cup_j B_r(\boldsymbol{z}_j)$, $\Omega_r=\Omega\setminus\omega_r$ and represent the energy E^{γ_k} as

$$E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\Omega) = E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\Omega_r) + E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\omega_r). \tag{3.40}$$

Since $\boldsymbol{n}^{\gamma_k} \rightharpoonup \boldsymbol{u}_*$ in $H^1(\Omega_r)$, employing Lemma A.3 we have

$$\liminf_{k\to\infty} E^{\gamma_k}(\boldsymbol{n}^{\gamma_k},\Omega_r) \geq \kappa\mathcal{D}(\boldsymbol{u}_*,\Omega_r) = -\pi|d|\,\kappa\ln r + \kappa\tilde{E}(\boldsymbol{z}_1,\dots,\boldsymbol{z}_{|d|},\phi) + \mathcal{O}(r\ln r). \tag{3.41}$$

Obtaining the exact lower bound for the energy $E^{\gamma_k}\big(\boldsymbol{n}^{\gamma_k},B_r(\boldsymbol{z}_j)\big)$ inside each ball $B_r(\boldsymbol{z}_j)$ is the so-called optimal profile problem. In essence, one can show that

$$\liminf_{k\to\infty}\Big[E^{\gamma_k}\big(\boldsymbol{n}^{\gamma_k},B_r(\boldsymbol{z}_j)\big) - \pi\kappa\ln\sqrt{\gamma_k}\Big] \geq \pi\kappa\ln r + \kappa E_0 + \mathcal{O}(r), \tag{3.42}$$

where κE_0 is $\mathcal{O}(1)$ contribution into the energy (as $\gamma\to\infty$) from the following minimization problem: minimize $E^{\gamma}\big(\boldsymbol{n},B_r(0)\big)$ given $\deg\big(\boldsymbol{n},\partial B_r(0)\big)=1$ and $\boldsymbol{n}(0)=0$. Since for sufficiently small r, $\omega_r=\cup_{j=1}^{|d|}B_r(\boldsymbol{z}_j)$, combining the estimates in (3.42) and (3.41) and sending $r\to 0$, we recover the asserted lower bound.

4. Concluding remarks

The study of the free energy functionals undertaken in this work provides information about the structure of equilibrium (or more generally, *tempered*) states of two-dimensional nematics. In order to explore their out-of-equilibrium properties, one has to look into the associated dynamics. The simplest dynamics are purely dissipative and describe the systems in which the solvent has already equilibrated and evolution is only manifested via diffusive transport of orientations. For example, the Doi dynamics [5] for the orientation probability density is governed by the following (kinetic) equation:

$$\partial_t\varrho(\varphi,\boldsymbol{z},t) = \partial_\varphi\left\{\varrho\,\partial_\varphi\frac{\delta\mathcal{E}(\varrho)}{\delta\varrho(\varphi,\boldsymbol{z})}\right\}. \tag{4.1}$$

At the same time, dissipative dynamics in order parameter-based theories, e.g, Landau-de Gennes theory, are described by the usual gradient flows for the functional $E(\boldsymbol{n},\Omega)$, e.g.,

$$\partial_t\boldsymbol{n}(\boldsymbol{z},t) = -\frac{\delta E(\boldsymbol{n})}{\delta\bar{\boldsymbol{n}}(\boldsymbol{z})}. \tag{4.2}$$

However the order parameter $\boldsymbol{n}(\boldsymbol{z})$ is a moment of the orientations probability density $\varrho(\varphi,\boldsymbol{z})$, cf. formula (2.2), thus equation (4.2), or its equivalent, must be derivable from the more general (4.1). This is a particular example of the general problem of derivation of hydrodynamic-type equations from kinetic-type equations. Since Theorem 2.1 provides an explicit decomposition of the total free energy into the Landau-de Gennes-type energy and relative entropy, our theory provides a natural setting for studying this problem, i.e., the relation between the Doi dynamics and Landau-de Gennes dynamics. The estimates in Theorem 2.2 and Remark 2.4 then provide essential ingredients for analysis of the vortex dynamics which arises in the high concentration limit.

Appendix A. Some properties of $\mathbb{S}^1$-maps. Recollect that the *Dirichlet energy* of a function $\boldsymbol{w}(\boldsymbol{z})=u(x,y)+\mathrm{i}v(x,y)$ in a domain $\Omega\subset\mathbb{C}$ is given by (denoting $w=|\boldsymbol{w}|$)

$$\begin{aligned}\mathcal{D}(\boldsymbol{w},\Omega) = \frac{1}{2}\int_\Omega|\nabla\boldsymbol{w}|^2\,\mathrm{d}\boldsymbol{z} &= \frac{1}{2}\int_\Omega\big(|\nabla w|^2 + w^2|\nabla\arg\boldsymbol{w}|^2\big)\,\mathrm{d}\boldsymbol{z}\\ &= \frac{1}{2}\int_\Omega\big(u_x^2+u_y^2+v_x^2+v_y^2\big)\,\mathrm{d}x\,\mathrm{d}y.\end{aligned} \tag{A.1}$$

We use the following lemmas.

LEMMA A.1 (Dirichlet energy of $\mathbb{S}^1$-maps in an annulus). *Consider an $\mathbb{S}^1$-map $\boldsymbol{u}\in H^1(A_{r,R})$. Let $d=\deg(\boldsymbol{u},\partial B_R)$, $\psi(\boldsymbol{z})=\arg\boldsymbol{u}(\boldsymbol{z})-d\arg\boldsymbol{z}$. Then the Dirichlet energy of $\boldsymbol{u}$ may be represented as*

$$\mathcal{D}(\boldsymbol{u},A_{r,R})=\mathcal{D}(\psi,A_{r,R})+\pi d^2\ln(R/r). \tag{A.2}$$

Proof. Since $|\boldsymbol{u}|=1$, $\mathcal{D}(\boldsymbol{u},A_{r,R})=\mathcal{D}(\arg\boldsymbol{u},A_{r,R})=\mathcal{D}(\psi+d\arg\boldsymbol{z},A_{r,R})$. Expanding the last expression we obtain

$$\mathcal{D}(\boldsymbol{u},A_{r,R})=\mathcal{D}(\psi,A_{r,R})+d\int_{A_{r,R}}\nabla\psi(\boldsymbol{z})\cdot\nabla\arg\boldsymbol{z}\,\mathrm{d}\boldsymbol{z}+\frac{d^2}{2}\int_{A_{r,R}}|\nabla\arg\boldsymbol{z}|^2\,\mathrm{d}\boldsymbol{z}. \tag{A.3}$$

The second term on the right-hand side of (A.3) is zero: integrate by parts using that $\arg\boldsymbol{z}$ is harmonic in $A_{r,R}$ and $\partial_\nu\arg\boldsymbol{z}=0$ on $\partial A_{r,R}$. The asserted formula (A.2) is then recovered computing the last term in (A.3) explicitly employing that $|\nabla\arg\boldsymbol{z}|=1/|\boldsymbol{z}|$. ∎

LEMMA A.2 (Multi-vortex maps). *Consider an $\mathbb{S}^1$-map $\boldsymbol{u}\in H^1_{\mathrm{loc}}(\Omega\setminus\{\boldsymbol{z}_1,\dots,\boldsymbol{z}_m\})$. Let $d_j=\deg(\boldsymbol{u},\boldsymbol{z}_j)$, $\sum d_j^2<\infty$. Suppose there exists a constant C such that for all sufficiently small r*

$$\mathcal{D}\big(\boldsymbol{u},\Omega\setminus\cup_{j=1}^m B_r(\boldsymbol{z}_j)\big)\le-\pi\sum_{j=1}^m d_j^2\ln r+C. \tag{A.4}$$

Then $\boldsymbol{u}$ is a multi-vortex map, i.e., it may be represented as

$$\boldsymbol{u}(\boldsymbol{z})=\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{z})}\prod_{j=1}^m\left[\frac{\boldsymbol{z}-\boldsymbol{z}_j}{|\boldsymbol{z}-\boldsymbol{z}_j|}\right]^{d_j}=\exp\Big\{\mathrm{i}\phi(\boldsymbol{z})+\mathrm{i}\sum_{j=1}^m d_j\arg(\boldsymbol{z}-\boldsymbol{z}_j)\Big\}$$
$$\text{with}\quad\nabla\phi\in L^2(\Omega). \tag{A.5}$$

Proof. Once some particular branch of $\arg(\cdot)$ is chosen, the function

$$\phi(\boldsymbol{z})=\arg\boldsymbol{u}(\boldsymbol{z})-\sum_{j=1}^m d_j\arg(\boldsymbol{z}-\boldsymbol{z}_j) \tag{A.6}$$

is well-defined (single-valued) in Ω, and satisfies equation (A.5). We have to prove that $\nabla\phi\in L^2(\Omega)$. Fix some j and represent the energy in the annulus $A_{r,R}(\boldsymbol{z}_j)$ as

$$\begin{aligned}\mathcal{D}\big(\boldsymbol{u},A_{r,R}(\boldsymbol{z}_j)\big)=&\mathcal{D}\big(\boldsymbol{u},\Omega\setminus\cup_{j=1}^m B_r(\boldsymbol{z}_j)\big)-\sum_{i=1,\ i\neq j}^m\mathcal{D}\big(\boldsymbol{u},A_{r,R}(\boldsymbol{z}_j)\big)\\&-\mathcal{D}\big(\boldsymbol{u},\Omega\setminus\cup_{j=1}^m B_R(\boldsymbol{z}_j)\big).\end{aligned} \tag{A.7}$$

Applying Lemma A.1 in the annuli $A_{r,R}(\boldsymbol{z}_i)$ we obtain $\mathcal{D}\big(\boldsymbol{u},A_{r,R}(\boldsymbol{z}_i)\big)\ge\pi d_i^2\ln(R/r)$, which together with the bound (A.4) implies

$$\mathcal{D}\big(\boldsymbol{u},A_{r,R}(\boldsymbol{z}_j)\big)\le-\pi d_j^2\ln r+C. \tag{A.8}$$

Using Lemma A.1 now in $A_{r,R}(\boldsymbol{z}_j)$, we obtain that ($\psi(\boldsymbol{z})$ below is defined as in Lemma A.1)

$$\mathcal{D}\big(\boldsymbol{u}, A_{r,R}(\boldsymbol{z}_j)\big) = \mathcal{D}\big(\psi, A_{r,R}(\boldsymbol{z}_j)\big) + \pi d_j^2 \ln(R/r) \le -\pi d_j^2 \ln r + C, \tag{A.9}$$

i.e., $\mathcal{D}(\psi, A_{r,R}(\boldsymbol{z}_j))$ is bounded as $r \to 0$ and thus $\nabla\psi \in L^2(B_R(\boldsymbol{z}_j))$. However for $\boldsymbol{z} \in B_R(\boldsymbol{z}_j)$,

$$\phi(\boldsymbol{z}) = \psi(\boldsymbol{z}) + \sum_{i=1,\ i\neq j}^{m} d_i \arg(\boldsymbol{z} - \boldsymbol{z}_i), \tag{A.10}$$

and since for sufficiently small R the right-hand side of formula (A.10) has no singularities in $B_R(\boldsymbol{z}_j)$, $\nabla\phi \in L^2(B_R(\boldsymbol{z}_j))$ for all j. At the same time $\boldsymbol{u} \in H^1(\Omega_R)$, where $\Omega_R = \Omega \setminus \cup_j B_R(\boldsymbol{z}_j)$, and since the right-hand side of (A.6) has no singularities in Ω_R, $\nabla\phi \in L^2(\Omega_R)$ and thus $\nabla\phi \in L^2(\Omega)$. ∎

LEMMA A.3 (Dirichlet energy of multi-vortex maps). *Let $\boldsymbol{u}$ be a multi-vortex map prescribed as in formula (A.5). Then, in the limit as $r \to 0$, its Dirichlet energy in $\Omega_r = \Omega \setminus \cup_j B_r(\boldsymbol{z}_j)$ admits the following asymptotic expansion:*

$$\begin{aligned}\mathcal{D}(\boldsymbol{u}, \Omega_r) = &-\pi \sum_{k=1}^{m} d_k^2 \ln r + \mathcal{D}(\phi, \Omega_r) - \pi \sum_{j,k=1,\ j\neq k}^{m} d_j d_k \ln|\boldsymbol{z}_j - \boldsymbol{z}_k| \\ &- \sum_{k=1}^{m} d_k \oint_{\partial\Omega} \ln|\boldsymbol{z} - \boldsymbol{z}_k| \, \partial_\tau \arg \boldsymbol{u}(\boldsymbol{z}) \, \mathrm{d}\ell(\boldsymbol{z}) \\ &- \frac{1}{2} \sum_{j,k=1}^{m} d_j d_k \oint_{\partial\Omega} \ln|\boldsymbol{z} - \boldsymbol{z}_j| \, \partial_\nu \ln|\boldsymbol{z} - \boldsymbol{z}_k| \, \mathrm{d}\ell(\boldsymbol{z}) + \mathcal{O}(r \ln r).\end{aligned} \tag{A.11}$$

Proof. First of all, observe the following simple identity:

$$\nabla \arg \boldsymbol{z} = \nabla_\perp \ln|\boldsymbol{z}| = \frac{(-y, x)}{|\boldsymbol{z}|^2}. \tag{A.12}$$

Substituting expression (A.5) into the formula for Dirichlet energy (A.1) and using (A.12) we obtain

$$\begin{aligned}\mathcal{D}(\boldsymbol{u}, \Omega_r) = \mathcal{D}(\phi, \Omega_r) &+ \sum_{k=1}^{m} d_k \int_{\Omega_r} \nabla\phi(\boldsymbol{z}) \cdot \nabla \arg(\boldsymbol{z} - \boldsymbol{z}_k) \, \mathrm{d}\boldsymbol{z} \\ &+ \frac{1}{2} \sum_{j,k=1}^{m} d_j d_k \int_{\Omega_r} \nabla \ln|\boldsymbol{z} - \boldsymbol{z}_j| \cdot \nabla \ln|\boldsymbol{z} - \boldsymbol{z}_k| \, \mathrm{d}\boldsymbol{z}.\end{aligned} \tag{A.13}$$

Integrating by parts using formula (A.12) and harmonicity of $\arg(\boldsymbol{z} - \boldsymbol{z}_k)$ and $\ln|\boldsymbol{z} - \boldsymbol{z}_k|$ in Ω_r, we obtain (recall that ∂_ν and ∂_τ denote the normal and tangential derivatives respectively)

$$\begin{aligned}\mathcal{D}(\boldsymbol{u}, \Omega_r) = \mathcal{D}(\phi, \Omega_r) &+ \sum_{k=1}^{m} d_k \oint_{\partial\Omega_r} \phi(\boldsymbol{z}) \, \partial_\tau \ln|\boldsymbol{z} - \boldsymbol{z}_k| \, \mathrm{d}\ell(\boldsymbol{z}) \\ &+ \frac{1}{2} \sum_{j,k=1}^{m} d_j d_k \oint_{\partial\Omega_r} \ln|\boldsymbol{z} - \boldsymbol{z}_j| \, \partial_\nu \ln|\boldsymbol{z} - \boldsymbol{z}_k| \, \mathrm{d}\ell(\boldsymbol{z}).\end{aligned} \tag{A.14}$$

Decomposing the integrals over $\partial\Omega_r$ into the integrals over $\partial\Omega$ and $\partial B_r(\boldsymbol{z}_l)$ ($l=1,\dots,m$) and employing the relations (A.16) below, we arrive at

$$\begin{aligned}\mathcal{D}(\boldsymbol{u},\Omega_r) =& -\pi\sum_{k=1}^m d_k^2\ln r+\mathcal{D}(\phi,\Omega_r)-\pi\sum_{j,k=1,\ j\neq k}^m d_jd_k\ln|\boldsymbol{z}_j-\boldsymbol{z}_k|\\ &+\sum_{k=1}^m d_k\oint_{\partial\Omega}\phi(\boldsymbol{z})\,\partial_\tau\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\mathrm{d}\ell(\boldsymbol{z})\\ &+\frac{1}{2}\sum_{j,k=1}^m d_jd_k\oint_{\partial\Omega}\ln|\boldsymbol{z}-\boldsymbol{z}_j|\,\partial_\nu\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\mathrm{d}\ell(\boldsymbol{z})+\mathcal{O}(r\ln r).\end{aligned}\tag{A.15}$$

Finally, we verify the assertion (A.11) integrating the first integral term in (A.15) by parts and using that $\phi=\arg\boldsymbol{u}-\sum_j d_j\arg(\boldsymbol{z}-\boldsymbol{z}_j)$. ∎

A few useful relations may be obtained via straightforward computation (estimate (A.16b) is obtained using integration by parts, the Cauchy-Schwarz inequality, and that $\big|\nabla\ln|\boldsymbol{z}|\big|=1/|\boldsymbol{z}|$):

$$\oint_{\partial B_r(\boldsymbol{z}_k)}\phi(\boldsymbol{z})\,\partial_\tau\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\mathrm{d}\ell(\boldsymbol{z})=0;\tag{A.16a}$$

$$\left|\oint_{\partial B_r(\boldsymbol{z}_l)}\phi(\boldsymbol{z})\,\partial_\tau\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\mathrm{d}\ell(\boldsymbol{z})\right|\le\frac{\sqrt{\pi}\,r\,\|\nabla\phi\|_{L^2(B_r(\boldsymbol{z}_l))}}{\big||\boldsymbol{z}_k-\boldsymbol{z}_l|-r\big|}=\mathcal{O}(r),\quad l\neq k;\tag{A.16b}$$

$$\left|\oint_{\partial B_r(\boldsymbol{z}_l)}\ln|\boldsymbol{z}-\boldsymbol{z}_j|\,\partial_\nu\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\mathrm{d}\ell(\boldsymbol{z})\right|\le 2\pi r\max_{\boldsymbol{z}\in\partial B_r(\boldsymbol{z}_l)}\frac{\big|\ln|\boldsymbol{z}-\boldsymbol{z}_j|\big|}{|\boldsymbol{z}-\boldsymbol{z}_k|}=\mathcal{O}(r),\quad l\neq j,k;\tag{A.16c}$$

$$\left|\oint_{\partial B_r(\boldsymbol{z}_j)}\ln|\boldsymbol{z}-\boldsymbol{z}_j|\,\partial_\nu\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\mathrm{d}\ell(\boldsymbol{z})\right|\le\frac{2\pi r|\ln r|}{\big||\boldsymbol{z}_j-\boldsymbol{z}_k|-r\big|}=\mathcal{O}(r\ln r),\qquad j\neq k;\tag{A.16d}$$

$$\oint_{\partial B_r(\boldsymbol{z}_k)}\ln|\boldsymbol{z}-\boldsymbol{z}_j|\,\partial_\nu\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\mathrm{d}\ell(\boldsymbol{z})=2\pi\ln|\boldsymbol{z}_k-\boldsymbol{z}_j|+\mathcal{O}(r),\qquad j\neq k;\tag{A.16e}$$

$$\oint_{\partial B_r(\boldsymbol{z}_k)}\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\partial_\nu\ln|\boldsymbol{z}-\boldsymbol{z}_k|\,\mathrm{d}\ell(\boldsymbol{z})=2\pi\ln r.\tag{A.16f}$$

The following theorem by Sandier [20] provides estimates on Dirichlet energy of $\mathbb{S}^1$-maps that are employed in our work.

THEOREM A.1 (Sandier '98, [20]). *Let $\bar\omega$ be a compact subset of a bounded domain $\Omega\subset\mathbb{C}$, $\boldsymbol{u}:\Omega\to\mathbb{S}^1$. Then*

$$\mathcal{D}(\boldsymbol{u},\Omega\setminus\bar\omega)\ge-\pi|d|\ln|\bar\omega|-C,\tag{A.17}$$

where C depends only on Ω and $H^{1/2+\epsilon}$ norm of $\boldsymbol{u}|_{\partial\Omega}$, and d is the winding number of $\boldsymbol{u}|_{\partial\Omega}$. Moreover, the energy of $\boldsymbol{u}$ may be localized: there exists $R>0$ (which depends on Ω) such that for any r satisfying $|\bar\omega|<r<R$, there exist k disjoint disks $\{B_j\}$, $j=1,\dots,k\le|d|$, with radii at most r such that

$$\mathcal{D}\big(\boldsymbol{u},\Omega\cap(\cup_{j=1}^k B_j)\setminus\bar\omega\big)\ge\pi|d|\ln(r/|\bar\omega|)-C,\tag{A.18}$$

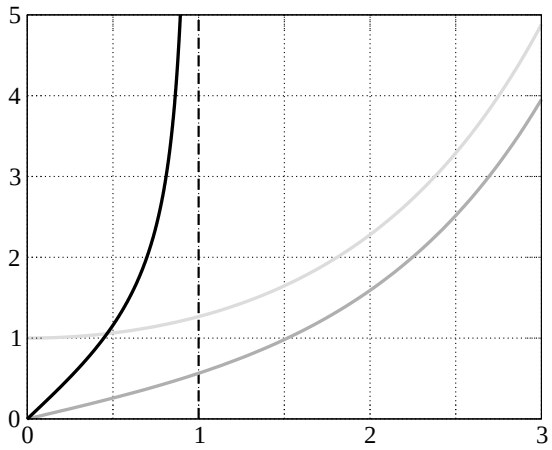

FIG. B.1. *Graphs of several special functions employed in this work. The light and dark grey lines, respectively, represent the modified Bessel functions* $\mathrm{I}_0(n)$, *and* $\mathrm{I}_1(n)$; *the black line corresponds to the function* $\mathrm{A}(n)$, *the inverse function of* $\mathrm{I}_1(n)/\mathrm{I}_0(n)$. $\mathrm{A}(n)$ *has a vertical asymptote at* $n=1$.

where C is the same constant as above.

Appendix B. Special functions and potential $W^\gamma(n)$. Finally, we review some properties of several special functions and provide more details regarding the potential $W^\gamma(n)$ employed in this work. These properties may be found in (or directly derived from) [1].

FACT B.1 (Sommerfeld representation of Bessel functions). *For any integer ν, we have*

$$\mathrm{I}_\nu(\boldsymbol{z}) = \frac{1}{\pi}\int_0^\pi \cos\nu\varphi\, \mathrm{e}^{\boldsymbol{z}\cos\varphi}\,\mathrm{d}\varphi. \tag{B.1}$$

FACT B.2 (Asymptotics of Bessel functions). *Let $|\arg\boldsymbol{z}|<\pi/2$, then for fixed ν, as $|\boldsymbol{z}|\to\infty$,*

$$\mathrm{I}_\nu(\boldsymbol{z}) \sim \frac{\mathrm{e}^{\boldsymbol{z}}}{\sqrt{2\pi\boldsymbol{z}}}\left[1-\frac{\mu-1}{8\boldsymbol{z}}+\frac{(\mu-1)(\mu-9)}{128\boldsymbol{z}^2}-\cdots\right], \qquad \mu=4\nu^2. \tag{B.2}$$

B.1. Properties of the potential. Recall, that potential $W^\gamma(n)$ is given by (its graphs are displayed in figure 1.1)

$$W^\gamma(n) = n\,\mathrm{A}(n) - \frac{\gamma n^2}{2} - \ln\mathrm{I}_0\big(\mathrm{A}(n)\big) + C_\gamma. \tag{B.3}$$

Here the function $\mathrm{A}(n)$ is the inverse function of $\mathrm{I}_1(n)/\mathrm{I}_0(n)$, see figure B.1 for the graphs. The constant C_γ is chosen so that $W^\gamma(n)\geq 0$ with equality achieved at $n=n^\gamma_{\mathrm{eq}}$, where n^γ_{eq} is the (nonzero for $\gamma>2$) solution of $\gamma n=\mathrm{A}(n)$. From the basic properties of Bessel functions (see above) it is not hard to establish the following facts:

FACT B.3 (Asymptotics of C_γ). *From the expansion (B.2) it is straightforward to establish that as* $n \nearrow 1$, $\mathrm{A}(n) = 1/[2(1-n)] + \mathcal{O}(1)$, *which implies that as* $\gamma \to \infty$, $n_{\mathrm{eq}}^{\gamma} = 1 - 1/2\gamma + \mathcal{O}(1/\gamma^2)$ *and*

$$C_\gamma = \frac{\gamma}{2} + \mathcal{O}(\ln\gamma). \tag{B.4}$$

FACT B.4 (Lower bound on the potential $W^\gamma(n)$). *From (B.1) we immediately get that* $\mathrm{I}_0'(n) = \mathrm{I}_1(n)$, *and thus* $\big[n\mathrm{A}(n) - \ln \mathrm{I}_0\big(\mathrm{A}(n)\big)\big]' = \mathrm{A}(n) \geq 0$. *This, in turn, implies that* $n\mathrm{A}(n) - \ln \mathrm{I}_0\big(\mathrm{A}(n)\big) \geq 0$ *and therefore for all* $n \in [0,1)$,

$$W^\gamma(n) \geq C_\gamma - \frac{\gamma n^2}{2} \geq \frac{\gamma}{2}(1-n^2) + \mathcal{O}(\ln\gamma). \tag{B.5}$$

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