A VARIATIONAL THEORY FOR POINT DEFECTS IN PATTERNS

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ABSTRACT. We derive a rigorous scaling law for minimizers in a natural version of the regularized Cross-Newell model for pattern formation far from threshold. These energy-minimizing solutions support defects having the same character as what is seen in experimental studies of the corresponding physical systems and in numerical simulations of the microscopic equations that describe these systems.

1. Introduction

This paper reports on some recent progress that has been made in the analytical modeling of defect formation, far from threshold, in pattern forming physical systems. We will take a moment here to very briefly sketch the physical and mathematical background that motivates what is done in this paper.

The relevant class of pattern-forming physical systems to consider are those in which the spatial physical field can be described as planar and the first bifurcation from a homogeneous state, having arbitrary translational symmetry in the plane, produces a striped pattern which has only a discrete periodic symmetry in one direction. This symmetry-breaking occurs at a critical threshold; above this threshold the pattern can deform and, further away, defects can form. It is the desire to understand and model this process of defect formation that motivates our study.

A good particular example of these kinds of physical systems is a high Prandtl number Rayleigh-Bénard convection experiment. The critical threshold in this example is the critical Rayleigh number at which fluid convection is initiated from the sub-threshold homogeneous conducting state. The ”striped pattern” here can be taken to be the horizontal cross-section of the temperature field at the vertical midpoint of the experimental cell in which convection rolls have formed.

Because of its periodic structure, the striped pattern can be described in terms of a periodic form function of a phase, \( \theta = \vec{k} \cdot \vec{x} \), where the magnitude of \( \vec{k} \) is the wavenumber of the pattern and the orientation of \( \vec{k} \) is perpendicular to the stripes. Here \( \vec{x} = (x, y) \) is a physical point in the plane. Even though the striped pattern will deform far from threshold, over most of the field (and in particular away from defects) it can be locally approximated as a function of a well-defined phase, \( \theta(\vec{x}) \), for which a local wavevector can be defined as \( \vec{k} = \nabla \theta \) which differs little from a constant vector unless one varies over distances on the order of many stripes in the pattern. This slowly-varying feature of pattern formation far from threshold motivates the introduction of a modulational ansatz in the microscopic equations describing these physical systems from which an order parameter equation for the behavior of the phase can be formally derived. This was originally done by Cross and Newell [3]. These equations are variational and from our perspective it is advantageous to
study their solutions by studying the behavior of the minimizers of the variational problem. The version of the variational problem that we study corresponds to the following energy functional on a given domain \( \Omega \) with specified Dirichlet boundary values.

\[
(1) \quad \mathcal{E}_\mu(\Theta) = \mu \int_{\Omega} (\Delta \mathbf{X} \Theta)^2 d\mathbf{X} + \frac{1}{\mu} \int_{\Omega} (1 - |\nabla \mathbf{X} \Theta|)^2 d\mathbf{X},
\]

which is expressed in terms of slow variables stemming from the modulational ansatz mentioned above: \( \mathbf{X} = (X, Y) = (\mu x, \mu y); \Theta = \frac{a}{\mu} \).

We refer to this functional as the regularized Cross-Newell (RCN) Energy. It consists of two parts: a non-convex functional of the gradient (the CN part) plus a quadratic functional of the Hessian matrix of \( \Theta \), which is the regularizing singular perturbation. Without this regularization, the CN variational equations admit non-physical caustic formation. Instead, by studying the limit of minimizers of \( \mathcal{E}_\mu \) as \( \mu \to 0 \), one may be able to identify the formation of a physical defect as a limiting jump discontinuity or other kind of singularity in the wavevector field associated to the \( \mu \)-indexed family of minimizing phase fields.

For more details on what has been rather tersely outlined above, we refer the reader to [4] where analytical results on the asymptotic limit of minimizers for RCN and their defects in certain geometries are also derived. See also [6] where further refinements and generalizations are developed. We further mention that the variational problem associated to (1) also arises in other physical contexts (unrelated to pattern formation) where it is known as the Aviles-Giga energy [2].

We now turn to the focus of this paper. The kind of defects that are seen to arise far from threshold are not supported by asymptotic minimizers of (1) if the class of functions over which one is varying is restricted to be single-valued phases. In particular, one can see for purely topological reasons that this restriction rules out disclinations [4]. In [5], physical, numerical and experimental arguments are developed which make a strong case in support of the hypothesis that the correct order parameter model for the phase in pattern forming systems far from threshold should come from a variational problem admitting test functions which are multi-valued and in particular two-valued. In physical parlance this is often expressed by saying that the wavefield \( \mathbf{k} \) should be allowed to be a director field; i.e. an unoriented vector field. One figure (see Fig. 1 below) from [5] will help to crystallize the issue and the focus of this paper.

This figure shows seven numerical simulations, each done in a horizontal strip, of a solution to the Swift-Hohenberg equation which is a generic model of microscopic equations for a pattern forming system. Each of these is run far from threshold but with differing boundary conditions imposed at the edges. In each case the boundary conditions impose a constant orientation of the stripe at the edges such that the normal to the stripe is \((\cos(\alpha), \sin(\alpha))\) along the top edge and \((\cos(\alpha), -\sin(\alpha))\) along the bottom edge. The only thing that changes from one simulation to the next is the value of \( \alpha \) which in the figure is recorded on the left in each respective cell. The results of [4] together with symmetry considerations establish that for an analogous domain and boundary values, the asymptotic minimizers of (1), within the class of single-valued phases, should have the form shown in the bottom-most cell of Figure (1). That is, they should have wavevectors very close to \((\cos(\alpha), \sin(\alpha))\) in the upper region of the cell and very close to \((\cos(\alpha), -\sin(\alpha))\) in the lower region of the
Figure 1. The “Swift-Hohenberg” zippers. The patterns are determined by minimizing the Swift-Hohenberg energy functional for various choices of the angle $\alpha$ that determines the slopes of the stripe patterns as $y \to \pm \infty$.

cell with a boundary layer around the mid-line in which the wavevector transitions smoothly but rapidly from one state to the other. These minimizers are dubbed knee solutions in [4] and in the limit as $\mu \to 0$, they tend to a configuration in which there is a sharp jump in the wavevector along the mid-line. This kind of defect is called a grain boundary. In other words, the theory for (1) with single-valued phases predicts that the grain boundary should be the limiting defect independent of the value of $\alpha$. The different result appearing in Figure (1) was one of the pieces of evidence sited in [5] to argue the necessity for the larger variational class of multi-valued phases, even in such simple geometries as those of Figure (1). In this paper we are going to carry out a careful analytical study of the RCN variational problem in exactly this geometry but within a larger class of two-valued phases. We will
firmly establish that the form of the asymptotic minimizers in this more general model does in fact depend non-trivially on $\alpha$. In addition, the construction of test functions in section 3 and the numerical simulations in section 5 gives some intuitive and experimental support to the belief that the stable solutions of the RCN equations qualitatively resemble what is seen in the Swift-Hohenberg simulations. In [5], the term Swift-Hohenberg “zippers” was coined to refer to the problem studied in Figure (1). In this paper we will be studying Cross-Newell zippers.

2. Setup

We are given an angle $\alpha$ that determines the boundary conditions on the pattern as $y \to \pm \infty$ by

$$\nabla \theta \to (\cos(\alpha), \pm \sin(\alpha))$$

as $y \to \pm \infty$.

Note that this differs from the setup underlying the Swift-Hohenberg zippers in that the boundary conditions are placed at $\pm \infty$ in the $y$-direction rather than at finite values of $y$. This simplifies our technical considerations in that we don’t need to worry about adjusting the location of these boundaries as $\alpha$ changes. Also, all of the patterns we want to consider here are shift-periodic in the $x$-direction. This allows us to reduce our study to domains that are periodic in $x$. We introduce the (small) parameter $\epsilon = \cos(\alpha)$ and we define the period $l = \pi/\epsilon$. We consider the following variational problem on the strip $S^\epsilon \equiv \{(x, y)|0 \leq x < l, y \geq 0\}$:

Minimize $F^\epsilon[\theta; a, \delta]$ given by

$$F^\epsilon[\theta; a, \delta] = \int \int_{S^\epsilon} \left\{[\Delta \theta]^2 + (1 - |\nabla \theta|^2)^2\right\} dxdy$$

over all $a \in [0, 1], \delta \in \mathbb{R}$ and $\theta$ satisfying the boundary conditions

(2)

$$\begin{align*}
\theta(x, 0) &= 0 \quad \text{for } 0 \leq x < al; \\
\theta_y(x, 0) &= 0 \quad \text{for } al \leq x < l; \\
\theta(x, y) - \epsilon x &\text{ is periodic in } x \text{ with period } l \text{ for each } y \geq 0; \\
\theta(x, y) - \left[\epsilon x + \sqrt{1 - \epsilon^2}y + \delta\right] &\in H^2(S^\epsilon).
\end{align*}$$

We take a moment here to explain the considerations that have motivated the mixed Dirichlet-Neumann boundary conditions here, the first two boundary conditions in (2) above. We argued in the introduction that in order to capture the physically relevant minimizers, the RCN variational problem needed to allow for multi-valued phases in its admissible class of test functions. However, the numerical results on the Swift-Hohenberg zippers suggest that in certain symmetrical geometries the appropriate multi-valuedness can be introduced in a tractable fashion. Indeed in the case of the SH zippers we see that the symmetry of the boundary conditions between the upper and lower edges of the domain is preserved in the symmetry of all of the exhibited solutions about the middle horizontal axis; i.e., the reflection in $y$ about the $y=0$ axis. This suggests that a single-valued phase could describe the solution in the upper half-plane with the solution in the lower half-plane given as a symmetric reflection of that in the upper half-plane about $y=0$.

Figure 2 illustrates two instances of the form that we expect these zippers to take in the infinite (in $y$) geometry. The figure on the left illustrates level curves (stripes in the parlance
of the introduction) of what we will shortly define to be a *self-dual knee solution*. This is indeed symmetric about the mid-axis, which we will take to be the $y = 0$ axis; moreover, one can see that its gradient field along $y = 0$ is tangential to this axis. Thus the gradient field in the upper half-plane is completely symmetrical to that in the lower half-plane under reflection about $y = 0$.

However, for the striped pattern on the right in figure 2, this is not the case. There are regions, illustrated for example by the darkened interval along $y = 0$, where the gradient field is tangential to this axis; but, there are other regions, illustrated for example by the lightened interval along $y = 0$, where the gradient field needs to be perpendicular to this axis. By reflection symmetry this field will point upwards in the upper half-plane and downward in the lower half-plane. This cannot be supported by a vector field but it is allowable for a director field. This indicates that in this region a two-valued phase is required.

To get at the conditions on the phase itself we observe that patterns of the type illustrated here are analytically given in terms of a form function $F$ of the phase $\theta = \theta(x, y)$ such that $F$ is locally periodic of period $2\pi$ in $\theta$ and such that $F(\theta(x, y))$ is even in $y$ and smooth in $(x, y)$. In order to allow $\theta$ to be two-valued we also require $F$ to be even in $\theta$. (An example of a global form function having these properties is $F = \cos$.) It follows from these requirements that either $\theta(x, y)$ is even in $y$, in which case $\theta_y(x, 0) = 0$, a Neumann boundary condition; or, $\theta(x, y)$ is an odd function of $y$ modulo $\pi$, in which case $\theta_y(x, 0) = n\pi$ for some integer $\pi$, a Dirichlet boundary condition. Thus to realize the pattern on the right in figure 2 in terms of a single-valued phase in the upper half-plane, we would need to take the Neumann boundary condition on the darkened interval and the Dirichlet boundary condition on the lightened interval. This is what we have done in (2). For the self-dual knee pattern on the left we would take the entire boundary condition to be Neumann.

The functional $\mathcal{F}'$ is the RCN energy functional but with the scaling $\mu$ removed. It is appropriate to do this because the demonstration that the nature of the RCN minimizers depends on $\alpha$ is independent of this scaling. The first and the second conditions impose
a mixed Dirichlet/Neumann boundary condition at \( y = 0 \), the third condition imposes (shifted-) periodicity in \( x \) and the last condition ensures that the test functions \( \theta \) approach the straight parallel roll patterns \( \epsilon x + \sqrt{1 - \epsilon^2} y + \delta \) as \( y \to \infty \).

Note that the dependence of the functional \( F^\epsilon \) on the parameter \( \epsilon \) is through the dependence of the domain \( S^\epsilon \) and the boundary conditions on \( \epsilon \). The parameters \( a \) and \( \delta \) are determined by minimization. The parameter \( a \) is a measure of the fraction of the boundary at \( y = 0 \) that has a Dirichlet boundary condition, and \( \delta \) represents the asymptotic phase shift, that is the difference in phases between the test function \( \theta \) and the roll pattern \( \hat{\theta}(x, y) = \epsilon x + \sqrt{1 - \epsilon^2} y \) which satisfies \( \hat{\theta}(0, 0) = \theta(0, 0) = 0 \).

The case where \( a \) is set to zero is considered in earlier references [4]. The test functions \( \theta(x, y) \) satisfy a pure Neumann boundary condition at \( y = 0 \) and the minimizers in this case are the self-dual knee solutions

\[
\theta_{\text{neu}}(x, y) = \epsilon x + \log(\cosh(\sqrt{1 - \epsilon^2} y)).
\]

These solutions have an asymptotic phase shift of \( -\log(2) \) and the energy of the minimizers in the strip \( S^\epsilon \) is given by

\[
(3) \quad F^\epsilon[\theta_{\text{neu}}, 0, -\log(2)] = \frac{4\pi \sqrt{1 - \epsilon^2}}{3\epsilon}.
\]

The existence of \( (\theta^\epsilon, a^\epsilon, \delta^\epsilon) \) minimizing \( F^\epsilon \) can be shown from the direct method in the calculus of variations. We also prove the following results about the minimizers, and their energy –

**Theorem 2.1. Upper bound**

There is a constant \( E_0 \) such that \( F^\epsilon[\theta^\epsilon; a^\epsilon, \delta^\epsilon] \leq E_0 \) for all \( \epsilon \in (0, 1] \).

We prove this result in sec. 3 by exhibiting an explicit test function satisfying this bound. Note the implication that the minimizers for sufficiently small \( \epsilon \) cannot be the self-dual solutions, since the energy in Eq. (3) diverges as \( \epsilon \to 0 \). Consequently, \( a^\epsilon > 0 \) for sufficiently small \( \epsilon \).

**Theorem 2.2. Lower bound**

There are constants \( E_1 > 0 \) and \( \epsilon_0 > 0 \) such that, even for the optimal test function \( \theta^\epsilon \) and the optimal parameter values \( a^\epsilon \) and \( \delta^\epsilon \), we have \( F^\epsilon[\theta^\epsilon; a^\epsilon, \delta^\epsilon] \geq E_1 \) for all \( \epsilon \leq \epsilon_0 \). Further, there are constants \( 0 < \alpha_1 < \alpha_2 \) such that \( 1 - \alpha_2 \epsilon < a^\epsilon < 1 - \alpha_1 \epsilon \) for sufficiently small \( \epsilon \).

We prove this result in sec. 4. Combining this result with the preceding theorem, we obtain a rigorous scaling law for the energy of the minimizer, and for the quantity \( (1 - a) \) as \( \epsilon \to 0 \). As a corollary to Theorem 2.2, we find that an \( O(1) \) part of the energy of the minimizer concentrates on the set, \( al \leq x \leq l, 0 \leq y \leq 1 \). This can be interpreted as saying that a nontrivial part of the energy of the minimizer lives in the region of the convex-concave disclination pair [5].

3. Upper bound

We will first show an upper bound for the energy functional \( F^\epsilon \), uniform in \( \epsilon \), by constructing a family of explicit test function whose energy is uniformly bounded. The idea for the construction of these test functions comes from the self-dual ansatz [4] which requires that
the energy density of the functional $F$ should be *equi-partitioned* between its two terms. Functions satisfying this ansatz solve the self-dual (resp., anti-self-dual) equation:

$$\Delta \theta = \pm (1 - |\nabla \theta|^2).$$

Solutions of this equation can be constructed via the logarithmic transform

$$\theta = \pm \log u$$

which reduces (4) to the linear Helmholtz equation (5). We refer the reader to [4, 6] for more background on self-dual reduction.

### 3.1. Self-dual test functions for the CN-Zipper problem.

#### 3.1.1. Existence.

We consider the Helmholtz equation in the upper half-plane,

$$\Delta u - u = 0$$

subject to the mixed boundary conditions

$$u(x, 0) = e^{-n\pi} \quad n\ell < x < (n + a)\ell$$

$$u_y(x, 0) = 0 \quad (n + a)\ell \leq x \leq (n + 1)\ell$$

and with asymptotic behavior for large $y$ given by $\text{const.} \exp(-\epsilon x - \sqrt{1 - \epsilon^2} y)$ where $\ell = \pi/\epsilon$ and $a \in (0, 1)$.

We seek a shift-periodic solution, meaning that we change variables to $w = e^{\epsilon x} u(x, y)$ and look for periodic solutions of

$$Lw = \Delta w - 2\epsilon \partial_x w - (1 - \epsilon^2) w = 0,$$

with boundary conditions of periodicity in $x$ of period $\ell$; mixed boundary conditions at $y = 0$,

$$w(x, 0) = e^{\epsilon x} \quad 0 < x < a\ell$$

$$w_y(x, 0) = 0 \quad a\ell \leq x \leq \ell,$$

and with asymptotic behavior for large $y$ given by $\text{const.} \exp(-\sqrt{1 - \epsilon^2} y)$. Given such a $u$, $\theta = -\log u$ would satisfy the boundary conditions (2). (However, for notational simplicity, in the remainder of this section we will set $\theta = \log u$.)

We now let $S^\epsilon$ denote the half-cylindrical domain, $\ell$-periodic in $x$ and with $y > 0$. The existence of a weak solution to (8) satisfying the above boundary conditions can be established via the Lax-Milgram theorem with appropriate energy estimates. However, in order to derive uniform asymptotic energy estimates (as $\epsilon \to 0$) for the CN Zipper problem we need to go beyond existence results and try to construct a more explicit representation of the solution to (5). Unfortunately, at present, the solutions one can construct using Greens function methods and the like do not yield sufficient a priori boundary regularity near $y = 0$ to control the asymptotic behavior of the energy in this finite part of $S^\epsilon$. We will therefore instead study solutions of a self-dual problem with modified boundary conditions (more precisely, with pure Dirichlet boundary conditions). Subsequently we will make a local modification of these solutions near the boundary to produce functions (no longer global self-dual solutions) whose asymptotic energy we can control and which are valid test functions for the Cross-Newell Zipper problem.

The modified boundary value problem we consider is (8) with (9-10) replaced by the pure Dirichlet boundary condition
\[
\begin{aligned}
\tag{9'}
w(x, 0) &= \begin{cases}
  e^{\epsilon x} & 0 < x < a\ell \\
  q_0(x) & a\ell \leq x \leq \ell
\end{cases}
\end{aligned}
\]

where \( q_0(x) \) is a function which smoothly interpolates, up through second derivatives, between \( e^{\epsilon x} \) at \( x = a\ell \) on the left and \( e^{\epsilon x - \pi} \) at \( x = \ell \) on the right. There are clearly many choices for such a function; the precise choice for our purposes will be made later at the end of subsection 3.2. By elliptic regularity \([7]\), the solution to this boundary value problem satisfies \( w(x, y) \in H^2(S^\epsilon) \). In the following sections we will construct the solutions to this problem and study its asymptotics relative to the RCN energy \( \mathcal{F}^\epsilon \).

3.1.2. Explicit Construction. The whole plane Green’s function for the Helmholtz equation (5) is explicitly given in terms of the Bessel potential \([7]\):

\[
\tag{11}
G(x, y; \xi, \eta) = \frac{1}{4\pi} \int_0^\infty e^{-t} \frac{dt}{t} \exp \left( -\frac{1}{4t} \{ (x - \xi)^2 + (y - \eta)^2 \} \right).
\]

In terms of this Green’s function we can then represent a solution to (5), with asymptotic behavior for large \( y \) given by const. \( \exp(-\epsilon x - \sqrt{1 - \epsilon^2|y|}) \), as

\[
\tag{12}
u^\epsilon(x, y) = \int_{-\infty}^\infty \rho^\epsilon(\xi) G(x, y; \xi, 0) d\xi.
\]

Note that

\[
\tag{13}
u^\epsilon_y(x, y) = \int_{-\infty}^\infty \rho^\epsilon(\xi) G_y(x, y; \xi, 0) d\xi
= -\int_{-\infty}^\infty \rho^\epsilon(\xi) G_\eta(x, y; \xi, 0) d\xi
\]

solves (5) with respect to the standard Dirichlet boundary condition which equals minus the jump of \( u^\epsilon_y \) along the \( x \)-axis. One may check directly (see (22)) that in fact \( \rho^\epsilon(\xi) = -2u^\epsilon_y(\xi, 0) \) almost everywhere. Integrating (13) with respect to \( y \) gives

\[
\tag{14}
u^\epsilon(x, y) + f(x) = \int_{-\infty}^\infty \rho^\epsilon(\xi) G(x, y; \xi, 0) d\xi.
\]

Since both \( u^\epsilon(x, y) \) and the RHS of (14) decay as \( y \uparrow \infty \), it follows that \( f(x) \equiv 0 \). This is consistent with the ansatz (12), taking \( \rho^\epsilon(\xi) \) to be the jump in the normal derivative of \( u^\epsilon \) along \( y = 0 \).

We make the following shift-periodic ansatz for \( \rho^\epsilon \),

\[
\rho^\epsilon(\xi + \ell)e^{\epsilon(\xi+\ell)} = \rho^\epsilon(\xi)e^{\epsilon\xi}.
\]

With this one can expand out (12) more explicitly as
\[ u^\epsilon(x, y) = \]

\[ (15) \quad \frac{1}{4\pi} \sum_{n \in \mathbb{Z}} \int_0^\infty \frac{dt}{t} e^{-(t + \frac{\epsilon^2}{4t})} \int_{n\ell}^{(n+1)\ell} \rho^\epsilon(\xi) \exp \left( \frac{(x - \xi)^2}{-4t} \right) d\xi \]

\[ (16) \quad \frac{1}{4\pi} \sum_{n \in \mathbb{Z}} \int_0^\infty \frac{dt}{t} e^{-(t + \frac{\epsilon^2}{4t})} \int_0^\ell e^{-n\pi \rho^\epsilon(\xi)} \exp \left( \frac{(x - (\xi + n\ell))^2}{-4t} \right) d\xi \]

\[ (17) \quad \frac{1}{4\pi} \int_0^\infty \frac{dt}{t} e^{-(t + \frac{\epsilon^2}{4t})} \int_0^\ell \rho^\epsilon(\xi) \sum_{n \in \mathbb{Z}} e^{-n\pi} \exp \left( \frac{(x - (\xi + n\ell))^2}{-4t} \right) d\xi \]

\[ (18) \quad \frac{e^{-\epsilon x}}{\sqrt{4\pi}} \int_0^\infty \frac{dt}{t} e^{-(1 - e^2)t + \frac{\epsilon^2}{4t^2}} \int_0^\ell d\xi \rho^\epsilon(\xi) e^{\epsilon \xi} \sum_{n \in \mathbb{Z}} \exp \left( \frac{((x - 2\epsilon t) - (\xi + n\ell))^2}{-4t} \right) \]

\[ (19) \quad \frac{e^{-\epsilon x}}{\sqrt{4\pi}} \int_0^\infty \frac{dt}{t^2} e^{-(1 - e^2)t + \frac{\epsilon^2}{4t^2}} \frac{1}{\ell} \int_0^\ell \rho^\epsilon(\xi) e^{\epsilon \xi} \vartheta_3 \left( \frac{-(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\pi t}{\ell^2} \right) d\xi \]

In (15) we have interchanged the order of integration which is justified by Tonelli’s Theorem; in (16) we’ve made the substitution \( \xi = \xi_n + n\ell \) and in (17) we’ve commuted the sum past the integrals which is justified by monotone convergence—all terms in the series are positive and hence the partial sums are monotonic. In (18) we write each summand as a single exponential and then appropriately complete the square in each exponent. Finally in (19) we apply Jacobi’s identity \([9]\). Here \( \vartheta_3 \) is one of the Jacobi theta functions, in this setting explicitly given as

\[ (20) \quad \vartheta_3 \left( \frac{-x + 2\epsilon t}{\ell}, \frac{-4\pi t}{\ell^2} \right) = 1 + 2 \sum_{n=1}^\infty e^{-\left(\frac{2\pi}{\ell}\right)^2 n^2 t} \cos \left( \frac{2\pi n}{\ell} \left( x - \frac{2\pi t}{\ell} \right) \right) \]

Finally, from (19) we can express our candidate for the solution to (8), (9’ – 10’) as

\[ (21) \quad w^\epsilon(x, y) = \frac{1}{\sqrt{4\pi}} \int_0^\infty \frac{dt}{t^2} e^{-(1 - e^2)t + \frac{\epsilon^2}{4t^2}} \frac{1}{\ell} \int_0^\ell \rho^\epsilon(\xi) \vartheta_3 \left( \frac{-(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\pi t}{\ell^2} \right) d\xi, \]

where \( \rho^\epsilon(\xi) = \rho^\epsilon(\xi) e^{\epsilon \xi} \).

3.1.3. Data Characterization, periodized and in Fourier Space. From the previous sections we have that \( \rho^\epsilon(\xi) \) is periodic of period \( \ell \); also \( w^\epsilon(x, y) \) is periodic in \( x \) of period \( \ell \) and \( = e^{\epsilon x} \) along \((0, \ell)\) when \( y = 0 \).

Moreover, taking the Fourier transform of (21) one finds that the Fourier coefficients, in \( x \), must satisfy

\[ (22) \quad \{w^\epsilon(x, y)\}(n, y) = \frac{1}{2} \frac{1}{\sqrt{1 + e^2(2n + i)^2}} \{p^\epsilon(\xi)\}(n) e^{-\sqrt{1 + e^2(2n + i)^2} y} \]

for each value of \( y \). Taking the limit as \( y \to 0 \) on both sides of (22) gives

\[ (23) \quad \{w^\epsilon(x, 0)\}(n) = \frac{1}{2} \frac{1}{\sqrt{1 + e^2(2n + i)^2}} \{p^\epsilon(\xi)\}(n). \]

This is a determining conditions for \( \rho^\epsilon(\xi) \). We note that differentiating (22) with respect to \( y \) and setting \( y = 0 \) demonstrates that \( \rho^\epsilon(x) = -2w^\epsilon_y(x, 0) \), at least in the \( L^2 \) sense.
Since \( w^\epsilon(x, 0) \in H^2(S^1) \), it follows, by comparison, that \( 2\sqrt{1 + \epsilon^2(2n + i)^2}\hat{w}^\epsilon(n) \in h^1(\mathbb{Z}) \). Given this we can now define

\[
(24) \quad p^\epsilon(x) = \left\{ 2\sqrt{1 + \epsilon^2(2n + i)^2}\hat{w}^\epsilon(n) \right\} \vee (x)
\]

which characterizes \( p^\epsilon \) as an element of \( H^1(S^1) \). It follows from Sobolev’s lemma \([7]\) that \( p^\epsilon \) can be taken to be continuous. This last observation also justifies the existence of the Fourier coefficients \( \{ \hat{p}^\epsilon \} (n) \) that were formally introduced in (22).

### 3.1.4. Large \( y \) asymptotics.

We now determine the large \( y \) asymptotics of (12). By (22), \( w^\epsilon \) has a Fourier representation given by

\[
\hat{w}^\epsilon(n) = \left. \sum_{n \in \mathbb{Z}} \hat{w}^\epsilon(n) e^{-\sqrt{1+\epsilon^2(2n+i)^2} y} e^{2\pi inx} \right|_{\tilde{\Theta}^\epsilon}.
\]

(We note that for large \( y \) this series converges uniformly to a smooth, in fact real-analytic, function of \( x \).) Moreover, \( \hat{w}^\epsilon(0) = \frac{1}{\ell} \int_0^\ell w^\epsilon(x, 0) \, dx \) is non-zero since by the maximum principle \([7]\) applied to the elliptic PDE (8) on the cylinder \([0, \ell] \times (-\infty, \infty)\), the integrand, \( w^\epsilon(x, 0) \), is non-negative and in fact, by \((9' - 10')\), non-vanishing on \([0, \ell]\) (the definition of \( q_\Theta \) which we give later will insure that this is so).

### 3.2. Energy Estimates.

We will now try to show that the regularized Cross-Newell energy of \( \theta(x, y) = \log u(x, y) \) is uniformly bounded in \( \epsilon \). This would establish a uniform (in \( \epsilon \)) upper bound for the energy minimizers. Recall that the energy is calculated by integrating the energy density over the domain \( S^\epsilon \). Making this estimate breaks naturally into the consideration of two regions: \([0, \ell] \times \{ y \geq M_\epsilon \} \) and \([0, \ell] \times \{ y < M_\epsilon \} \) where \( M_\epsilon \) is to be determined.

We remark that the so-called ”knee solution” of the self-dual equation provides an upper bound for the energy for values of \( \epsilon \) bounded away from zero. So we only need to be concerned with small values of \( \epsilon \). Since \( u^\epsilon(x, y) = e^{-\epsilon\theta} w^\epsilon(x, y) \) solves the Helmholtz equation, it will suffice to bound the density \((1 - |\nabla \theta^\epsilon|^2)^2\) (since the integral of this density equals that of \((\Delta \theta^\epsilon)^2\) for self-dual solutions).

#### 3.2.1. Estimates in \([0, \ell] \times \{ y \geq M_\epsilon \} \).

We begin by considering the domain for large \( y \). Since

\[
\nabla \theta^\epsilon(x, y) = \frac{\nabla u^\epsilon(x, y)}{u^\epsilon(x, y)} = \left( \begin{array}{c} -\epsilon \\ 0 \end{array} \right) + \frac{\nabla w^\epsilon(x, y)}{w^\epsilon(x, y)},
\]

we may reduce our considerations to studying the asymptotics of \( w^\epsilon \) and its first derivatives. It will be convenient to replace the convolution integral in (21) by the Fourier series whose coefficients are the product of the Fourier coefficients of \( p^\epsilon \) and the \( \vartheta_3 \) series. This results in the following alternative representation of \( w^\epsilon \):

\[
w^\epsilon(x, y) = \frac{1}{\sqrt{4\pi}} \sum_{n \in \mathbb{Z}} \int_0^\infty \frac{dt}{t^{\frac{1}{2}}} e^{-\left(1+\epsilon^2(2n+i)^2\right)t+i\frac{x^2}{t}} \hat{p}^\epsilon(n) e^{2\pi inx}.
\]
With the change of variables, 

\[ s = \frac{t}{y} \]

this representation takes the form

\begin{equation}
(25) \quad w^\theta(x, y) = \sqrt{\frac{y}{4\pi}} \sum_{n \in \mathbb{Z}} \frac{1}{s_n} e^{-\frac{y}{s_n}} \int_{-1}^{\infty} \frac{dz}{(1 + z)^{\frac{s_n}{2}}} e^{-\frac{y}{s_n} \left(z^2 + O(z^3)\right)} \hat{P}(n) e^{2\pi inz},
\end{equation}

where \( s_n = \frac{1}{2\sqrt{1 + \epsilon^2(2n + 1)^2}} \). The critical point of the exponent is \( s = s_n \) and the expansion of the exponent in the \( nth \) term of the series near this critical point has the form

\[ \frac{s}{s_n^2} + \frac{1}{s} = \frac{2}{s_n} \left(1 + \frac{(s - s_n)^2}{s_n^2} + O\left(\frac{(s - s_n)^3}{s_n^3}\right)\right). \]

An asymptotic expansion in large \( y \) may be developed for the integral in each term of the series \( (25) \) by the method of Laplace. By the uniform convergence of the series (for large \( y \), the asymptotic expansion of the series is equivalent to the sum of the asymptotic expansions from each term. We implement this strategy to find the leading order, large \( y \) behavior, and next corrections, for \( w^\theta, w^\xi \) and \( w^\eta \):

\[ w^\xi(x, y) = \sqrt{\frac{y}{4\pi}} \sum_{n \in \mathbb{Z}} \frac{1}{s_n} e^{-\frac{y}{s_n}} \int_{-1}^{\infty} \frac{dz}{(1 + z)^{\frac{s_n}{2}}} e^{-\frac{y}{s_n} \left(z^2 + O(z^3)\right)} \hat{P}(n) e^{2\pi inz}, \]

\[ w^\eta(x, y) = \frac{1}{2y} w^\xi - \frac{1}{2} \sqrt{\frac{y}{4\pi}} \sum_{n \in \mathbb{Z}} s_n^{-\frac{1}{2}} e^{-\frac{y}{s_n^2}} \int_{-1}^{\infty} \frac{dz}{(1 + z)^{\frac{s_n}{2}}} e^{-\frac{y}{s_n^2} \left(z^2 + O(z^3)\right)} \hat{P}(n) e^{2\pi inz}, \]

where in the \( nth \) term of each series, \( z = \frac{z^2}{s_n} \), respectively. We can now apply Laplace’s method to each term and then observe that the dominant contributions for large \( y \) come from the \( 0, +1, -1 \) Fourier modes. Retaining just these we derive the following asymptotic behavior for \( \nabla \log w^\xi \):

\[ \frac{w^\xi_x(x, y)}{w^\xi(x, y)} = -\frac{4\epsilon \sqrt{1 - \epsilon^2}}{\hat{P}(0)} e^{-2\epsilon^2 y} \Im \left( \hat{P}(1) e^{-2i\epsilon^2 y} \right) = O\left(\epsilon e^{-2\epsilon^2 y}\right) \]

\[ \frac{w^\xi_y(x, y)}{w^\xi(x, y)} = \frac{1}{2y} \sqrt{1 - \epsilon^2} - \frac{1 + \Re \left( \hat{P}(1) e^{2i(\epsilon x - \epsilon^2 y)} \right) e^{-2\epsilon^2 y} + O\left(\epsilon^2 e^{-2\epsilon^2 y}\right)}{1 + \Re \left( \hat{P}(1) e^{2i(\epsilon x - \epsilon^2 y)} \right) e^{-2\epsilon^2 y} + O\left(\epsilon^2 e^{-2\epsilon^2 y}\right)} \]

\[ = -\frac{1}{2y} + \frac{1}{2y} + O\left(\epsilon^2 e^{-2\epsilon^2 y}\right). \]

Based on these asymptotics we can now estimate the energy in the large \( y \) domain.

\[ \nabla \theta^\xi = \left( -\frac{-\epsilon}{\sqrt{1 - \epsilon^2}} \right) + \left( O\left(\epsilon e^{-2\epsilon^2 y}\right) \right) \]

\[ \left( O\left(\frac{1}{y^2} + \epsilon^2 e^{-2\epsilon^2 y}\right) \right). \]
from which it follows that
\[ |\nabla \theta^\epsilon|^2 = 1 + \mathcal{O}\left(\epsilon^2 e^{-2\epsilon^2 y}\right) + \mathcal{O}\left(\frac{1}{y}\right) \]
and so the energy density
\[ (1 - |\nabla \theta^\epsilon|^2)^2 = \mathcal{O}\left(\epsilon^4 e^{-4\epsilon^2 y}\right) + \mathcal{O}\left(\frac{\epsilon^2}{y} e^{-2\epsilon^2 y}\right) + \mathcal{O}\left(\frac{1}{y^2}\right). \]
From this it follows that the "large y" part of the total energy is bounded as
\[ \mathcal{F}_{y \geq M_\epsilon} \lesssim \frac{1}{\epsilon M_\epsilon}. \]
Thus, if we take \( M_\epsilon = c/\epsilon \), this part of the total energy will remain finite as \( \epsilon \to 0 \).

3.2.2. Estimates in \([0, \ell] \times \{y < M_\epsilon\}\). We next turn to consideration of the energy density in the finite part of the domain. To facilitate this consideration we will sometimes make the uniformizing change of variables \( z = \epsilon \xi \) and \( h = \epsilon x \) in the Jacobi theta function (20):
\[ \vartheta_3\left(\frac{(h - z) + 2\epsilon^2 t}{\pi}, \frac{-4\epsilon^2 t}{\pi}\right) = \vartheta_3\left(\frac{(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\epsilon t}{\ell^2}\right) \]
In what follows we will assume that \( a \) is chosen to depend on \( \epsilon \) in such a way that \( 1 - a^\epsilon = \mathcal{O}(\epsilon) \).

We will make use here of the following single-layer potential counterpart of the double-layer potential representation (21), which in fact can be deduced directly from a change of variables in (25):
\[ w^\epsilon(x, y) = \frac{-y}{\sqrt{4\pi}} \int_0^\infty \frac{dt}{t^2} e^{-(1 - \epsilon^2)t + \frac{\pi^2}{4t^2}} \frac{1}{\ell} \int_0^\ell w^\epsilon(\xi, 0) \vartheta_3\left(\frac{(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\epsilon t}{\ell^2}\right) d\xi, \]
We study the asymptotic behavior of the convolution integral in (27) for \( x \in (0, a\ell) \) and for times \( t \) of order less than \( 1/\epsilon \):
\[ \frac{1}{\ell} \int_0^\ell w^\epsilon(\xi) \vartheta_3\left(\frac{(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\epsilon t}{\ell^2}\right) d\xi \]
\[ = \frac{1}{\ell} \int_0^\ell e^{\epsilon \xi} \vartheta_3\left(\frac{(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\epsilon t}{\ell^2}\right) d\xi + \frac{1}{\ell} \int_{a\ell}^\ell (w^\epsilon(\xi) - e^{\epsilon \xi}) \vartheta_3\left(\frac{(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\epsilon t}{\ell^2}\right) d\xi \]
\[ = \frac{1}{\pi} \int_0^\pi e^{\epsilon z} \vartheta_3\left(\frac{-(h - z) + 2\epsilon^2 t}{\pi}, \frac{-4\epsilon^2 t}{\pi}\right) dz + \frac{1}{\pi} \int_0^\pi \left(q_0\left(\frac{z}{\epsilon}\right) - e^{\epsilon z}\right) \vartheta_3\left(\frac{-(h - z) + 2\epsilon^2 t}{\pi}, \frac{-4\epsilon^2 t}{\pi}\right) dz \]
\[ = e^{\epsilon x} + o(\epsilon), \]
where in the third line above, the form of the integrals follows from making the change of
variables as in (26). In the second integral we smoothly extend \( q_0(\frac{z}{\epsilon}) - e^z \) to be zero on
\((0, a\pi)\). The final line follows for \( t \) of order less than \( 1/\epsilon \) because in this regime the Jacobi
theta function inside the convolution behaves as a Dirac comb as \( \epsilon \to 0 \). The second term has
this asymptotic behavior because \( h \in (0, a\pi) \) and the support of \( q_0(\frac{z}{\epsilon}) - e^z \) is complementary
to this interval, so that this integral decays exponentially to zero with \( \epsilon \), as with a Dirac
sequence away form its support.

Based on (28) we can estimate \( w^\epsilon \) as

\[
\begin{align*}
w^\epsilon(h, y) &= -\frac{y}{\sqrt{4\pi}} \left[ \int_0^{1/\epsilon} \frac{dt}{t^2} e^{-((1-\epsilon^2)t + \frac{z^2}{4t})} \left( e^{tx} + o(\epsilon) \right) \right] + O\left( e^{-1/\epsilon} \right) \\
&= e^{tx} e^{-\sqrt{1-\epsilon^2}y} + o(\epsilon).
\end{align*}
\]

(29)

The evaluation of the previous integral may be deduced from a basic Bessel identity (see [1]
9.6.23).

In order to estimate \( \nabla \theta^\epsilon \), we also need to estimate the \( x \) and \( y \) derivatives of \( w^\epsilon(x, y) \). To
this end we first consider the \( x \)-derivative of the internal convolution integral which equals

\[
\begin{align*}
\partial_x \frac{1}{\pi} \int_0^\pi \left( q_0(\frac{z}{\epsilon}) - e^z \right) \varphi_3 \left( -\frac{(h - z) + 2\epsilon^2t}{\pi}, -\frac{4\epsilon^2t}{\pi} \right) dz \\
&= \frac{1}{\pi} \int_0^\pi \left( q_0(\frac{z}{\epsilon}) - e^z \right) \varphi_3 \left( -\frac{(h - z) + 2\epsilon^2t}{\pi}, -\frac{4\epsilon^2t}{\pi} \right) dz \\
&= -\frac{1}{\pi} \int_0^\pi \left( q_0(\frac{z}{\epsilon}) - e^z \right) \varphi_3 \left( -\frac{(h - z) + 2\epsilon^2t}{\pi}, -\frac{4\epsilon^2t}{\pi} \right) dz.
\end{align*}
\]

(30)

(31)

Integrating by parts, the above derivative may be rewritten as

\[
\begin{align*}
\frac{1}{\pi} \int_0^\pi \epsilon \partial_z \left( q_0(\frac{z}{\epsilon}) - e^z \right) \partial_3 \left( -\frac{(h - z) + 2\epsilon^2t}{\pi}, -\frac{4\epsilon^2t}{\pi} \right) dz \\
&= o(\epsilon) \text{ for } h \in (0, a\pi),
\end{align*}
\]

(32)

as for the second integral in the last line of (28). Thus,

\[
\begin{align*}
\frac{w^\epsilon_x}{w^\epsilon} &= -\epsilon + \frac{y}{\sqrt{4\pi}} \int_0^{1/\epsilon} \frac{dt}{t^2} e^{-((1-\epsilon^2)t + \frac{z^2}{4t})} \frac{1}{\pi} \int_0^\pi \epsilon \partial_z \left( q_0(\frac{z}{\epsilon}) - e^z \right) \varphi_3 \left( -\frac{(h - z) + 2\epsilon^2t}{\pi}, -\frac{4\epsilon^2t}{\pi} \right) dz \\
&= -\epsilon + \frac{y}{\sqrt{4\pi}} \int_0^{1/\epsilon} \frac{dt}{t^2} e^{-((1-\epsilon^2)t + \frac{z^2}{4t})} \frac{1}{\pi} \int_0^\pi \left( q_0(\frac{z}{\epsilon}) - e^z \right) \varphi_3 \left( -\frac{(h - z) + 2\epsilon^2t}{\pi}, -\frac{4\epsilon^2t}{\pi} \right) dz \\
&= -\epsilon + \frac{o(\epsilon)}{e^{tx} + o(\epsilon)} = O(\epsilon)
\end{align*}
\]

(33)

For the \( y \) logarithmic derivative we have
\[
\frac{u_0'}{u'} = \frac{1}{y} - \frac{y}{2} \int_0^\infty \frac{dt}{t^2} e^{-(1-\epsilon^2)\frac{t^2}{4t^2}} \int_0^\ell w'(\xi, 0) \vartheta_3 \left( \frac{-(x-\xi) + 2\epsilon t}{t}, \frac{-4\pi t}{2t^2} \right) d\xi \\
= \frac{1}{y} - \frac{y}{2} \int_0^\infty \frac{dt}{t^2} e^{-(1-\epsilon^2)\frac{t^2}{4t^2}} \left( e^{ct} + o(\epsilon) \right) \\
= \frac{1}{y} - \frac{K_{-\frac{3}{2}}(y)}{K_{-\frac{1}{2}}(y)} + o(\epsilon) = -1 + o(\epsilon).
\]

The last equivalence follows from a Bessel recurrence identity \[1\], formula 9.6.26, together with formula 9.6.6.

Thus we finally have

\[
\nabla \theta' = \left( \begin{array}{c} 0 \\ -1 \end{array} \right) + \mathcal{O}(\epsilon)
\]

and hence \((1 - |\nabla \theta'|^2)^2 = \mathcal{O}(\epsilon^2)\). Since the domain \([0, a\ell] \times \{ y < M_\epsilon \}\) has dimensions \(1/\epsilon \times 1/\epsilon\), the total energy in this region is also asymptotically finite.

3.2.3. Modification of the Self-dual Test Function. It remains to estimate the energy in the region \([a\ell, \ell] \times \{ y < M_\epsilon \}\) which has dimensions \(\mathcal{O}(1) \times 1/\epsilon\). The question of the finiteness of the energy of the \(\theta'\) we have been considering in this region is beside the point for general purpose of but, this self-dual solution does not satisfy the boundary condition (10) in this region.

As stated earlier we are going to modify the self-dual test function in this region so that the boundary condition (10) is satisfied. To that end we fix a small value of \(\delta\) and let \(B(\delta)\) denote the \(\delta\)-neighborhood of \([a\ell, \ell]\) in \(S^\epsilon\). We modify \(w'\) in this neighborhood as follows. Define

\[
\tilde{w'}(x, y) = \phi_1(x, y)w'(x, y) + \phi_2(x, y)w_2(x, y)
\]

where \(\{\phi_1, \phi_2\}\) is a partition of unity subordinate to the cover of \(S^\epsilon\) given by

\[
U_1 = S^\epsilon \setminus B(\delta/2) \\
U_2 = B(\delta)
\]

and \(w_2(x, y) = w'(x, 0) \cosh(y)\), where \(w'(x, 0)\) here is defined as in (9' - 10'). One has

\[
\phi_1 = \begin{cases} 1 & U_1 \setminus B(\delta) \\ 0 & B(\delta/2) \end{cases} \\
\phi_2 = \begin{cases} 1 & B(\delta/2) \\ 0 & U_1 \setminus B(\delta) \end{cases}
\]

and \(\phi_1 + \phi_2 \equiv 1\).
It is straightforward to check that \( \tilde{w}^\varepsilon(x, y) \) satisfies the boundary conditions (9) and (10):
\[
\lim_{y \to 0} \tilde{w}^\varepsilon(x, y) = \phi_1(x, 0) w^\varepsilon(x, 0) + \phi_2(x, 0) w^\varepsilon(x, 0) \\
= (\phi_1(x, 0) + \phi_2(x, 0)) w^\varepsilon(x, 0) \\
= w^\varepsilon(x, 0) \\
= e^{\varepsilon x}
\]
for \( x \in [0, a\ell] \).
For \( x \in [a\ell, \ell] \),
\[
\lim_{y \to 0} \tilde{w}^\varepsilon_y(x, y) = (\phi_1 y(x, 0) + \phi_2 y(x, 0)) w^\varepsilon(x, 0) + \phi_2(x, 0) w^\varepsilon(x, 0) \sinh(0) \\
= (\phi_1 + \phi_2) y(x, 0) w^\varepsilon(x, 0) + 0 \\
= 0.
\]
Thus, \( \log \tilde{w}^\varepsilon \) is an admissible test function for the regularized Cross-Newell variational problem. We can now estimate the energy of this test function in \( B(\delta) \). The energy density in this region is bounded and therefore the energy in \( B(\delta) \) is finite.

3.2.4. Estimates for the "outer" solution in \( ([a\ell, \ell] \times \{ y < M_1 \}) \). It remains to estimate the energy in \( ([a\ell, \ell] \times \{ y < M_1 \}) \setminus B(\delta) \). To proceed with this we will need a more specific definition of \( q_0 \) which we now give.

Note first that by our assumption that \( 1 - a^\varepsilon = O(\varepsilon) \), the interval \([a\ell, \ell]\) remains of size \( O(1) \) for arbitrarily small values of \( \varepsilon \). We will now further pin this down by setting \( 1 - a^\varepsilon = c\varepsilon \) for a value of \( c \) that is fixed, independent of \( \varepsilon \). Consequently, \([a\ell, \ell]\) is now an interval of fixed length \( c\pi \) which can therefore also be represented as \([\ell - c\pi, \ell]\). Recall that \( q_0 \) needs to be built so that on this interval it matches, through second order, to \( e^{\varepsilon x} \) at the left endpoint and similarly to \( e^{\varepsilon x - \pi} \) at the right endpoint. Toward this end we observe that the required leading order value on the right is 1, independent of \( \varepsilon \) while on the left the leading order value limits to the stable value of \( e^\pi \) as \( \varepsilon \to 0 \).

Choosing a value \( \nu > 0 \) that is small with respect to \( c\pi \), we define a compressed \( \tanh \)-profile that interpolates between the point \((x_0, y_0) = (\ell - c\pi + \nu, e^\pi + \gamma) \) and the point \((x_1, y_1) = (\ell - \nu, 1 - \gamma) \) and where \( \gamma > 0 \) is another chosen value required to be smaller than 1. (This last requirement will insure that the positivity claim made at the end of subsection 3.1 holds.) Explicitly this \( \tanh \)-profile is given by
\[
T(x) = \frac{e^\pi + 1}{2} + \left( \frac{e^\pi - 1}{2} + \gamma \right) \tanh \left( \frac{x - (\ell - c\pi)}{(x - (\ell - \nu))(x - (\ell - c\pi + \nu))} \right).
\]
Note that the profile of \( T(x) \) is independent of \( \varepsilon \). The only way in which \( T \) depends on \( \varepsilon \) is that this profile translates uniformly with \( \ell \) as \( \varepsilon \) changes. We will define \( q_0(x) = T(x) \) on the subinterval \([x_0, x_1] = [\ell - c\pi + \nu, \ell - \nu] \) of \([\ell - c\pi, \ell]\).

Next we will define the piece of \( q_0(x) \) on the left that interpolates between the point \((\ell - c\pi, e^{\pi - c\pi}) \) and the point \((x_0, y_0) \). Choose a value \( \sigma > 0 \) that is small with respect to \( \nu \). Consider the covering of \([\ell - c\pi, \ell - c\pi + \nu] \) by the two sets \( V_1 = [\ell - c\pi, x_0 - \sigma] \) and \( V_2 = (\ell - c\pi + \sigma, x_0] \) and let \( \{ \psi_1(x), \psi_2(x) \} \) be a partition of unity subordinate to this cover which means, in particular, that
On \([\ell - c\pi, x_0]\) we define

\[
q_a(x) = \psi_1(x)e^{\epsilon x} + \psi_2(x)(e^{\pi} + \gamma).
\]

(37)

It is straightforward to see that with these choices \(q_a(x)\) is smooth throughout \([\ell - c\pi, \ell - \nu]\) and satisfies the smooth matching conditions on the left. Moreover, it is clear from the functions comprising (37) that \(q_a\) and its derivatives remain bounded on \([\ell - c\pi, \ell - \nu]\) as \(\epsilon \to 0\). A similar construction may be made on the right; i.e., on \((\ell - c\pi + \nu, \ell]\). This completes our description of \(q_a(x)\).

The study of the convolution integral in (27) in the region where \(x \in [a\ell, \ell]\) now proceeds similarly to what was done in (28) and subsequent formulae. In particular, the analogous result to (28) is that for \(x \in (a\ell, \ell]\) and for times \(t\) of order less than \(1/\epsilon\):

\[
\frac{1}{\ell} \int_0^\ell w^\epsilon(\xi) \vartheta_3 \left( \frac{-(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\pi t}{\ell^2} \right) d\xi
= \frac{1}{\ell} \int_0^\ell q_a(\xi) \vartheta_3 \left( \frac{-(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\pi t}{\ell^2} \right) d\xi
+ \frac{1}{\ell} \int_{a\ell}^\ell (w^\epsilon(\xi) - q_a(\xi)) \vartheta_3 \left( \frac{-(x - \xi) + 2\epsilon t}{\ell}, \frac{-4\pi t}{\ell^2} \right) d\xi
= \frac{1}{\pi} \int_0^\pi q_a \left( \frac{z}{\epsilon} \right) \vartheta_3 \left( \frac{-(h - z) + 2\epsilon^2 t}{\pi}, \frac{-4\epsilon^2 t}{\pi} \right) dz
+ \frac{1}{\pi} \int_0^\pi \left( w^\epsilon \left( \frac{z}{\epsilon} \right) - q_a \left( \frac{z}{\epsilon} \right) \right) \vartheta_3 \left( \frac{-(h - z) + 2\epsilon^2 t}{\pi}, \frac{-4\epsilon^2 t}{\pi} \right) dz
= q_a(x) + o(\epsilon),
\]

with \(q_a(x)\) here bounded away from zero, independent of \(\epsilon\), by our earlier choice of \(\gamma\). Hence the denominators in the estimates analogous to (33) and (34) are under control. In the subsequent formulae the roles of \(e^{\epsilon x}\) and \(q_a(x)\) are effectively interchanged as above and all proceeds as before. The result is that the energy in \((a\ell, \ell] \times \{y < M_\epsilon\}) \setminus \mathcal{B}(\delta)\) is asymptotically bounded like \(O(\epsilon)\).

It thus follows that the total energy of our family of test functions is uniformly bounded in \(\epsilon\).

4. LOWER BOUND

Following the ideas of Jin and Kohn \[8\], we will prove \textit{ansatz-free} lower bounds for the functional \(\mathcal{F}^\epsilon\) by identifying vector fields \(\Sigma(\nabla\theta)\) such that

\[
\mathcal{F}^\epsilon[\theta; a, \delta] \geq C^{-1} \left| \int_{S^*} \nabla \cdot \Sigma(\nabla\theta) dx dy \right|.
\]
This allows us to obtain information about the energy $\mathcal{F}^\varepsilon$ purely in terms of the boundary conditions on $\theta$. To avoid the proliferation of symbols, here and henceforth, $C, C', C_1, \text{ etc}$ denote (finite) constants whose precise value is unimportant, and different occurrences of the same symbol might denote different values of the constants. $e_1, e_2, K, K_1, \text{ etc}$ denote constants that have the same value in all their occurrences.

**Definition 1.** A smooth vector function $\Sigma(p,q) = (\Sigma_1, \Sigma_2)$ is **subordinate to the energy** if

\[
|\nabla \cdot \Sigma(\nabla \theta)| \leq C|1 - p^2 - q^2|
\]

for some $C < \infty$.

If $\Sigma$ is subordinate to the energy, it follows that

\[
|\nabla \cdot \Sigma(\nabla \theta)| \leq C|1 - \theta_x^2 - \theta_y^2||\nabla \nabla \theta|,
\]

where we use the identification $p = \theta_x, q = \theta_y$ and $|\nabla \nabla \theta|^2 = \theta_{xx}^2 + 2\theta_{xy}^2 + \theta_{yy}^2$. Consequently,

\[
\mathcal{F}^\varepsilon[\theta; a, \delta] = \iint_{S^\varepsilon} \left\{ |\nabla \nabla \theta|^2 + (1 - |\nabla \theta|^2)^2 \right\} dxdy - 2 \int_{\partial S^\varepsilon} \theta_x d\theta_y
\]

\[
\geq 2 \iint_{S^\varepsilon} |\nabla \nabla \theta|^2 |1 - |\nabla \theta|^2|^2 dxdy - 2 \int_{\partial S^\varepsilon} \theta_x d\theta_y
\]

\[
\geq \frac{2}{C} \left\{ \iint_{S^\varepsilon} \nabla \cdot \Sigma(\nabla \theta)dxdy \right\} - 2 \int_{\partial S^\varepsilon} \theta_x d\theta_y
\]

\[
\geq C^{-1} \left\{ \iint_{S^\varepsilon} \nabla \cdot \Sigma(\nabla \theta)dxdy \right\}.
\]

In obtaining the last equation, we use the fact that

\[
\int_{\partial S^\varepsilon} \theta_x d\theta_y = 0
\]

for the boundary conditions in (2).

**Lemma 4.1.** There are constants $e_1, K_1 > 0$ such that for all $\varepsilon \in (0, 1], a \in [0, 1]$ and $\delta \in \mathbb{R}$, we have

\[
\mathcal{F}^\varepsilon[\theta; a, \delta] \geq \frac{e_1 \varepsilon^2}{(1 - a)^2} - K_1 \varepsilon^2.
\]

**Proof.** Let $\phi \geq 0$ be a smooth, compactly supported function such that

\[
\phi(0) = 1,
\]

\[
\phi(1) < \phi(0),
\]

\[
\phi(p) = p\phi(p^2) \text{ has a single maximum at } p = 1.
\]

An explicit example of a function $\phi$ with these properties is

\[
\phi(p) = \begin{cases} 
\exp \left[ \frac{1}{2} - \frac{1}{(2-p)(p+1)} - \frac{p}{4} \right] & p \in (-1, 2) \\
0 & \text{otherwise}
\end{cases}
\]

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Let \( b = (1 - a)/\epsilon \). Define the vector field \( \Sigma(p, q) \) by

\[
\Sigma_2(p, q) = p \phi(b^2 p^2)
\]

\[
\Sigma_1(p, q) = - \int_0^q \left[ \phi(b^2(1 - \eta^2)) + 2(b^2(1 - \eta^2)\phi'(b^2(1 - \eta^2)) \right] d\eta.
\]

Since \( \phi \) has compact support, it follows that \( \Sigma \) is bounded on \( \mathbb{R}^2 \). An explicit calculation shows that the quantities \( \Sigma_1, p \) and \( \Sigma_2, q \) are zero. Also,

\[
\left| \frac{\partial \Sigma_1(p, q)}{\partial q} + \frac{\partial \Sigma_2(p, q)}{\partial p} \right| = \left| \phi(b^2 p^2) + 2b^2 p^2 \phi'(b^2 p^2) - \phi(b^2(1 - q^2)) \right|
\]

\[
-2b^2(1 - q^2)\phi'(b^2(1 - q^2))
\]

\[
\leq Cb^2 \left| (1 - p^2 - q^2) \right|
\]

where

\[
C = \sup_{x,y} \left| \phi(x) + 2x\phi'(x) - \phi(y) - 2y\phi'(y) \right| \leq \sup_z \left| 3\phi'(z) + 2z\phi''(z) \right|
\]

is clearly finite since \( \phi \) is compactly supported and twice differentiable. This proves that \( \Sigma \) is subordinate to the energy.

Since \( \nabla \cdot \Sigma(\nabla \theta) = (\Sigma_2, p + \Sigma_1, q)\theta_{xy} \) we obtain

\[
\left| \iint \nabla \cdot \Sigma(\nabla \theta) \, dxdy \right| \leq Cb^2 \iint \left| (1 - \theta_x^2 - \theta_y^2)\theta_{xy} \right| \, dxdy
\]

\[
\leq \frac{C b^2}{2} \left[ \iint (1 - \theta_x^2 - \theta_y^2)^2 \, dxdy + \iint [\nabla\nabla \theta]^2 \, dxdy \right]
\]

\[
= \frac{C b^2}{2} \mathcal{F}^\epsilon[\theta, a, \delta]
\]

(40)

Integrating by parts, we have

\[
\iint \nabla \cdot \Sigma(\nabla \theta) \, dxdy = \Sigma_2(\epsilon, \sqrt{1 - \epsilon^2}) - \int_0^{a\pi/\epsilon} \Sigma_2(0, \theta_0(x, 0)) \, dx
\]

\[
- \int_{a\pi/\epsilon}^{\pi/\epsilon} \Sigma_2(\theta_0(x, 0), 0) \, dx,
\]

where the contributions from the boundaries at \( x = 0 \) and \( x = \pi/\epsilon \) cancel due to the periodicity. By construction, \( \Sigma_2(p, 0) = 0 \) and \( \Sigma_2(p, q) \) has a maximum value at \( p = 1/b \). Consequently,

\[
\int_0^{a\pi/\epsilon} \Sigma_2(0, \theta_0(x, 0)) \, dx = 0
\]

\[
\int_{a\pi/\epsilon}^{\pi/\epsilon} \Sigma_2(\theta_0(x, 0), 0) \, dx \leq \frac{(1 - a)\pi \phi(1)}{\epsilon b} = \pi \phi(1).
\]

Also, \( \phi(0) = 1 \) and \( \phi \) is Lipschitz so that

\[
\Sigma_2(\epsilon, \sqrt{1 - \epsilon^2}) = c\phi(b^2 \epsilon^2) = c\phi((1 - a)^2) \geq \epsilon(1 - C'(1 - a)^2),
\]

\[
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\]
for some finite $C'$. Combining these estimates with (40), we obtain

$$F^c[\theta; a, \delta] \geq \frac{2\pi}{C_b^2} \left[ \phi(0) - \phi(1) - C'(1 - a)^2 \right],$$

and rewriting $b$ in terms of $a$ and $\epsilon$ yields the desired conclusion. □

The above lemma shows that the energy grows without bound as the quantity $(1 - a)$ becomes small. However, we do not have a priori control on the size of $(1 - a)$. Consequently, to obtain a lower bound for the energy, we need a complementary estimate which shows that the energy grows as the quantity $(1 - a)$ becomes large.

To prove this result, we first construct a vector field $\Sigma$ subordinate to the energy functional as follows:

Let $\psi \geq 0$ be a smooth, compactly supported function such that

$$\psi(0) = 1$$

$$\int_0^{\infty} (1 - \xi^2)\psi(\xi^2)d\xi = 0$$

We can always construct such a function, given $\chi \geq 0$, a compactly supported function with $\chi(0) = 1$. Observe that

$$\int_0^{\infty} (1 - \xi^2)\chi \left( \frac{\xi^2}{\eta^2} \right) d\xi = \eta(A_0 - \eta^2A_1),$$

where $A_0, A_1 > 0$. Consequently, by an appropriate choice of $\eta$, we get $\psi(x) = \chi(x/\eta^2)$ with the required properties.

We define the functions $\zeta(q^2)$ and $\sigma(q^2)$ by

$$\zeta(q^2) = \int_0^q (q - \eta)\psi(\eta^2)d\eta$$

$$\sigma(q^2) = \int_0^q (q - \eta)(1 - \eta^2)\psi(\eta^2)d\eta$$

(42)

Note that the functions $\zeta$ and $\sigma$ are well defined for positive values of their arguments, that is the expressions on the right hand sides of the above equations are even functions of $q$. From these expressions, we have

$$\frac{\partial^2}{\partial q^2}\zeta(q^2) = \psi(q^2); \quad \zeta(0) = 0$$

$$\frac{\partial^2}{\partial q^2}\sigma(q^2) = (1 - q^2)\psi(q^2); \quad \sigma(0) = 0$$

We will also use the same letters $\zeta$ and $\sigma$ to denote smooth extensions of the functions defined above to all of $\mathbb{R}$. We will pick extensions such that the supports of $\zeta$ and $\sigma$ are contained in $[-1, \infty)$.

Let $\varphi \geq 0$ be a compactly supported function and set

$$V(p, q) = \varphi(p^2) \left[ \sigma(q^2) - p^2\zeta(q^2) \right]$$

$$- \int_0^p (p - \xi) \left\{ \sigma(1 - \xi^2) \left[ \frac{\partial^2}{\partial \xi^2}\varphi(\xi^2) \right] - \zeta(1 - \xi^2) \left[ \frac{\partial^2}{\partial \xi^2}(\xi^2\varphi(\xi^2)) \right] \right\} d\xi.$$  

(43)
$V$ is now an even function of $p$ and $q$. Define the vector field $\Sigma$ by

\begin{equation}
\Sigma(p, q) = \left( \frac{-\partial}{\partial p} V, \frac{\partial}{\partial q} V \right)
\end{equation}

From (44) it follows that

\[ \frac{\partial \Sigma_1(p, q)}{\partial q} + \frac{\partial \Sigma_2(p, q)}{\partial p} = 0. \]

Also,

\[ \left| \frac{\partial \Sigma_2(p, q)}{\partial q} \right| = \left| \frac{\partial^2 V(p, q)}{\partial q^2} \right| = |\varphi(p^2)\psi(q^2)||1 - p^2 - q^2| \leq C_1|1 - p^2 - q^2|. \]

With $C_1 = \sup |\varphi(p^2)\psi(q^2)| < \infty$. Finally, an explicit calculation yields

\begin{equation}
\left| \frac{\partial \Sigma_1(p, q)}{\partial p} \right| = \left| \left[ \frac{\partial^2}{\partial p^2} \varphi(p^2) \right] (\sigma(q^2) - \sigma(1 - p^2)) - \left[ \frac{\partial^2}{\partial p^2} p^2 \varphi(p^2) \right] (\zeta(q^2) - \zeta(1 - p^2)) \right|
\end{equation}

\[ \leq C_2|1 - p^2 - q^2| \]

where $C_2$ can be bounded in terms of the support of $\varphi$ and the maximum values of $|\varphi|$, $|\varphi'|$, $|\varphi''|$, $|\zeta'|$ and $|\sigma'|$. Clearly $\varphi$ and all its derivatives are uniformly bounded since it is smooth and compactly supported. From (42), we have

\[ \zeta'(q^2) = \frac{1}{2q} \int_0^q \psi(\eta^2) d\eta \]

\[ \sigma'(q^2) = \frac{1}{2q} \int_0^q (1 - \eta^2) \psi(\eta^2) d\eta \]

Since $\psi$ is compactly supported, these derivatives vanish as $q^2 \to \infty$, implying that $\zeta'$ and $\sigma'$ are bounded for all positive values of the argument. Since $\sigma$ and $\zeta$ are smooth and are identically zero if their arguments are sufficiently negative, it follows that $C_2 < \infty$. It thus follows that the vector field $\Sigma$ is subordinate to the energy functional.

For future use, let us record a few observations that follow directly from the construction:

**Observation 1.** $\Sigma_2(p, 0) = 0$ since $\Sigma_2$ is an odd function of $q$.

**Observation 2.**

\[ \Sigma_{2,q}(0, q) = V_{qq}(0, q) = \psi(q^2)(1 - q^2). \]

Consequently, the non-degenerate critical points are at $q = \pm 1$. Differentiating in $q$, we get

\[ \Sigma_{2,qq}(0, \pm 1) = \mp 2\psi(1), \]

so that $\Sigma_2(0, q)$ has a maximum at $q = 1$ and a minimum at $q = -1$.

Finally,

\[ \Sigma_2(0, q) = 2q\sigma'(q^2) = \int_0^q (1 - \xi^2)\psi(\xi^2) d\xi, \]

so that $\Sigma_2(0, 1) > 0$ and $\Sigma_2(0, q) \to 0$ as $q \to \infty$.

\[ M = \int_0^1 (1 - \xi^2)\psi(\xi^2) d\xi \] will denote the maximum value of $\Sigma_2(0, q)$. 


Observation 3.

\[
\Sigma_2(\epsilon, \sqrt{1 - \epsilon^2}) = \varphi(\epsilon^2) \int_0^{\sqrt{1 - \epsilon^2}} (1 - \epsilon^2 - \xi^2) \psi(\xi^2) d\xi \geq M - K\epsilon^2
\]

for a constant \( K < \infty \). In obtaining the last line, we use

\[
|1 - \varphi(\epsilon^2)| \leq C_1 \epsilon^2
\]

\[
\left| \int_0^{\sqrt{1 - \epsilon^2}} \psi(\xi^2) d\xi \right| \leq C_2
\]

\[
\left| \int_0^1 (1 - \xi^2) \psi(\xi^2) d\xi \right| \leq C_3 \epsilon^2
\]

for some bounded constants \( C_1, C_2, C_3 \).

Lemma 4.2. There are constants \( e_2, K_2 > 0 \) such that for all \( \epsilon \in (0, 1], a \in [0, 1] \) and \( \delta \in \mathbb{R} \), we have

\[
\mathcal{F}[\theta; a, \delta] \geq \frac{e_2(1 - a)}{\epsilon} - K_2\epsilon.
\]

Remark. For the case \( a = 0 \), corresponding to the self-dual minimizers, this estimate captures the right scaling of the minimum energy as \( \epsilon \to 0 \).

Proof. The proof of the lemma follows from estimating a lower bound for the functional \( \mathcal{F}[\theta; a, \delta] \) using the vector field \( \Sigma \) that we constructed above.

For the vector field \( \Sigma \) we have

\[
\int \int \nabla \cdot (\nabla \theta) \, dx \, dy = \Sigma_2(\epsilon, \sqrt{1 - \epsilon^2}) \frac{\pi}{\epsilon} - \int_0^{a\pi/\epsilon} \Sigma_2(0, \theta_y(x, 0)) \, dx
\]

\[
- \int_{a\pi/\epsilon}^{\pi/\epsilon} \Sigma_2(\theta_x(x, 0), 0) \, dx.
\]

As before, the contributions from the boundaries at \( x = 0 \) and \( x = \pi/\epsilon \) cancel due to the periodicity. By construction, \( \Sigma_2(p, 0) = 0 \) and \( \Sigma_2(0, q) \) has a maximum value \( M \) at \( q = 1 \). Consequently,

\[
\int_0^{a\pi/\epsilon} \Sigma_2(0, \theta_y(x, 0)) \, dx \leq \frac{M \pi}{\epsilon}
\]

From observation 3, we obtain

\[
\Sigma_2(\epsilon, \sqrt{1 - \epsilon^2}) \frac{\pi}{\epsilon} \geq \frac{M \pi}{\epsilon} - K\pi\epsilon,
\]

Since \( \Sigma \) is subordinate to the energy,

\[
\mathcal{F}[\theta; a, \delta] \geq \frac{M \pi}{C\epsilon} \left[ 1 - a - K\epsilon^2 \right],
\]

which yields the desired conclusion. \( \square \)

We can now prove theorem 2.2 using lemma 4.1 and lemma 4.2.
Proof. Let $b$ denote the quantity $(1 - a)/\epsilon$. From lemma 4.1 we get
\[
\mathcal{F}^\epsilon[\theta; a, \delta] \geq \frac{e_1}{b^2} - K_1\epsilon^2 \geq 3 \left( e_1 e_2^2 \right)^{1/3} - 2e_2b - K_1\epsilon^2
\]
where the last inequality comes from linearizing the convex function $e_1 b^{-2}$ at $b = (e_1/e_2)^{1/3}$. Combining this estimate with the conclusion of lemma 4.2, we get
\[
\mathcal{F}^\epsilon[\theta; a, \delta] \geq \max \left( 3 \left( e_1 e_2^2 \right)^{1/3} - 2e_2b - K_1\epsilon^2, e_2b - K_2\epsilon \right) \geq \left( e_1 e_2^2 \right)^{1/3} - \frac{2K_2\epsilon + K_1\epsilon^2}{3}.
\]
If we set
\[
\epsilon_* = \min \left( \frac{(e_1 e_2^2)^{1/6}}{\sqrt{K_1}}, \frac{(e_1 e_2^2)^{1/3}}{2K_2} \right),
\]
for all $\epsilon < \epsilon_*$, all $a \in [0, 1]$ and all $\theta$ satisfying the boundary conditions in (2), we have
\[
\mathcal{F}^\epsilon[\theta; a, \delta] \geq \frac{(e_1 e_2^2)^{1/3}}{3} \equiv E_1.
\]
Combining the upper bound $\mathcal{F}^\epsilon[\theta^\epsilon; a^\epsilon, \delta^\epsilon] \leq E_0$ in theorem 2.1 with the lower bounds for $\mathcal{F}^\epsilon$ in lemma 4.1 and lemma 4.2, it follows that for
\[
\epsilon < \min \left( \sqrt{\frac{E_0}{K_1}} \frac{E_0}{K_2} \right),
\]
we have
\[
\sqrt{\frac{e_1}{2E_0}} < \frac{1 - a^\epsilon}{\epsilon} < \frac{2E_0}{e_2}.
\]
Consequently,
\[
1 - \alpha_2\epsilon < a^\epsilon < 1 - \alpha_1\epsilon,
\]
for sufficiently small $\epsilon$ with $\alpha_1 = \sqrt{e_1/(2E_0)}$ and $\alpha_2 = 2E_0/e_2$. □

5. Numerical Results

In this section, we will present the results of numerical simulations that illustrate and clarify our analysis of the energy and also the structure of the minimizers for the regularized Cross-Newell energy $\mathcal{F}^\epsilon$ within the class of functions given by (2).

For our numerical simulations, we restrict ourself to the finite domain, $\mathcal{R}^\epsilon = \{(x, y) \mid 0 \leq x \leq l = \pi/\epsilon, 0 \leq y \leq L\}$, where $L \gg 1$ is a length scale much larger than the typical wavelength of the pattern. The boundary conditions in (2) which are appropriate for the semi-infinite strip $\mathcal{S}^\epsilon$ are modified for the finite domain as follows –
\[
\theta(x, 0) = 0 \quad \text{for } 0 \leq x < al;
\]
\[
\theta_y(x, 0) = 0 \quad \text{for } al \leq x < l;
\]
\[
\theta(x, y) - \epsilon x \text{ is periodic in } x \text{ with period } l \text{ for each } y \in [0, L];
\]
\[
\theta(x, L) = \left[ \epsilon x + \sqrt{1 - \epsilon^2L + \delta} \right]
\]
(47)

It is rather straightforward to show that there exist $\theta^\epsilon \in H^2(\mathcal{R}^\epsilon)$ satisfying (47) for an $a^\epsilon \in [0, 1)$ and $\delta^\epsilon \in \mathbb{R}$ minimizing the functional
\[
\mathcal{F}^\epsilon[\theta; a, \delta] = \iint_{\mathcal{R}^\epsilon} \left\{ |\Delta \theta|^2 + (1 - |\nabla \theta|^2)^2 \right\} \, dx dy.
\]
The existence of a minimizer is immediate from the following lemma:

**Lemma 5.1.** Let $0 \leq a < 1$, and $\delta \in \mathbb{R}$ be given. $\rho_j \in L^2(\mathcal{R}^e)$ is a sequence of functions that converges weakly to zero. $H^2_{per}$ denotes the completion of periodic (in $x$) functions on $\mathcal{R}^e$ with respect to the $H^2$ norm. If $\theta_j \in H^2_{per}(\mathcal{R}^e)$ is a sequence satisfying (in the sense of trace)

$$
\Delta \theta_j = \rho_j \\
\theta_j(x,0) = 0 \quad \text{for } 0 \leq x < al; \\
\partial_y \theta_j(x,0) = 0 \quad \text{for } al \leq x < l; \\
\theta(x,L) = 0
$$

(48)

it follows that, up to extraction of a subsequence and relabelling, we have $\nabla \theta_j \to 0$ in $L^4(\mathcal{R}^e, \mathbb{R}^2)$.

**Proof.** Elliptic regularity along with the given boundary conditions implies that the sequence $\theta_j$ is bounded in $H^2(\mathcal{R}^e)$. The compactness of the embedding $H^2(\mathcal{R}^e) \hookrightarrow W^{1,4}(\mathcal{R}^e)$ [7] proves the lemma. □

If $\tilde{\theta}_j$ is an infimizing sequence for $F^e[\theta; a, \delta]$ subject to the boundary conditions in (47), then let $\theta_j = \tilde{\theta}_j - \varphi$, where $\varphi$ is a smooth function on $\mathcal{R}^e$ satisfying the boundary conditions in (47). It then follows from the form of $F^e$ and the fact that $\tilde{\theta}_j$ is infimizing that $\Delta \theta_j$ is a bounded sequence in $L^2$, and so converges weakly to a limit $\rho^\ast$. Applying the compactness result of the preceding lemma with reference to the sequence $\rho_j = \Delta \theta_j - \rho^\ast$, we obtain the existence of a minimizer for the functional $F^e[\theta; a, \delta]$ for a fixed $a$ and $\delta$.

Note that, for a given $a$ it is easy to construct smooth transformations $\psi_t : \mathcal{R}^e \to \mathcal{R}^e$ such that $\psi_0$ is the identity, if $\theta$ satisfies the boundary conditions in (47), then $\theta \circ \psi_t$ satisfies the same boundary conditions with the fraction of the boundary with a Dirichlet boundary condition equaling $a(1 + t)$. Further, the energy $F^e[\theta \circ \psi_t; a(1 + t), \delta]$ is a smooth function of $t$ for sufficiently small $t$. A standard argument now implies that, for a given $\delta$ the map

$$
a \mapsto \inf_{\theta} F^e[\theta; a, \delta]
$$

is continuous for $a \in (0, 1)$. A similar argument shows that the map is also continuous at $a = 0$. In Lemma 4.1 we showed that $\lim_{a \to 1} \inf_{\theta} F^e[\theta; a, \delta] = \infty$. Combining these results, we see that

$$
\inf_{a,\delta} F^e[\theta; a, \delta] = \inf_{a} \left[ \inf_{\theta} F^e[\theta; a, \delta] \right].
$$

We now consider variations $\theta \to \theta_t = \theta + t\chi(y/L)$, where $\chi$ is a smooth function vanishing identically on $[0, 1/3]$ and equal to 1 on $[2/3, 1]$. The functions $\theta_t$ satisfy the boundary conditions in (47), except the asymptotic phase shift is given by $\delta + t$. A similar argument as above shows that the map

$$
\delta \mapsto \inf_{\theta} F^e[\theta; a, \delta]
$$

is continuous and it is easy to see that $F^e[\theta; a, \delta] \to \infty$ as $\delta \to \pm\infty$. In particular, this proves the existence of an optimal $\delta$, and combining with the results from above, we see that the minimizer $\theta^e, a^e, \delta^e$, can be obtained by successive minimization in each of the factors.
This suggests the following discretization for the functional $F^\epsilon$, which should converge as the grid spacings $\eta,\zeta \to 0$. We define a grid by $x_i = i\eta, i = 0, 1, 2, \ldots, m - 1, y_j = j\zeta, j = 0, 1, 2, \ldots, n$, where $\eta = l/m, \zeta = L/n$. The discretization of the test function $\theta(x,y)$ is
\[
\theta_{i,j} = \theta(i\eta,j\zeta)
\]
We define the difference operator $\delta^\pm_x$ by
\[
(\delta^\pm_x \theta)_{i,j} = \pm \frac{\theta_{i\pm 1,j} - \theta_{i,j}}{\eta}
\]
with similar definitions for $\delta^\pm_y$. In terms of the discretization, the boundary conditions are
\[
\theta_{i,0} = 0 \quad \text{for } 0 \leq i < k;
\]
\[
\delta^+_y \theta_{i,0} = 0 \quad \text{for } k \leq i < m;
\]
\[
\theta_{m,j} = \theta_{0,j} + \pi \quad j = 0, 1, 2, \ldots, n
\]
\[
\theta_{i,n} = \frac{\pi i}{m} + \sqrt{1 - \epsilon^2(L + \delta)} \quad i = 0, 1, 2, \ldots, m - 1
\]
and the Energy functional is discretized as
\[
F^\epsilon \approx \eta \zeta \sum_{i=0}^{m-1} \sum_{j=0}^{n} \left[ (\delta^+_x \delta^-_x + \delta^+_y \delta^-_y) \theta_{i,j} \right]^2 + \left[ \frac{(\delta^+_x \theta)^2_{i,j} + (\delta^-_x \theta)^2_{i,j} + (\delta^+_y \theta)^2_{i,j} + (\delta^-_y \theta)^2_{i,j}}{2} - 1 \right]^2
\]
Computing this functional requires assigning values for $\theta_{i,j}$ with $i = -1, j = -1$ and $j = n+1$. The values for $i = -1$ are obtained form the shift-periodicity of $\theta$ by $\theta_{-1,j} = \theta_{m-1,j} - \pi$. The values for $j = n+1$ are assigned using the Dirichlet boundary condition $\theta_{i,n+1} = \frac{\pi i}{m} + \sqrt{1 - \epsilon^2(L + \zeta)} + \delta$. This functional is minimized using MATLAB’s conjugate-gradient minimization.

Fig. 3 shows the results from minimizing the RCN energy over the pattern $\theta$ and also the phase shift $\delta$, for different values of $\epsilon$, and for a range of values of $a \approx k/m$. The results do indeed suggest that the (partial) minimization with respect to the pattern and the asymptotic phase yields a functional that depends continuously on $a$. Further, this functional has first-order (discontinuous) phase transition at a bifurcation value $\epsilon^*$, below which the global minimizer has $a \neq 0$.  

Fig. 4 shows the energy of the minimizer (minimizing over the pattern, asymptotic phase and the parameter $a$) as a function of $\epsilon$. Note that the minimum energy is a non-differentiable function of $\epsilon$, as one would expect for a first-order phase transition.

Figure 5 show the numerically obtained minimizing patterns at various values of $\epsilon$. Note that, for sufficiently large $\epsilon$, the minimizers are the knee-solutions (3) with $a = 0$, whereas for sufficiently small $\epsilon$, the minimizers have convex-concave disclination pairs, and have $a \neq 0$.

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