Single droplet pattern in the cylindrical phase of diblock copolymer morphology *

Xiaofeng Ren †‡
Department of Mathematics and Statistics
Utah State University
Logan, UT 84322-3900, USA

Juncheng Wei §
Department of Mathematics
Chinese University of Hong Kong
Hong Kong, PRC

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Abstract

The Ohta-Kawasaki density functional theory of diblock copolymers gives rise to a nonlocal free boundary problem. Under a proper condition between the block composition fraction and the nonlocal interaction parameter, a pattern of a single droplet is proved to exist in a general planar domain. A smaller parameter range is identified where the droplet solution is stable. The droplet is a set which is close to a round disc. The boundary of the droplet satisfies an equation that involves the curvature of the boundary and a quantity that depends nonlocally on the whole pattern. The location of the droplet is determined by the regular part of a Green's function of the domain. This droplet pattern describes one cylinder in space in the cylindrical phase of diblock copolymer morphology.

Key words. Cylindrical phase, diblock copolymer morphology, single droplet pattern.

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Abbreviated title. Single droplet pattern.

1 Introduction

A diblock copolymer melt is a soft material, characterized by fluid-like disorder on the molecular scale and a high degree of order at a longer length scale. A molecule in a diblock copolymer is a linear sub-chain of A-monomers grafted covalently to another sub-chain of B-monomers. Because of the repulsion between the unlike monomers, the different type sub-chains tend to segregate, but as they are chemically bonded in chain molecules, segregation of sub-chains cannot lead to a macroscopic phase separation. Only a local micro-phase separation occurs: micro-domains rich in A monomers

*Abbreviated title: single droplet pattern

†Corresponding author. Phone: 1 435 797-0755; Fax: 1 435 797-1822; E-mail: ren@math.usu.edu

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and micro-domains rich in B monomers emerge as a result. These micro-domains form patterns that are know as morphology phases. Various phases, including lamellar, cylindrical, spherical, gyroid, have been observed in experiments.

Powerful methods in statistical physics have made it possible to derive a macroscopic model for monomer density fields from a microscopic model based on chain molecule formation and monomer interaction. A self consistent field theory (SCFT, see Helfand [13], Helfand and Wasserman [14, 15, 16], Hong and Noolandi [17, 18]) was developed, which was followed naturally by a density functional theory (DFT, see Ohta and Kawasaki [27]).

However there is generic criticism (see Bates and Fredrickson [4]) about the existing theoretical techniques of free energy minimization in the physics literature. They proceed by assuming a periodic structure, computing its free energy and then comparing that free energy to the free energy of other candidate test fields, (see, for instance, Matsen and Schick [21]). These test fields in general do not satisfy the Euler-Lagrange equation of the free energy.

In this paper we rigorously study the cylindrical phase of the diblock copolymer morphology by constructing an exact analytic solution that models one cylinder in a block copolymer melt. We identify two parameter ranges, one for the existence of a cylinder and one for the stability of the cylinder. The cross section of the cylinder is proved to be approximately a small, round disc. The location of this disc is determined by the geometry of the copolymer sample via a Green's function.

Consider a two dimensional bounded and sufficiently smooth domain D, which is a cross section of a diblock copolymer melt and perpendicular to a cylinder in the melt. The A-monomers occupy the subset E and the B-monomers occupy the compliment $D\backslash E$. The interface between the A-monomer regions and B-monomer regions is $\partial_D E$, which is the part of the boundary of E that is in D. Denote the Lebesgue measure of E by $|E|$ and set χ_E to be the characteristic function of E, i.e. $\chi_E(x) = 1$ if $x \in E$, and $\chi_E(x) = 0$ if $x \in D\backslash E$. Let a be the block composition fraction, i.e. the number of the A-monomers divided by the number of all the A- and B- monomers in a polymer chain. Given a fixed number $a \in (0, 1)$ we look for a subset E of D and a number λ such that $\partial_D E$ is a smooth curve, or a union of several smooth curves, $|E| = a|D|$, and at every point on $\partial_D E$,

$$H(\partial_D E) + \gamma(-\Delta)^{-1}(\chi_E - a) = \lambda. \tag{1.1}$$

Here $H(\partial_D E)$ is the curvature of $\partial_D E$ viewed from E and γ is a given positive parameter. The expression $(-\Delta)^{-1}(\chi_E - a)$ is the solution v of the problem

$$-\Delta v = \chi_E - a \text{ in } D, \ \ \partial_\nu v = 0 \text{ on the boundary of } D, \ \ \overline{v} = 0$$

where the bar over a function is the average of the function over its domain, i.e.

$$\overline{v} = \frac{1}{|D|} \int_D v(x)\, dx.$$

Because $(-\Delta)^{-1}$ is a nonlocal operator, the free boundary problem (1.1) is nonlocal.

The equation (1.1) is the Euler-Lagrange equation of the following variational problem.

$$J(E) = |D\chi_E|(D) + \frac{\gamma}{2} \int_D |(-\Delta)^{-1/2}(\chi_E - a)|^2\, dx. \tag{1.2}$$

The admissible set Σ of the functional J is the collection of all measurable subsets of D of measure $a|D|$ and of finite perimeter, i.e.

$$\Sigma = \{E \subset D : E \text{ is Lebesgue measurable}, \ \ |E| = a|D|, \ \ \chi_E \in BV(D)\}. \tag{1.3}$$

Here $BV(D)$ is the space of functions of bounded variation on D. The nonlocal integral operator $(-\Delta)^{-1}$ is defined by solving

$$-\Delta v = q \text{ in } D, \ \partial_\nu v = 0 \text{ on the boundary of } D, \overline{v} = 0$$

for $q \in L^2(D)$, $\overline{q} = 0$. Then $(-\Delta)^{-1/2}$ is the positive square root of $(-\Delta)^{-1}$. There are two parameters in (1.2): a and γ.

Since $\chi_E \in BV(D)$, we view $D\chi_E$, the derivative of χ_E, as a vector valued, signed measure, and let $|D\chi_E|$ be the positive total variation measure of $D\chi_E$. The first term in (1.2), $|D\chi_E|(D)$, is the $|D\chi_E|$ measure of the entire domain D. When $\partial_D E$ is a smooth curve, or a union of smooth curves, $|D\chi_E|(D)$ is just the length of $\partial_D E$. The constant λ in (1.1) comes as a Lagrange multiplier from the constraint $|E| = a|D|$.

Nishiura and Ohnishi [25] formulated the Ohta-Kawasaki theory on a bounded domain as a singularly perturbed variational problem with a nonlocal term and also identified the free boundary problem (1.1). Ren and Wei [31] showed that (1.2) is a Γ-limit of the singularly perturbed variational problem. See the last section for more discussion on the Ohta-Kawasaki theory and Γ-convergence.

Since then much work has been done to these problems. The lamellar phase is studied in Ren and Wei [31, 33, 34, 38, 39], Fife and Hilhorst [12], Chen and Oshita [5], and Choksi and Sternberg [9]. The work of Müller [24] is related to the lamellar phase in the case $a = 1/2$, as observed in [25]. Radially symmetric bubble and ring patterns are studied in Ren and Wei [32, 37, 40]. A triblock copolymer is studied in Ren and Wei [36]. Teramoto and Nishiura [41] studied the gyroid phase numerically. Mathematically strict derivations of the density functional theories for diblock copolymers, triblock copolymers and polymer blends are given in Choksi and Ren [7, 8], and Ren and Wei [35]. Also see Ohnishi and Nishiura [26], Ohnishi *et al* [26], and Choksi [6].

An explicit solution is easily found when the domain D itself is a disc and E a concentric disc of smaller radius. On a general domain Oshita [28] proved that for any $a \in (0,1)$, there is γ_0 such that if $\gamma < \gamma_0$, (1.1) admits a solution of measure $a|D|$, which is close to a disc. The bound γ_0 for γ depends on a.

The cylindrical phase occurs in a diblock copolymer melt only if a is relatively close to 0 (or close to 1) and γ is sufficiently large. Then the A-monomers (or B-monomers respectively) form parallel cylinders in a sample and the B-monomers (or A-monomers respectively) occupy the rest of the sample. If we look at a cross section, then the A-monomers form a number of droplets in a two dimensional region. Unfortunately Oshita's result does not cover this parameter range.

In this paper we prove a stronger result that contains Oshita's as a special case, and also covers the relevant parameter range for the cylindrical phase of diblock copolymer morphology.

We look for a solution which is close to a disc in a general domain, i.e. a single droplet pattern. Set $\rho > 0$ so that

$$\pi\rho^2 = a|D|. \tag{1.4}$$

From now on ρ replaces a as one of the two parameters of the problem. We need a crucial gap condition. Given any $\epsilon > 0$ assume that ρ, γ satisfy

$$|\gamma\rho^3 - 2n(n+1)| > \epsilon n^2, \quad \text{for all } n = 2, 3, 4, ... \tag{1.5}$$

Under (1.5), a gap condition, there exists $\delta > 0$ such that a single droplet solution exists if

$$\gamma\rho^4 < \delta \tag{1.6}$$

The situation studied by Oshita, i.e. ρ is fixed and γ is sufficiently small depending on ρ, is a special case included in our study. This is because for any ϵ, when ρ is fixed, one may take γ to be sufficiently small so that both (1.5) and (1.6) hold. Our result also allows ρ to be small and γ to be large, as long as (1.5) and (1.6) hold. The latter is the situation for a diblock copolymer in the cylindrical phase.

When intervals around $2n(n+1)$, $n = 2, 3, \ldots$, in (1.5) are deleted, the width of the intervals, $2\epsilon n^2$, grows as n becomes large. At some point an interval will include nearby members in the sequence $2n(n+1)$. When this happens, $\gamma\rho^3$ can not be placed above such $2n(n+1)$. This implies that there exists $C > 0$ depending on ϵ such that

$$\gamma\rho^3 < C. \tag{1.7}$$

Whether the solution found here is stable depends on how (1.5) is satisfied. It is stable, if

$$\gamma\rho^3 - 2n(n+1) < -\epsilon n^2, \text{ for all } n \geq 2, \tag{1.8}$$

Otherwise the solution is unstable. The solution found by Oshita satisfies (1.8) and hence is stable.

Although ρ may not be small, one needs to impose an upper bound, as in [28]. Let

$$G(x,y) = \frac{1}{2\pi} \log \frac{1}{|x-y|} + R(x,y) \tag{1.9}$$

be the Green's function of $-\Delta$ with the Neumann boundary condition. In this paper the Green's function G satisfies

$$-\Delta_x G(x,y) = \delta(x-y) - \frac{1}{|D|} \text{ in } D, \ \ \partial_{\nu(x)} G(x,y) = 0 \text{ on } \partial D, \ \ \overline{G(\cdot, y)} = 0 \text{ for every } y \in D. \tag{1.10}$$

Here Δ_x is the Laplacian with respect to the x-variable of G and $\partial_{\nu(x)}$ is the outward normal derivative at $x \in \partial D$. The function R is the regular part of G. Let $\tilde{R}(x) = R(x,x)$. Since $\tilde{R}(x)$ tends to ∞ as x tends to ∂D, $\tilde{R}$ has a at least global minimum in D. The distance from any global minimum of $\tilde{R}$ to the boundary of D must be strictly greater than ρ, i.e.

$$\rho < \min\{|x-y| : \ y \in \partial D, \ x \in D, \ \tilde{R}(x) = \min_{z \in D} \tilde{R}(z)\}. \tag{1.11}$$

The main result of this paper is the following.

Theorem 1.1 *For any $\epsilon > 0$ there exists $\delta > 0$ such that when ρ and γ satisfy (1.5) and (1.6), (1.1) admits a solution of a single droplet pattern. Moreover*

1. *the radius of the droplet is $\rho + O(\gamma\rho^5)$;*
2. *the center of the droplet is near a global minimum of $\tilde{R}$ in D;*
3. *if (1.5) is satisfied and*

$$\gamma\rho^3 - 2n(n+1) < -\epsilon n^2, \ \textit{for all } n \geq 2,$$

then the droplet solution is stable;

4. if (1.5) is satisfied and

$$\epsilon n^2 < \gamma\rho^3 - 2n(n+1), \ \text{and}\ \gamma\rho^3 - 2(n+1)(n+2) < -\epsilon(n+1)^2$$

for some $n \geq 2$, then the droplet solution is unstable.

Therefore in order to have a solution, we take $\gamma\rho^3$ to be of order $O(1)$, make sure that $\gamma\rho^3$ stays away from the sequence $2n(n+1)$, $n = 2, 3, 4, ...$, and make $\gamma\rho^4$ small. To have a stable solution we simply take

$$\gamma\rho^3 < 12 - 4\epsilon \ \text{ and } \ \gamma\rho^4 \ll 1. \tag{1.12}$$

The theorem is proved by a variant of the Lyapunov-Schmidt reduction procedure. In Section 2 we construct a family of approximate solutions of round discs parametrized by their centers. They form a two dimensional manifold. In Section 3 we perturb each disc a bit to find a set which solves (1.1) up to translation in a subspace approximately normal to the manifold. These perturbed discs form a new manifold that consists of solutions of (1.1) modulo translation. In this step we use a fixed point argument, for which the linearization of (1.1) at each approximate solution must be analyzed and the second Fréchet derivative computed. The obstacle to the invertibility of the linear operator is an oscillation phenomenon, i.e. oscillation of the boundary of the perturbed disc. The gap condition (1.5) ensures that oscillation does not happen. In Section 4 a particular perturbed disc in the new manifold is found, which solves (1.1) exactly. The location of this particular perturbed disc is determined by minimizing J on the new manifold. To show that the minimizer is indeed an exact solution of (1.1), we use a tricky re-parametrization argument.

The main difficulty in this approach for the wide parameter range (1.6) lies in the analysis of the nonlocal part of (1.1), such as the proofs of Lemmas 3.1 and 3.3. It involves a singular integral operator similar to the Hilbert transform. In the case that γ is small, studied in [28], one does not need these sharp estimates. Only when ρ is small, it is crucial to carry out estimates to such extend.

The gap condition (1.5) suggests bifurcations to non-circular shapes, when $\gamma\rho^3$ becomes close to $2n(n+1)$. Gap conditions have appeared before in constructing layered solutions for singularly perturbed problems. See Malchiodi and Montenegro [20], del Pino, Kowalczyk and Wei [11], Pacard and Ritoré [29], and the references therein.

Denote by S^1 the interval $[0, 2\pi]$ with 0 and 2π identified. The L^2 space on S^1 is $L^2(S^1)$. The inner product in $L^2(S^1)$ is denoted by $\langle\cdot,\cdot\rangle$. Let $\{u_1, u_2, ...\}^\perp$ be the closed subspace of $L^2(S^1)$ whose elements are perpendicular to u_1, u_2, ... The L^2 norm is denoted by $\|\cdot\|_{L^2}$, and the L^∞ norm by $\|\cdot\|_{L^\infty}$. The Sobolev $W^{2,k}$ space is denoted by $H^k(S^1)$ where $k \geq 1$ is an integer. The $W^{2,k}$ norm is denoted by $\|\cdot\|_{H^k}$.

We use C to denote a positive constant which is independent of a, ρ, γ, and the points ξ in U, where U is a subset of D given in Section 2. C can only depend on D and ϵ. The value of C may change from place to place.

The complex $e^{i\theta}$ is written instead of $(\cos\theta, \sin\theta)$ for a simpler notation even though no complex structure is assumed on R^2. The reader will see things like $e^{i\theta}\cdot x$ which is simply the inner product of two real vectors $e^{i\theta}$ and x.

From now on we assume that $\epsilon > 0$ is given and (1.5) is satisfied.

2 Approximate solutions

Let U be an open neighborhood of the set $\{x \in D : \tilde{R}(x) = \min_{y\in D} \tilde{R}(y)\}$. The last set consists of the global minima of $\tilde{R}$ and is compact. By taking U to be sufficiently close to $\{x \in D : \tilde{R}(x) = \min_{y\in D} \tilde{R}(y)\}$ we assume that the closure of U, $\overline{U}$, is also a subset of D.

For each $\xi \in U$ let

$$B_\xi = \{x \in D : |x - \xi| < \rho\} \tag{2.1}$$

be an approximate solution which is a disc of radius ρ and centered at ξ. Because of (1.11) by taking U to be sufficiently close to $\{x \in D : \tilde{R}(x) = \min_{y\in D} \tilde{R}(y)\}$ we have $B_\xi \subset D$ for all $\xi \in U$.

A perturbed disc E_ϕ is characterized by a 2π periodic function $\phi(\theta)$ so that

$$E_\phi = \{\xi + \alpha e^{i\theta} : \theta \in [0, 2\pi],\ \alpha \in [0, \sqrt{\rho^2 + \phi(\theta)})\}, \tag{2.2}$$

and the boundary of the perturbed disc E_ϕ is a curve parametrized by θ: $\xi + \sqrt{\rho^2 + \phi(\theta)}e^{i\theta}$. We will restrict the size of ϕ so that $\rho^2 + \phi$ is always positive. Moreover it is always assumed that

$$\int_0^{2\pi} \phi(\theta)\, d\theta = 0. \tag{2.3}$$

This ensures that the size of E_ϕ remains $a|D|$:

$$|E_\phi| = \int_0^{2\pi} \int_0^{\sqrt{\rho^2+\phi(\theta)}} r\, dr d\theta = \int_0^{2\pi} \frac{\rho^2 + \phi(\theta)}{2}\, d\theta = \pi\rho^2 = a|D|$$

The arc-length of $\partial_D E_\phi$ can be expressed as

$$|D\chi_{E_\phi}|(D) = \int_0^{2\pi} \sqrt{\rho^2 + \phi(\theta) + \frac{(\phi'(\theta))^2}{4(\rho^2 + \phi(\theta))}}\, d\theta \tag{2.4}$$

The nonlocal part of J in (1.2) may be written in terms of ϕ as

$$\begin{aligned} &\frac{\gamma}{2}\int_D |(-\Delta)^{-1/2}(\chi_{E_\phi} - a)|^2\, dx = \frac{\gamma}{2}\int_{E_\phi}\int_{E_\phi} G(x,y)\, dxdy \\ =\ & \frac{\gamma}{2}\int_0^{2\pi} d\theta \int_0^{\sqrt{\rho^2+\phi(\theta)}} dr \int_0^{2\pi} d\omega \int_0^{\sqrt{\rho^2+\phi(\omega)}} dt\ G(\xi + re^{i\theta}, \xi + te^{i\omega}) rt. \end{aligned} \tag{2.5}$$

In terms of ϕ the curvature at a point on $\partial_D E_\phi$ corresponding to θ is

$$\mathcal{H}(\phi)(\theta) = \frac{\rho^2 + \phi(\theta) + \frac{3(\phi'(\theta))^2}{4(\rho^2+\phi(\theta))} - \frac{\phi''(\theta)}{2}}{(\rho^2 + \phi(\theta) + \frac{(\phi'(\theta))^2}{4(\rho^2+\phi(\theta))})^{3/2}} \tag{2.6}$$

The nonlocal part in (1.1) may be written as

$$\begin{aligned} &\gamma(-\Delta)^{-1}(\chi_{E_\phi} - a)(\theta) \\ =\ & \gamma\int_{E_\phi} G(\xi + \sqrt{\rho^2 + \phi(\theta)}e^{i\theta}, y)\, dy \end{aligned}$$

$$
\begin{aligned}
&= \gamma\int_0^{2\pi}\int_0^{\sqrt{\rho^2+\phi(\omega)}} G(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},\xi+te^{i\omega})t\,dtd\omega \\
&= -\frac{\gamma\log\rho}{2\pi}|E_\phi| - \frac{\gamma}{2\pi}\int_0^{2\pi}\int_0^{\sqrt{\rho^2+\phi(\omega)}} \log|\sqrt{1+\frac{\phi(\theta)}{\rho^2}}e^{i\theta} - \frac{te^{i\omega}}{\rho}|t\,dtd\omega \\
&\quad +\gamma\int_0^{2\pi}\int_0^{\sqrt{\rho^2+\phi(\omega)}} R(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},\xi+te^{i\omega})t\,dtd\omega \qquad (2.7)
\end{aligned}
$$

The first term in (2.7) is only a constant. The second and the third terms are defined to be

$$
\mathcal{A}(\phi) = -\frac{\gamma\rho^2}{2\pi}\int_0^{2\pi}\int_0^{\sqrt{1+\phi(\omega)/\rho^2}} \log|\sqrt{1+\frac{\phi(\theta)}{\rho^2}}e^{i\theta} - se^{i\omega}|s\,dsd\omega \qquad (2.8)
$$

$$
\mathcal{B}_\xi(\phi) = \gamma\int_0^{2\pi}\int_0^{\sqrt{\rho^2+\phi(\omega)}} R(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},\xi+te^{i\omega})t\,dtd\omega \qquad (2.9)
$$

Note that the operators $\mathcal{H}$ and $\mathcal{A}$ are independent of ξ while the operator $\mathcal{B}_\xi$ does depend on ξ.

Remark 2.1 *The expressions (2.6) and (2.7) may be obtained by calculating the variations of (2.4) and (2.5) with respect to ϕ. Then there will be an extra $\frac{1}{2}$ in front of both (2.6) and (2.7).*

Let S_ξ be the operator that appears on the left side of (1.1) projected to $\{1\}^\perp$, i.e.

$$
S_\xi(\phi) = \mathcal{H}(\phi) + \mathcal{A}(\phi) + \mathcal{B}_\xi(\phi) + \lambda_\xi(\phi) \qquad (2.10)
$$

Here $\lambda_\xi(\phi) \in R$ is a number so chosen that

$$
\overline{S_\xi(\phi)} := \frac{1}{2\pi}\int_0^{2\pi} S_\xi(\phi)\,d\theta = 0. \qquad (2.11)
$$

The subscript ξ indicates that S_ξ depends on ξ, because $\mathcal{B}_\xi$ (and consequently λ_ξ) does. E_ϕ is a solution of (1.1) if and only if

$$
S_\xi(\phi) = 0. \qquad (2.12)
$$

The first Fréchet derivative of S_ξ is given by

$$
\begin{aligned}
\mathcal{H}'(\phi)(u) &= \mathcal{H}_1(\phi)u + \mathcal{H}_2(\phi)u' + \mathcal{H}_3(\phi)u'' \qquad (2.13) \\
\mathcal{A}'(\phi)(u)(\theta) &= -\frac{\gamma}{4\pi}\int_0^{2\pi} u(\omega)\log|\sqrt{1+\frac{\phi(\theta)}{\rho^2}}e^{i\theta} - \sqrt{1+\frac{\phi(\omega)}{\rho^2}}e^{i\omega}|\,d\omega - \\
&\quad \frac{\gamma u(\theta)}{4\pi\sqrt{1+\phi(\theta)/\rho^2}}\int_0^{2\pi}\int_0^{\sqrt{1+\phi(\omega)/\rho^2}} \frac{(\sqrt{1+\frac{\phi(\theta)}{\rho^2}}e^{i\theta} - se^{i\omega})\cdot e^{i\theta}}{|\sqrt{1+\frac{\phi(\theta)}{\rho^2}}e^{i\theta} - se^{i\omega}|^2} s\,dsd\omega. \qquad (2.14) \\
\mathcal{B}'_\xi(\phi)(u)(\theta) &= \frac{\gamma}{2}\int_0^{2\pi} u(\omega)R(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},\xi+\sqrt{\rho^2+\phi(\omega)}e^{i\omega})\,d\omega \\
&\quad +\frac{\gamma u(\theta)}{2\sqrt{\rho^2+\phi(\theta)}}\int_{E_\phi} \nabla R(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},y)\cdot e^{i\theta}\,dy. \qquad (2.15)
\end{aligned}
$$

The derivative of the operator λ_ξ is so chosen that

$$S'_\xi(\phi) = \mathcal{H}'(\phi) + \mathcal{A}'(\phi) + \mathcal{B}'_\xi(\phi) + \lambda'_\xi(\phi), \quad \overline{S'_\xi(\phi)(u)} = 0. \tag{2.16}$$

We have abused the notations a bit in (2.13). The operator $\mathcal{H}$ is also viewed as a function of ϕ, ϕ' and ϕ'', i.e.

$$\mathcal{H}(\phi, \phi', \phi'') = \frac{\rho^2 + \phi + \frac{3(\phi')^2}{4(\rho^2+\phi)} - \frac{\phi''}{2}}{(\rho^2 + \phi + \frac{(\phi')^2}{4(\rho^2+\phi)})^{3/2}}.$$

The derivatives of $\mathcal{H}$ with respect to ϕ, ϕ' and ϕ'' are denoted by $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_3$ respectively.

Lemma 2.2 $\|S_\xi(0)\|_{L^\infty} = O(\gamma\rho^3)$.

Proof. Compute $v = (-\Delta)^{-1}(\chi_{B_\xi} - a)$. Define

$$P(x) = \begin{cases} -\frac{|x|^2}{4} + \frac{\rho^2}{4} - \frac{\rho^2}{2}\log\rho, & \text{if } |x| < \rho \\ -\frac{\rho^2}{2}\log|x|, & \text{if } |x| \geq \rho \end{cases}.$$

Then $-\Delta P(\cdot - \xi) = \chi_{B_\xi}$. Write $v = P(\cdot - \xi) + Q(\cdot, \xi)$. Clearly

$$-\Delta Q(x,\xi) = -a, \ \partial_{\nu(x)}Q(x,\xi) = \partial_\nu \frac{\rho^2}{2}\log|x-\xi| \text{ on } \partial D, \ \overline{Q(\cdot,\xi)} = -\overline{P(|\cdot - \xi|)}.$$

Here the Laplacian Δ and the outward normal derivative $\partial_{\nu(x)}$ are taken with respect to x. Note that the Green's function G satisfies the equation (1.10). Recall that the regular part of the Green function G is denoted by R. Then one sees that $Q(x,\xi)$ and $\pi\rho^2 R(x,\xi)$ satisfy the same equation and the same boundary condition. Therefore they can differ only by a constant. This constant is $\overline{Q(\cdot,\xi)} - \pi\rho^2\overline{R(\cdot,\xi)}$. But $\overline{v} = \overline{G(\cdot,\xi)} = 0$ implies that this constant is also equal to

$$-\frac{\rho^2}{2}\overline{\log|\cdot - \xi|} - \overline{P(\cdot - \xi)} = \frac{\pi\rho^4}{8|D|}.$$

Hence

$$Q(x,\xi) = \pi\rho^2 R(x,\xi) + \frac{\pi\rho^4}{8|D|}. \tag{2.17}$$

Therefore at each $\xi + \rho e^{i\theta}$,

$$\begin{aligned}
\mathcal{H}(0)(\theta) + \gamma(-\Delta)^{-1}(\chi_{B_\xi} - a)(\theta) &= \frac{1}{\rho} + \gamma v(\xi + \rho e^{i\theta}) \\
&= \frac{1}{\rho} + \gamma[-\frac{\rho^2\log\rho}{2} + \pi\rho^2 R(\xi + \rho e^{i\theta}, \xi) + \frac{\pi\rho^4}{8|D|}] \\
&= \frac{1}{\rho} + \gamma[-\frac{\rho^2\log\rho}{2} + \pi\rho^2 R(\xi,\xi) + \frac{\pi\rho^4}{8|D|}] + O(\gamma\rho^3)
\end{aligned}$$

Note that on the last line every term except $O(\gamma\rho^3)$ is independent of θ. Since $\mathcal{H}(0)+\gamma(-\Delta)^{-1}(\chi_{B_\xi} - a)$ and $S_\xi(0)$ also differ by a constant only,

$$S_\xi(0) = \mathcal{H}(0) + \gamma(-\Delta)^{-1}(\chi_{B_\xi} - a) + \frac{\gamma\log\rho}{2\pi}|B_\xi| + \lambda_\xi(0) = \frac{1}{\rho} + \gamma[\pi\rho^2 R(\xi,\xi) + \frac{\pi\rho^4}{8|D|}] + \lambda_\xi(0) + O(\gamma\rho^3).$$

If we integrate $S_\xi(0)$ with respect to θ over $[0,2\pi]$, then $\overline{S_\xi(0)}=0$ implies that

$$\frac{1}{\rho}+\gamma[\pi\rho^2 R(\xi,\xi)+\frac{\pi\rho^4}{8|D|}]+\lambda_\xi(0)=O(\gamma\rho^3).$$

Hence $S_\xi(0)=O(\gamma\rho^3)$. □

Lemma 2.3 $J(B_\xi)=2\pi\rho+\frac{\pi^2\gamma\rho^4}{2}[\frac{-\log\rho}{2\pi}+\frac{1}{8\pi}+\tilde{R}(\xi)+\frac{\rho^2}{4|D|}]$.

Proof. Let $v=(-\Delta)^{-1}(\chi_{B_\xi}-a)=P(\cdot-\xi)+Q(\cdot,\xi)$ as in the proof of Lemma 2.2. The local part of $J(B_\xi)$ is just the arc length

$$2\pi\rho. \tag{2.18}$$

The nonlocal part of $J(B_\xi)$ is

$$\begin{aligned}
&\frac{\gamma}{2}\int_D |(-\Delta)^{-1/2}(\chi_{B_\xi}-a)|^2\,dx\\
&= \frac{\gamma}{2}\int_D(\chi_{B_\xi}-a)v(x)\,dx \;=\; \frac{\gamma}{2}\int_D\chi_{B_\xi}v(x)\,dx \;=\; \frac{\gamma}{2}\int_{B_\xi}v(x)\,dx\\
&= \frac{\gamma}{2}[\int_{B_0}P(x)\,dx+\int_{B_\xi}Q(x,\xi)\,dx]
\end{aligned} \tag{2.19}$$

From the definition of P one finds that

$$\int_{B_0}P(x)\,dx=\frac{\pi\rho^4}{8}-\frac{\pi\rho^4\log\rho}{2}. \tag{2.20}$$

For the integral of Q, note that, since $\Delta Q(\cdot,\xi)=a$, $Q(x,\xi)-\frac{a}{4}|x-\xi|^2$ is harmonic in x. By the Mean Value Theorem for harmonic functions

$$\begin{aligned}
\int_{B_\xi}Q(x,\xi)\,dx &= \int_{B_\xi}(Q(x,\xi)-\frac{a}{4}|x-\xi|^2)\,dx+\int_{B_\xi}\frac{a}{4}|x-\xi|^2\,dx\\
&= \pi\rho^2Q(\xi,\xi)+\frac{\pi^2\rho^6}{8|D|} \;=\; \pi^2\rho^4R(\xi,\xi)+\frac{\pi^2\rho^6}{4|D|}
\end{aligned} \tag{2.21}$$

The lemma then follows from (2.18), (2.19), (2.20) and (2.21). □

3 Reduction to two dimensions

One views S_ξ as a nonlinear operator from $H^2(S^1)\cap\{1\}^\perp$ to $L^2(S^1)\cap\{1\}^\perp$. In this section it will be proved that, for each $\xi\in U$, a function $\varphi(\cdot,\xi)$ exists such that $\varphi(\cdot,\xi)\perp\cos\theta$, $\varphi(\cdot,\xi)\perp\sin\theta$ and

$$S_\xi(\varphi(\cdot,\xi))(\theta)=A_{1,\xi}\cos\theta+A_{2,\xi}\sin\theta \tag{3.1}$$

for some $A_{1,\xi},A_{2,\xi}\in R$. The equation (3.1) is written as

$$\Pi S_\xi(\varphi(\cdot,\xi))=0 \tag{3.2}$$

where Π is the orthogonal projection operator from $L^2(S^1) \cap \{1\}^\perp$ to $L^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$.

Roughly speaking the functions $\cos\theta$ and $\sin\theta$ correspond to translations in space. By solving (3.2) we are solving (1.1) modulo translation. In the next section we will find a particular ξ, say ζ, such that $A_{1,\zeta} = A_{2,\zeta} = 0$, i.e. $S_\zeta(\varphi(\cdot, \zeta)) = 0$. This means that by finding φ in this section one reduces the original problem (1.1) to a problem of finding a ζ in a two dimensional set U.

Let L_ξ be the linearized operator of S_ξ at $\phi = 0$, i.e.

$$L_\xi(u) = S'_\xi(0)(u). \tag{3.3}$$

L_ξ maps from $H^2(S^1) \cap \{1\}^\perp$ to $L^2(S^1) \cap \{1\}^\perp$. Expand $S_\xi(\phi)$ as

$$S_\xi(\phi) = S_\xi(0) + L_\xi(\phi) + N_\xi(\phi) \tag{3.4}$$

where N_ξ is a higher order term defined by (3.4). Rewrite (3.2) in a fixed point form:

$$\phi = -(\Pi L_\xi)^{-1}(\Pi S_\xi(0) + \Pi N_\xi(\phi)) \tag{3.5}$$

Before solving (3.5), one must estimate the linear operator ΠL_ξ.

Lemma 3.1 *Let γ and ρ satisfy the gap condition (1.5).*

1. *There exists $C > 0$ independent of ξ, ρ and γ such that*

$$\|u\|_{L^2} \leq C\rho^3 \|\Pi L_\xi(u)\|_{L^2}$$

   for all $u \in H^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$.

2. *If (1.8) is satisfied, then*

$$\|u\|_{L^2}^2 \leq C\rho^3 \langle \Pi L_\xi(u), u\rangle.$$

3. *The operator ΠL_ξ is invertible from $H^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$ onto $L^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$ and there exists $C > 0$ independent of ξ, ρ and γ such that*

$$\|u\|_{H^2} \leq C\rho^3 \|\Pi L_\xi(u)\|_{L^2}$$

   for all $u \in H^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$.

4. *Under (1.8), Part 2 can be improved to*

$$\|u\|_{H^1}^2 \leq C\rho^3 \langle \Pi L_\xi(u), u\rangle.$$

Proof. Without the loss of generality assume that $\xi = 0$ and set $\mathcal{B} = \mathcal{B}_\xi$, $L = L_\xi$, etc, in this proof.

The derivative of $\mathcal{H} + \mathcal{A}$ at 0 is calculated in Appendix A. Denote it by L_1, which is

$$\begin{aligned} L_1(u) &= (\mathcal{H}'(0) + \mathcal{A}'(0))(u) \\ &= -\frac{1}{2\rho^3}(u'' + u) - \frac{\gamma}{8\pi}\int_0^{2\pi} u(\omega)\log(1 - \cos(\theta - \omega))\, d\omega - \frac{\gamma u}{4} \end{aligned} \tag{3.6}$$

Note that $\Pi L_1 = L_1$ on $H^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$ because L_1 maps from $H^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$ to $L^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$.

The Fourier coefficients of $\log(1 - \cos(\theta))$ is given by

$$\int_0^{2\pi} \log(1-\cos\theta)e^{-in\theta}\, d\theta = -\frac{2\pi}{|n|}, \quad |n| \geq 1. \tag{3.7}$$

Because $u \perp 1$, the $n = 0$ coefficient is not needed. The formula (3.7) is equivalent to the well known formula

$$-\log|2\sin(\frac{\theta}{2})| = \sum_{n=1}^{\infty} \frac{\cos n\theta}{n}.$$

(See Tolstov [42, Page 93], e.g.)

In the Fourier space, L_1 is diagonalized and written as

$$\widehat{L_1(u)}(n) = \widehat{u}(n)[\frac{n^2-1}{2\rho^3} - \gamma(\frac{1}{4} - \frac{1}{4|n|})], \; |n| = 1, 2, 3, ..., \tag{3.8}$$

where

$$\widehat{u}(n) = \int_0^{2\pi} u(\theta)e^{-in\theta}\, d\theta$$

is the n-th Fourier coefficient of u.

The eigen pairs, in $H^2(S^1) \cap \{1\}^\perp$, are

$$\lambda_n = \frac{n^2-1}{2\rho^3} - \frac{\gamma(n-1)}{4n}, \quad e_n = \cos n\theta, \; \sin n\theta; \quad n = 1, 2, ... \tag{3.9}$$

In this lemma the operator ΠL's domain is perpendicular to $\cos\theta$ and $\sin\theta$, so we discard the eigen pair λ_1 and $e_1 = \cos\theta, \sin\theta$. The gap condition (1.5) ensures that, with $n \geq 2$,

$$|\lambda_n| > \frac{\epsilon(n-1)n}{4\rho^3} \geq \frac{\epsilon}{2\rho^3}, \tag{3.10}$$

which implies

$$\|u\|_{L^2} \leq C\rho^3 \|L_1(u)\|_{L^2}, \tag{3.11}$$

for all $u \in H^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$. Under the condition (1.8)

$$\lambda_n > \frac{\epsilon}{2\rho^3}, \tag{3.12}$$

which implies

$$\|u\|_{L^2}^2 \leq C\rho^3 \langle \Pi(L_1(u), u\rangle. \tag{3.13}$$

Moreover the gap condition also asserts that

$$\frac{|\lambda_n|}{n^2} > \frac{\epsilon(n-1)n}{4n^2\rho^3} \geq \frac{\epsilon}{8\rho^3}, \tag{3.14}$$

which implies that

$$\|u''\|_{L^2} \leq C\rho^3 \|L_1(u)\|_{L^2}.$$

Consequently

$$\|u\|_{H^2} \le C\rho^3 \|L_1(u)\|_{L^2}. \tag{3.15}$$

To estimate $\mathcal{B}'(0)$ note from (2.15) that

$$\mathcal{B}'(0)(u) = \frac{\gamma}{2}\int_0^{2\pi} u(\omega) R(\xi+\rho e^{i\theta}, \xi+\rho e^{i\omega})\, d\omega + \frac{\gamma u(\theta)}{2\rho}\int_B \nabla R(\xi+\rho e^{i\theta}, y)\cdot e^{i\theta}\, dy \tag{3.16}$$

where B is the ball centered at ξ of radius ρ. For the first part we write it as

$$\frac{\gamma}{2}\int_0^{2\pi} u(\omega) R(\xi+\rho e^{i\theta}, \xi+\rho e^{i\omega})\, d\omega = \frac{\gamma}{2}\int_0^{2\pi} u(\omega)(R(\xi+\rho e^{i\theta}, \xi+\rho e^{i\omega}) - R(\xi,\xi))\, d\omega$$

since $\int_0^{2\pi} u(\omega)\, d\omega = 0$. And by the smoothness of R, we find

$$\|R(\xi+\rho e^{i\theta}, \xi+\rho e^{i\omega}) - R(\xi,\xi)\|_{L^\infty} = O(\rho),$$

and consequently

$$\|\mathcal{B}'(0)(u)\|_{L^2} \le C\gamma\rho\|u\|_{L^2}. \tag{3.17}$$

The last part $\lambda'(0)$ of L maps $u \in H^2(S^1)\cap\{1,\cos\theta,\sin\theta\}^\perp$ into R. Therefore

$$\langle \Pi\lambda'(0)(u), u\rangle = \lambda'(0)(u)\int_0^{2\pi} u\, d\theta = 0. \tag{3.18}$$

Since

$$\overline{\mathcal{B}'(0)(u)} + \lambda'(0)(u) = 0,$$

by (3.17)

$$|\lambda'(0)(u)| \le C\gamma\rho\|u\|_{L^2}. \tag{3.19}$$

When $\gamma\rho^4$ is sufficiently small (3.11), (3.17) and (3.19) imply that

$$\begin{aligned} \|\Pi L(u)\|_{L^2} &\ge \|L_1(u)\|_{L^2} - \|(\mathcal{B}'(0)+\lambda'(0))(u)\|_{L^2} \\ &\ge \frac{C}{\rho^3}\|u\|_{L^2} - C\gamma\rho\|u\|_{L^2} \;\ge\; \frac{C}{\rho^3}\|u\|_{L^2} \end{aligned}$$

This proves Part 1 of the Lemma.

If (1.8) holds we derive from (3.13), (3.17) and (3.18) that

$$\langle \Pi L(u), u\rangle \ge \frac{C}{\rho^3}\|u\|^2_{L^2} - C\gamma\rho\|u\|^2_{L^2} \ge \frac{C}{\rho^3}\|u\|^2_{L^2}.$$

This proves Part 2.

Part 1 ensures that ΠL is one-to-one from $H^2(S^1)\cap\{1,\cos\theta,\sin\theta\}^\perp$ to $L^2(S^1)\cap\{1,\cos\theta,\sin\theta\}^\perp$. Since ΠL is self-adjoint and hence closed, (3) also ensures that the range of ΠL is closed. The Closed Range Theorem (See Yosida [44, Page 205], e.g.) then implies that ΠL is onto.

To prove Part 3 set $\Pi L(u) = g$. There exist $c_1, c_2 \in R$ such that

$$L_1(u) + \mathcal{B}'(0)(u) + \lambda'(0)(u) + c_1\cos\theta + c_2\sin\theta = g. \tag{3.20}$$

If we multiply (3.20) by $\cos\theta$ and integrate, then

$$\langle \mathcal{B}'(0)u, \cos\theta\rangle + c_1\|\cos\theta\|_{L^2}^2 = 0$$

from which we derive, with the help of (3.17), that

$$|c_1| \le C\gamma\rho\|u\|_{L^2}. \tag{3.21}$$

Similarly we have

$$|c_2| \le C\gamma\rho\|u\|_{L^2}. \tag{3.22}$$

Therefore by (3.15), (3.17), (3.19), (3.21), (3.22) and Part 1,

$$\begin{aligned}
\|u\|_{H^2} &\le C\rho^3\|L_1(u)\|_{L^2} \\
&\le C\rho^3\|g - \mathcal{B}'(0)(u) - \lambda'(0)(u) - c_1\cos\theta - c_2\sin\theta\|_{L^2} \\
&\le C\rho^3(\|g\|_{L^2} + \gamma\rho\|u\|_{L^2}) \\
&\le C\rho^3(\|g\|_{L^2} + C\gamma\rho^4\|\Pi L(u)\|_{L^2}) \\
&\le C\rho^3\|g\|_{L^2}
\end{aligned}$$

which proves Part 3 of the lemma.

To show Part 4 under (1.8), let

$$u(\theta) = \sum_{|n|=2}^{\infty} \widehat{u}(n)\frac{e^{in\theta}}{2\pi}$$

be the Fourier series of u. Then (1.8) asserts that

$$\frac{\lambda_n}{n^2} > \frac{\epsilon(n-1)}{4\rho^3 n} \tag{3.23}$$

which implies that

$$\begin{aligned}
\langle L_1(u), u\rangle &= \langle \sum_{|n|=2}^{\infty} \lambda_{|n|}\widehat{u}(n)\frac{e^{in\theta}}{2\pi}, \sum_{|n|=2}^{\infty}\widehat{u}(n)\frac{e^{in\theta}}{2\pi}\rangle \\
&= \sum_{|n|=2}^{\infty}\frac{\lambda_{|n|}|\widehat{u}(n)|^2}{2\pi} \;\ge\; \frac{C}{\rho^3}\sum_{|n|=2}^{\infty} n^2|\widehat{u}(n)|^2 \\
&\ge \frac{C}{\rho^3}\|u\|_{H^1}^2.
\end{aligned}$$

Finally by (3.17),

$$\langle \Pi L(u), u\rangle = \langle L(u), u\rangle = \langle L_1(u), u\rangle + \langle \mathcal{B}'(0)u, u\rangle \ge \frac{C}{\rho^3}\|u\|_{H^1}^2 - C\gamma\rho\|u\|_{L^2}^2 \ge \frac{C}{\rho^3}\|u\|_{H^1}^2. \quad \square$$

We also estimate the second Fréchet derivative of $S_\xi = \mathcal{H} + \mathcal{A} + \mathcal{B}_\xi + \lambda_\xi$.

Lemma 3.2 *There exists $c > 0$ such that if $\|\phi\|_{H^2} \le c\rho^2$, the following holds.*

1. $\|\mathcal{H}''(\phi)(u,v)\|_{L^2} \leq \dfrac{C}{\rho^5}\|u\|_{H^2}\|v\|_{H^2}$.

2. $\|\mathcal{A}''(\phi)(u,v)\|_{L^2} \leq \dfrac{C\gamma}{\rho^2}\|u\|_{H^1}\|v\|_{H^1}$.

3. $\|\mathcal{B}''_\xi(\phi)(u,v)\|_{L^2} \leq \dfrac{C\gamma}{\rho}\|u\|_{H^1}\|v\|_{H^1}$.

4. $|\lambda''_\xi(\phi)(u,v)| \leq (\dfrac{C}{\rho^5} + \dfrac{C\gamma}{\rho^2})\|u\|_{H^2}\|v\|_{H^2}$.

Proof. Note that by taking c small, we keep $\rho^2 + \phi$ positive, so E_ϕ is a perturbed disc.

$\mathcal{H}$ may be better understood after re-scaling. Introduce

$$\Phi = \frac{\phi}{\rho^2},\ \Phi' = \frac{\phi'}{\rho^2},\ \Phi'' = \frac{\phi''}{\rho^2},$$

and

$$\tilde{H}(\Phi, \Phi', \Phi'') = \rho\mathcal{H}(\phi, \phi', \phi'').$$

Then

$$\tilde{H}(\Phi, \Phi', \Phi'') = \frac{1 + \Phi + \frac{3(\Phi')^2}{4(1+\Phi)} - \frac{\Phi''}{2}}{(1 + \Phi + \frac{(\Phi')^2}{4(1+\Phi)})^{3/2}}$$

does not involve ρ. With a small c in the condition $\|\phi\|_{H^2} \leq c\rho^2$, $\|\Phi\|_{H^2}$ becomes small compared to 1. With $\tilde{H}_1(\Phi)$, $\tilde{H}_2(\Phi)$, and $\tilde{H}_3(\Phi)$ denoting the derivatives of $H(\Phi, \Phi', \Phi'')$ with respect to its three arguments, the second Fréchet derivative of $\tilde{H}$ is

$$\begin{aligned} &\tilde{H}''(\Phi, \Phi', \Phi'')(u, v) \\ &= \tilde{H}_{11}(\Phi)uv + \tilde{H}_{22}(\Phi)u'v' + \tilde{H}_{12}(\Phi)(u'v + uv') + \tilde{H}_{23}(\Phi)(u'v'' + u''v') + \tilde{H}_{31}(u''v + uv'')\end{aligned}$$

Note that we do not have $u''v''$ on the right side since $\tilde{H}_{33} = 0$. Because of this absence, the Sobolev Embedding Theorem implies

$$\|\tilde{H}''(\Phi)(u, v)\|_{L^2} \leq C\|u\|_{H^2}\|v\|_{H^2}$$

In terms of $\mathcal{H}$ and ϕ,

$$\|\mathcal{H}''(\phi)(u, v)\|_{L^2} \leq \frac{C}{\rho^5}\|u\|_{H^2}\|v\|_{H^2} \tag{3.24}$$

This proves Part 1.

To prove Part 2, let us again set $\Phi = \frac{\phi}{\rho^2}$ and introduce

$$A(\Phi)(\theta) = \int_0^{2\pi}\int_0^{\sqrt{1+\Phi(\omega)}} \log|\sqrt{1 + \Phi(\theta)}e^{i\theta} - se^{i\omega}|s\, ds d\omega. \tag{3.25}$$

Then

$$\mathcal{A}(\phi) = -\frac{\rho^2\gamma}{2\pi}A(\Phi) \tag{3.26}$$

The change from ϕ and $\mathcal{A}$ to Φ and A scales away ρ. The first Fréchet derivative of A is given by

$$\begin{aligned} A'(\Phi)(u)(\theta) &= \frac{1}{2}\int_0^{2\pi} u(\omega)\log|\sqrt{1+\Phi(\theta)}e^{i\theta}-\sqrt{1+\Phi(\omega)}e^{i\omega}|\,d\omega \\ &\quad +\frac{u(\theta)}{2\sqrt{1+\Phi(\theta)}}\int_0^{2\pi}\int_0^{\sqrt{1+\Phi(\omega)}} \frac{(\sqrt{1+\Phi(\theta)}e^{i\theta}-se^{i\omega})\cdot e^{i\theta}}{|\sqrt{1+\Phi(\theta)}e^{i\theta}-se^{i\omega}|^2} s\,dsd\omega \end{aligned} \tag{3.27}$$

The second Fréchet derivative of A is

$$A''(\Phi)(u,v) = A_1(\Phi)(u,v) + A_2(\Phi)(u,v) + A_3(\Phi)(u,v) + A_4(\Phi)(u,v) + A_5(\Phi)(u,v) \tag{3.28}$$

where

$$\begin{aligned} A_1(\Phi)(u,v) &= \frac{v(\theta)e^{i\theta}}{4\sqrt{1+\Phi(\theta)}}\cdot\int_0^{2\pi} K(\theta,\omega)u(\omega)\,d\omega \\ A_2(\Phi)(u,v) &= \frac{u(\theta)e^{i\theta}}{4\sqrt{1+\Phi(\theta)}}\cdot\int_0^{2\pi} K(\theta,\omega)v(\omega)\,d\omega \\ A_3(\Phi)(u,v) &= -\frac{1}{4}\int_0^{2\pi} K(\theta,\omega)\cdot\frac{u(\omega)v(\omega)e^{i\theta}}{\sqrt{1+\Phi(\omega)}}\,d\omega \\ A_4(\Phi)(u,v) &= \frac{u(\theta)v(\theta)}{4(1+\Phi(\theta))}\int_{E_\Phi} \frac{|\sqrt{1+\Phi(\theta)}e^{i\theta}-y|^2 - 2(\sqrt{1+\Phi(\theta)}-e^{i\theta}\cdot y)^2}{|\sqrt{1+\Phi(\theta)}e^{i\theta}-y|^4}\,dy \\ A_5(\Phi)(u,v) &= -\frac{u(\theta)v(\theta)}{4(1+\Phi(\theta))^{3/2}}\int_0^{2\pi}\int_0^{\sqrt{1+\Phi(\omega)}} \frac{(\sqrt{1+\Phi(\theta)}e^{i\theta}-se^{i\omega})\cdot e^{i\theta}}{|\sqrt{1+\Phi(\theta)}e^{i\theta}-se^{i\omega}|^2} s\,dsd\omega. \end{aligned}$$

The set E_Φ is a shifted and re-scaled version of E_ϕ:

$$E_\Phi = \{t\sqrt{1+\Phi(\theta)} : \theta\in[0,2\pi],\ t\in[0,1)\}. \tag{3.29}$$

The kernel K is

$$K(\theta,\omega) = \frac{\sqrt{1+\Phi(\theta)}e^{i\theta}-\sqrt{1+\Phi(\omega)}e^{i\omega}}{|\sqrt{1+\Phi(\theta)}e^{i\theta}-\sqrt{1+\Phi(\omega)}e^{i\omega}|^2} \tag{3.30}$$

Here we encounter a singular integral operator

$$K(u)(\theta) = \int_0^{2\pi} K(\theta,\omega)u(\omega)\,d\omega \tag{3.31}$$

since the singularity of $K(\theta,\omega)$ is of the type $\frac{\theta-\omega}{|\theta-\omega|^2}$. This operator is very much like the Hilbert transform. To define the operator properly, we first write

$$K(u)(\theta) = \int_0^{2\pi} K(\theta,\omega)(u(\omega)-u(\theta))\,d\omega + u(\theta)\int_0^{2\pi} K(\theta,\omega)\,d\omega. \tag{3.32}$$

For $u\in H^2(S^1)\subset H^1(S^1)$, u is Hölder continuous. Hence

$$|u(\omega)-u(\theta)| \le |\omega-\theta|^\alpha \|u\|_{C^\alpha}$$

for some $\alpha \in (0,1)$. Therefore

$$|K(\theta,\omega)(u(\omega)-u(\theta))| \le C|\omega-\theta|^{-1+\alpha}\|u\|_{C^\alpha},$$

and the first term in (3.32) is convergent. Here $\|u\|_\alpha$ is the C^α norm of u. The second term is defined by its principal part:

$$\int_0^{2\pi} K(\theta,\omega)\,d\omega = \lim_{\epsilon\to 0}\int_{|\omega-\theta|>\epsilon} K(\theta,\omega)\,d\omega.$$

The limit converges due to the cancellation effect for ω before and after θ. We have derived

$$\|K(u)\|_{L^\infty} \le C\|u\|_{C^\alpha} \le C\|u\|_{H^1}. \tag{3.33}$$

We can now estimate A_1, A_2 and A_3. By (3.33)

$$\|A_1(\Phi)(u,v)\|_{L^2} \le C\|u\|_{H^1}\|v\|_{L^2} \tag{3.34}$$

Similarly

$$\|A_2(\Phi)(u,v)\|_{L^2} \le C\|u\|_{L^2}\|v\|_{H^1}. \tag{3.35}$$

For A_3 we have

$$\|A_3(\Phi)(u,v)\|_{L^\infty} \le C\|uv\|_{C^\alpha} \le C\|u\|_{H^1}\|v\|_{H^1}. \tag{3.36}$$

We now turn to A_4. The integral

$$\int_{E_\Phi} \frac{|\sqrt{1+\Phi(\theta)}e^{i\theta}-y|^2 - 2(\sqrt{1+\Phi(\theta)}-e^{i\theta}\cdot y)^2}{|\sqrt{1+\Phi(\theta)}e^{i\theta}-y|^4}\,dy$$

is a convergent improper integral defined by its principal part. It is uniformly bounded with respect to θ. In the case of Φ equal to 0, it may be explicitly computed. (See Appendix B.) Therefore

$$\|A_4(\Phi)(u,v)\|_{L^\infty} \le C\|u\|_{H^1}\|v\|_{H^1} \tag{3.37}$$

For A_5, because of the mild singularity, we easily find

$$\|A_5(\Phi)(u,v)\|_{L^\infty} \le C\|u\|_{H^1}\|v\|_{H^1}. \tag{3.38}$$

Following (3.34), (3.35), (3.36), (3.37) and (3.38) we obtain

$$\|A''(\Phi)(u,v)\|_{L^2} \le C\|u\|_{H^1}\|v\|_{H^1}, \tag{3.39}$$

and by (3.26) we have

$$\|\mathcal{A}''(\phi)(u,v)\|_{L^2} \le \frac{C\gamma}{\rho^2}\|u\|_{H^1}\|v\|_{H^1},$$

proving Part 2.

The kernel R in B_ξ is a smooth function. Calculations show that

$$\begin{aligned}
\mathcal{B}''_\xi(\phi)(u,v) &= \frac{\gamma v(\theta)}{4\sqrt{\rho^2+\phi(\theta)}}\int_0^{2\pi} u(\omega)\nabla_1 R(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},\xi+\sqrt{\rho^2+\phi(\omega)}e^{i\omega})\cdot e^{i\theta}\,d\omega \\
&+\frac{\gamma u(\theta)}{4\sqrt{\rho^2+\phi(\theta)}}\int_0^{2\pi} v(\omega)\nabla_1 R(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},\xi+\sqrt{\rho^2+\phi(\omega)}e^{i\omega})\cdot e^{i\theta}\,d\omega \\
&+\frac{\gamma}{4}\int_0^{2\pi}\frac{u(\omega)v(\omega)}{\sqrt{\rho^2+\phi(\omega)}}\nabla_2 R(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},\xi+\sqrt{\rho^2+\phi(\omega)}e^{i\omega})\cdot e^{i\omega}\,d\omega \\
&+\frac{\gamma u(\theta)v(\theta)}{4(\rho^2+\phi(\theta))}\int_{E_\phi}(D_1^2 R(\xi+\sqrt{\rho^2+\phi(\theta)},y)e^{i\theta}\cdot e^{i\theta})\,dy \\
&-\frac{\gamma u(\theta)v(\theta)}{4(\rho^2+\phi(\theta))^{3/2}}\int_{E_\phi}\nabla_1 R(\xi+\sqrt{\rho^2+\phi(\theta)}e^{i\theta},y)\cdot e^{i\theta}\,dy
\end{aligned}$$

where ∇_1 and ∇_2 refer to the derivatives of R with respect to its first and second arguments respectively. $D_1^2 R$ is the second derivative matrix of R with respect to the first argument of R. Part 3 is now proved easily.

Part 4 follows from Parts 1-3 and the fact that

$$0=\overline{S''_\xi(\phi)(u,v)}=\overline{\mathcal{H}''(\phi)(u,v)}+\overline{\mathcal{A}''(\phi)(u,v)}+\overline{\mathcal{B}''_\xi(\phi)(u,v)}+\lambda''_\xi(\phi)(u,v).\ \square$$

Lemma 3.3 *There exists $\varphi=\varphi(\theta,\xi)$ such that for every $\xi\in U$, $\varphi(\cdot,\xi)\in H^2(S^1)\cap\{1,\cos\theta,\sin\theta\}^\perp$ solves (3.5) and $\|\varphi(\cdot,\xi)\|_{H^2}\le c\gamma\rho^6$ where c is a sufficiently large constant independent of ξ, ρ and γ.*

Proof. For simplicity we again assume that $\xi=0$ and set $B_\xi=B$, $L_\xi=L$, etc. Recall the fixed point setting (3.5). To use the Contraction Mapping Principle, let

$$T(\phi)=-(\Pi L)^{-1}(\Pi S(0)+\Pi N(\phi)) \tag{3.40}$$

be an operator defined on

$$D(T)=\{\phi\in H^2(S^1)\cap\{1,\cos\theta,\sin\theta\}^\perp:\|\phi\|_{H^2}\le c\rho^6\gamma\} \tag{3.41}$$

where the constant c is sufficiently large which will be made more transparent later.

It is clear from Lemmas 2.2 and 3.1 that

$$\|(\Pi L)^{-1}\Pi S(0)\|_{H^2}\le C\gamma\rho^6. \tag{3.42}$$

More difficult is the estimation of $N(\phi)$. We decompose $N(\phi)$ into three parts. The first is

$$N_1(\phi)=\mathcal{H}(\phi)-\frac{1}{\rho}+\frac{1}{2\rho^3}(\phi''+\phi)=\mathcal{H}(\phi)-\mathcal{H}(0)-\mathcal{H}'(0)(\phi) \tag{3.43}$$

which is $\mathcal{H}(\phi)$ minus its linear approximation at ϕ equal to 0. Lemma 3.2, Part 1, shows that

$$\|N_1(\phi)\|_{L^2}\le\frac{C}{\rho^5}\|\phi\|_{H^2}^2. \tag{3.44}$$

The second part of N, which we denote by N_2, is $\mathcal{A}(\phi)+\mathcal{B}(\phi)$ minus its linear approximation, i.e.

$$N_2(\phi)=\mathcal{A}(\phi)-\mathcal{A}(0)-\mathcal{A}'(0)(\phi)+\mathcal{B}(\phi)-\mathcal{B}(0)-\mathcal{B}'(0)(\phi). \tag{3.45}$$

Lemma 3.2, Parts 2 and 3, implies that

$$\|N_2(\phi)\|_{L^2}\le\frac{C\gamma}{\rho^2}\|\phi\|^2_{H^1} \tag{3.46}$$

The third part of N, which is denoted by N_3, merely gives a constant so that

$$\overline{N(\phi)}=\overline{N_1(\phi)}+\overline{N_2(\phi)}+N_3(\phi)=0.$$

It follows that

$$|N_3(\phi)|\le\frac{C}{\rho^5}\|\phi\|^2_{H^2}+\frac{C\gamma}{\rho^2}\|\phi\|^2_{H^1}. \tag{3.47}$$

Therefore we deduce, from (3.44), (3.46), (3.47) and with the help of Lemma 3.1, that

$$\begin{aligned}\|N(\phi)\|_{L^2} &\le \frac{C}{\rho^5}\|\phi\|^2_{H^2}+\frac{C\gamma}{\rho^2}\|\phi\|^2_{H^1} && (3.48)\\ \|(\Pi L)^{-1}\Pi N(\phi)\|_{H^2} &\le \frac{C}{\rho^2}\|\phi\|^2_{H^2}+C\gamma\rho\|\phi\|^2_{H^1} && (3.49)\end{aligned}$$

Using (1.7), (3.42), (3.41), and (3.49) we find

$$\|T(\phi)\|_{H^2}\le C\gamma\rho^6+Cc^2\gamma^2\rho^{10}+Cc^2\gamma^3\rho^{13}\le c\gamma\rho^6$$

if c is sufficiently large and $\gamma\rho^4$ sufficiently small. Therefore T is a map from $D(T)$ into itself.

Finally we show that T is a contraction. Let $\phi_1,\phi_2\in D(T)$. To estimate $N_1(\phi_1)-N_1(\phi_2)$ we proceed as in the proof of Lemma 3.2, Part 1. Let $\Phi_1=\frac{\phi_1}{\rho^2}$ and $\Phi_2=\frac{\phi_2}{\rho^2}$. Then, writing $\tilde H(\Phi_1)$ for $\tilde H(\Phi_1,\Phi_1',\Phi_1'')$ for simplicity, we find

$$\begin{aligned}
&\rho|N_1(\phi_1)-N_1(\phi_2)|\\
&= |\tilde H(\Phi_1)-\tilde H(\Phi_2)-\tilde H_1(0)(\Phi_1-\Phi_2)-\tilde H_2(0)(\Phi_1'-\Phi_2')-\tilde H_3(0)(\Phi_1''-\Phi_2'')|\\
&= |\tilde H_1(\Phi_2)(\Phi_1-\Phi_2)+\tilde H_2(\Phi_2)(\Phi_1'-\Phi_2')+\tilde H_3(\Phi_2)(\Phi_1''-\Phi_2'')\\
&\quad +\frac{1}{2}\tilde H_{11}(t\Phi_1-(1-t)\Phi_2)(\Phi_1-\Phi_2)^2+\frac{1}{2}\tilde H_{22}(t\Phi_1-(1-t)\Phi_2)(\Phi_1'-\Phi_2')^2\\
&\quad +\tilde H_{12}(t\Phi_1-(1-t)\Phi_2)(\Phi_1-\Phi_2)(\Phi_1'-\Phi_2')+\tilde H_{23}(t\Phi_1-(1-t)\Phi_2)(\Phi_1'-\Phi_2')(\Phi_1''-\Phi_2'')\\
&\quad +\tilde H_{31}(t\Phi_1-(1-t)\Phi_2)(\Phi_1''-\Phi_2'')(\Phi_1-\Phi_2)\\
&\quad -\tilde H_1(0)(\Phi_1-\Phi_2)-\tilde H_2(0)(\Phi_1'-\Phi_2')-\tilde H_3(0)(\Phi_1''-\Phi_2'')|\\
&\le C[(|\Phi_1|+|\Phi_2|)|\Phi_1-\Phi_2|+(|\Phi_1'|+|\Phi_2'|)|\Phi_1'-\Phi_2'|\\
&\quad +(|\Phi_1|+|\Phi_2|)|\Phi_1'-\Phi_2'|+(|\Phi_1'|+|\Phi_2'|)|\Phi_1-\Phi_2|\\
&\quad +(|\Phi_1'|+|\Phi_2'|)|\Phi_1''-\Phi_2''|+(|\Phi_1''|+|\Phi_2''|)|\Phi_1'-\Phi_2'|\\
&\quad +(|\Phi_1''|+|\Phi_2''|)|\Phi_1-\Phi_2|+(|\Phi_1|+|\Phi_2|)|\Phi_1''-\Phi_2''|].
\end{aligned}$$

Since there is no $(|\Phi_1''|+|\Phi_2''|)|\Phi_1''-\Phi_2''|$ term, by the Sobolev Embedding Theorem we deduce, after returning to ϕ_1 and ϕ_2,

$$\|N_1(\phi_1)-N_1(\phi_2)\|_{L^2} \le \frac{C}{\rho^5}(\|\phi_1\|_{H^2}+\|\phi\|_{H^2})\|\phi_1-\phi_2\|_{H^2} \le C\gamma\rho\|\phi_1-\phi_2\|_{H^2}. \tag{3.50}$$

For N_2 we note that

$$N_2(\phi_1)-N_2(\phi_2) = \mathcal{A}(\phi_1)-\mathcal{A}(\phi_2)-\mathcal{A}'(0)(\phi_1-\phi_2)+\mathcal{B}(\phi_1)-\mathcal{B}(\phi_2)-\mathcal{B}'(0)(\phi_1-\phi_2). \tag{3.51}$$

Therefore using Lemma 3.2, Part 2, we obtain

$$\begin{aligned}
&\|\mathcal{A}(\phi_1)-\mathcal{A}(\phi_2)-\mathcal{A}'(0)(\phi_1-\phi_2)\|_{L^2} \\
\le\ & \|\mathcal{A}'(\phi_2)(\phi_1-\phi_2)-\mathcal{A}'(0)(\phi_1-\phi_2)\|_{L^2}+\frac{C\gamma}{\rho^2}\|\phi_1-\phi_2\|_{H^1}^2 \\
\le\ & \frac{C\gamma}{\rho^2}\|\phi_2\|_{H^1}\|\phi_1-\phi_2\|_{H^1}+\frac{C\gamma}{\rho^2}\|\phi_1-\phi_2\|_{H^1}^2 \\
\le\ & \frac{C\gamma}{\rho^2}(\|\phi_1\|_{H^1}+\|\phi_2\|_{H^1})\|\phi_1-\phi_2\|_{H^1}.
\end{aligned}$$

Similarly using Lemma 3.2, Part 3, we deduce

$$\|\mathcal{B}(\phi_1)-\mathcal{B}(\phi_2)-\mathcal{B}'(0)(\phi_1-\phi_2)\|_{L^2} \le \frac{C\gamma}{\rho}(\|\phi_1\|_{H^1}+\|\phi_2\|_{H^1})\|\phi_1-\phi_2\|_{H^1}.$$

From (3.51) we conclude that

$$\|N_2(\phi_1)-N_2(\phi_2)\|_{L^2} \le \frac{C\gamma}{\rho^2}(\|\phi_1\|_{H^1}+\|\phi_2\|_{H^1})\|\phi_1-\phi_2\|_{H^1} \le C\gamma^2\rho^4\|\phi_1-\phi_2\|_{H^1} \tag{3.52}$$

We also have

$$\|N_3(\phi_1)-N_3(\phi_2)\|_{L^2} \le C(\gamma\rho+\gamma^2\rho^4)\|\phi_1-\phi_2\|_{H^2}. \tag{3.53}$$

Hence, following (3.50), (3.52), and (3.53), we find that

$$\|T(\phi_1)-T(\phi_2)\|_{H^2} \le C(\gamma\rho^4+\gamma^2\rho^7)\|\phi_1-\phi_2\|_{H^2}, \tag{3.54}$$

i.e. that T is a contraction map if $\gamma\rho^4$ is sufficiently small, with the help of (1.7). A fixed point φ is found. $\square$

Since φ satisfies $\|\phi\|_{H^2} \le c\gamma\rho^6$, by taking δ small we see that $c\gamma\rho^4$ is small and hence $\rho^2+\varphi$ remains positive. E_φ is a perturbed disc.

4 Existence

We prove Theorem 1.1 in this section. From Lemma 3.3 we know that for every $\xi=(\xi_1,\xi_2)\in U$ there exists $\varphi(\cdot,\xi)\in H^2(S^1)\cap\{1,\sin\theta,\cos\theta\}^\perp$ such that $\Pi S_\xi(\varphi(\cdot,\xi))=0$, i.e. (3.1) holds. In this section we find a particular ξ, denoted by ζ, in U such that $S_\zeta(\varphi(\cdot,\zeta))=0$.

But first we state a result regarding the linearization of S_ξ at $\varphi(\cdot,\xi)$. Denote the linearized operator by $\tilde{L}_\xi$. We have the following analog to Lemma 3.1.

Lemma 4.1 *Let Π be the same projection operator to $L^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$.*

1. *There exists $C > 0$ such that for all $u \in H^2(S^1) \cap \{1, \cos\theta, \sin\theta\}^\perp$*

$$\|u\|_{H^2} \leq C\rho^3 \|\Pi \tilde{L}_\xi(u)\|_{L^2}$$

2. *If (1.8) holds,*

$$\|u\|_{H^1}^2 \leq C\rho^3 \langle \Pi \tilde{L}_\xi(u), u\rangle.$$

Proof. In this proof we again assume, without the loss of generality, that $\xi = 0$, and write L, $\tilde{L}$ for L_ξ, $\tilde{L}_\xi$, etc.

By Lemma 3.1, Part 3, Lemma 3.2, (1.7), and the fact $\|\varphi\|_{H^2} = O(\gamma\rho^6)$, we deduce

$$\begin{aligned}
\|\Pi\tilde{L}(u)\|_{L^2} &\geq \|\Pi L(u)\|_{L^2} - \|\Pi(\tilde{L} - L)(u)\|_{L^2} \\
&\geq \frac{C}{\rho^3}\|u\|_{H^2} - (\frac{C}{\rho^5} + \frac{C\gamma}{\rho^2})\|\varphi\|_{H^2}\|u\|_{H^2} \\
&\geq \frac{C}{\rho^3}\|u\|_{H^2} - C(\gamma\rho + \gamma^2\rho^4)\|u\|_{H^2} \\
&\geq \frac{C}{\rho^3}\|u\|_{H^2}
\end{aligned}$$

when $\gamma\rho^4$ is small.

Write $\tilde{L} = \mathcal{H}'(\varphi) + \mathcal{A}'(\varphi) + \mathcal{B}'(\varphi) + \lambda'_\xi(\varphi)$. Let

$$Q(\varphi, \varphi') = 2\sqrt{\rho^2 + \varphi + \frac{(\varphi')^2}{4(\rho^2 + \varphi)}}. \tag{4.1}$$

Then

$$\langle \mathcal{H}'(\varphi)(u), u\rangle = \int_0^{2\pi} [Q_{11}(\varphi, \varphi')u^2 + 2Q_{12}(\varphi, \varphi')uu' + Q_{22}(\varphi, \varphi')(u')^2]\, d\theta.$$

and a similar expression holds for L if we replace φ and φ' by 0 in the last formula. Here Q_{11} is the second derivative with respect to the first argument of Q, etc. With $\|\varphi\|_{H^2} = O(\gamma\rho^6)$ calculations show that

$$\begin{aligned}
|\langle(\mathcal{H}''(\varphi) - \mathcal{H}'(0))u, u\rangle| &\leq |\int_0^{2\pi} (Q_{11}(\varphi, \varphi') - Q_{11}(0,0))u^2\, d\theta| \\
&\quad + |\int_0^{2\pi} 2(Q_{12}(\varphi, \varphi') - Q_{12}(0,0))uu'\, d\theta| \\
&\quad + |\int_0^{2\pi} (Q_{22}(\varphi, \varphi') - Q_{22}(0,0))(u')^2\, d\theta| \\
&\leq C\gamma\rho\|u\|_{L^2}^2 + C\gamma\rho\|u\|_{L^2}\|u'\|_{L^2} + C\gamma\rho\|u'\|_{L^2}^2 \\
&\leq C\gamma\rho\|u\|_{H^1}^2
\end{aligned} \tag{4.2}$$

Lemma 3.2, Parts 2 and 3, and the fact $\|\varphi\|_{H^2} = O(\gamma\rho^6)$ show that

$$\|(\mathcal{A}'(\varphi) + \mathcal{B}'(\varphi) - \mathcal{A}'(0) - \mathcal{B}'(0))u\|_{L^2} \leq C\gamma^2\rho^4\|u\|_{H^1}. \tag{4.3}$$

Finally we combine Lemma 3.1, Part 4, (4.2), (4.3) and (1.7) to deduce that

$$\langle \Pi\tilde{L}(u), u\rangle = \langle \Pi L(u), u\rangle + \langle \Pi(\tilde{L}-L)u, u\rangle \geq \frac{C}{\rho^3}\|u\|_{H^1}^2 - C\gamma\rho\|u\|_{H^1}^2 - C\gamma^2\rho^4\|u\|_{H^1}^2 \geq \frac{C}{\rho^3}\|u\|_{H^1}^2,$$

proving the lemma. □

One consequence of this lemma is an estimate of $\frac{\partial\varphi}{\partial\xi_j}$.

Lemma 4.2 *For each $\xi \in U$, φ satisfies $\|\frac{\partial\varphi}{\partial\xi_j}\|_{H^2} = O(\gamma\rho^5)$, $j = 1, 2$.*

Proof. We prove this lemma by the Implicit Function Theorem. Differentiating $\Pi S_\xi(\varphi)$ with respect to ξ_j finds that

$$\begin{aligned} 0 &= \frac{\partial \Pi S_\xi(\varphi)}{\partial\xi_j} \\ &= \Pi\tilde{L}_\xi(\frac{\partial\varphi}{\partial\xi_j}) + \Pi\gamma\int_{E_\varphi}[\frac{\partial R(\xi+\sqrt{\rho^2+\varphi(\theta)}e^{i\theta}, y)}{\partial x_j} + \frac{\partial R(\xi+\sqrt{\rho^2+\varphi(\theta)}e^{i\theta}, y)}{\partial y_j}]\,dy \\ &\quad \overline{-\gamma\int_{E_\varphi}[\frac{\partial R(\xi+\sqrt{\rho^2+\varphi(\theta)}e^{i\theta}, y)}{\partial x_j} + \frac{\partial R(\xi+\sqrt{\rho^2+\varphi(\theta)}e^{i\theta}, y)}{\partial y_j}]\,dy} \end{aligned}$$

where $R = R(x, y)$. It is clear that

$$\|\int_{E_\varphi}[\frac{\partial R(\xi+\sqrt{\rho^2+\varphi(\theta)}e^{i\theta}, y)}{\partial x_j} + \frac{\partial R(\xi+\sqrt{\rho^2+\varphi(\theta)}e^{i\theta}, y)}{\partial y_j}]\,dy\|_{L^2} = O(\rho^2),$$

and

$$\|\overline{\int_{E_\varphi}[\frac{\partial R(\xi+\sqrt{\rho^2+\varphi(\theta)}e^{i\theta}, y)}{\partial x_j} + \frac{\partial R(\xi+\sqrt{\rho^2+\varphi(\theta)}e^{i\theta}, y)}{\partial y_j}]\,dy}\|_{L^2} = O(\rho^2).$$

With the help of Lemma 4.1 we deduce that

$$\|\frac{\partial\varphi}{\partial\xi_j}\|_{H^2} \leq C\rho^3\rho^2\gamma = C\gamma\rho^5. \quad \square$$

We now turn to solve $S_\xi(\phi) = 0$.

Lemma 4.3 $J(E_{\varphi(\cdot,\xi)}) = J(B_\xi) + O(\gamma^2\rho^9)$.

Proof. In this proof without the loss of generality we take $\xi = 0$. Expanding $J(E_\varphi)$ yields

$$J(E_\varphi) = J(B) + \frac{1}{2}\int_0^{2\pi} S(0)\varphi\,d\theta + \frac{1}{4}\int_0^{2\pi} L(\varphi)\varphi\,d\theta + O(\gamma^3\rho^{13}) + O(\gamma^4\rho^{16}). \tag{4.4}$$

The two error terms in (4.4) are obtained in the same way that (3.48) is derived.

On the other hand $\Pi S_\xi(\varphi) = 0$ implies that

$$\Pi(S(0) + L(\varphi) + N(\varphi)) = 0$$

where N is given in (3.4) and estimated in (3.48). We multiply the last equation by φ and integrate to derive

$$\int_0^{2\pi} S(0)\varphi\,d\theta + \int_0^{2\pi} L(\varphi)\varphi\,d\theta = O(\gamma^3\rho^{13}) + O(\gamma^4\rho^{16}).$$

We can now rewrite (4.4) as

$$J(E_\varphi) = J(B) + \frac{1}{4}\int_0^{2\pi} S(0)\varphi\,d\theta + O(\gamma^3\rho^{13}) + O(\gamma^4\rho^{16}).$$

Lemma 2.2 implies that

$$J(E_\varphi) = J(B) + O(\gamma^2\rho^9) + O(\gamma^3\rho^{13}) + O(\gamma^4\rho^{16}) = J(B) + O(\gamma^2\rho^9).$$

because of (1.6) and (1.7). □

If we consider $J(\varphi(\cdot,\xi))$ as a function of ξ, then Lemmas 2.3 and 4.3 imply that

$$J(E_{\varphi(\cdot,\xi)}) = 2\pi\rho + \frac{\pi^2\gamma\rho^4}{2}[\frac{-\log\rho}{2\pi} + \frac{1}{8\pi} + \tilde{R}(\xi) + \frac{\rho^2}{4|D|}] + O(\gamma^2\rho^9). \tag{4.5}$$

Because of the definition of U, (1.6) and (4.5), there is $\zeta \in U$ such that $J(E_{\varphi(\cdot,\xi)})$ is minimized at $\xi = \zeta$. This ζ is close to a global minimum of $\tilde{R}$. We prove the existence of a solution in the next lemma. It uses a tricky re-parametrization technique.

Lemma 4.4 *At* $\xi = \zeta$, $S_\zeta(\varphi(\cdot,\zeta)) = 0$.

Proof. For $\xi = (\xi_1, \xi_2)$ near ζ we re-parametrize $\partial_D E_{\varphi(\cdot,\xi)}$. Let ζ be the center of a new polar coordinates, $\rho^2 + \psi$ the new radius square and η the new angle. A point on $\partial_D E_{\varphi(\cdot,\xi)}$ is described as $\zeta + \sqrt{\rho^2+\psi}e^{i\eta}$. It is related to the old polar coordinates via

$$\zeta + \sqrt{\rho^2+\psi}e^{i\eta} = \xi + \sqrt{\rho^2+\varphi}e^{i\theta} \tag{4.6}$$

In the new coordinates E_φ becomes E_ψ. It is viewed as a perturbation of the disc centered at ζ with radius ρ. The perturbation is described by ψ which is a function of η and ξ.

The main effect of the new coordinates is to "freeze" the center. The center of the new polar system is ζ which is fixed while the center of the old polar system is ξ which varies in U.

We now consider the derivative of $J(E_{\varphi(\cdot,\xi)}) = J(E_{\psi(\cdot,\xi)})$ with respect to ξ. On one hand, at $\xi = \zeta$,

$$\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial \xi_j}|_{\xi=\zeta} = \frac{\partial J(E_{\varphi(\cdot,\xi)})}{\partial \xi_j}|_{\xi=\zeta} = 0, \quad j = 1, 2, \tag{4.7}$$

since ζ is a minimum.

On the other hand calculations show that

$$\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial \xi_j} = \frac{1}{2}\int_0^{2\pi} S_\zeta(\psi(\cdot,\xi))(\eta)\frac{\partial\psi}{\partial\xi_j}\,d\eta. \tag{4.8}$$

We emphasize that (4.8) is obtained under the re-parametrized coordinates, in which the dependence of $J(E_{\psi(\cdot,\xi)})$ on ξ is only reflected in the dependence of ψ on ξ. Had we calculated in the original coordinates, ξ would have appeared also in the nonlocal part of J through $R(\xi+..., \xi+...)$. The result would have been very different from (4.8). See the proof of Lemma 4.2 which involves differentiation with respect to ξ in the original coordinates. In the derivation of (4.8) we have used the fact that $\int_0^{2\pi} \psi\, d\eta = 0$ which implies that $\int_0^{2\pi} \frac{\partial \psi}{\partial \xi_j}\, d\eta = 0$, so that $\int_0^{2\pi} \lambda_\zeta(\psi) \frac{\partial \psi}{\partial \xi_j}\, d\eta = 0$ where $\lambda_\zeta(\psi)$ is part of

$$S_\zeta(\psi) = \mathcal{H}(\psi) + \mathcal{A}(\psi) + \mathcal{B}_\zeta(\psi) + \lambda_\zeta(\psi),$$

and we can reach the right side of (4.8). See Remark 2.1 for the coefficient $\frac{1}{2}$ in (4.8).

The expression $S_\xi(\phi)$ is invariant under re-parametrization, i.e.

$$S_\xi(\varphi(\cdot,\xi))(\theta) = S_\zeta(\psi(\cdot,\xi))(\eta). \tag{4.9}$$

Now we return to the original coordinate system and integrate with respect to θ in (4.8). Then

$$\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial \xi_j} = \frac{1}{2} \int_0^{2\pi} S_\xi(\varphi(\cdot,\xi))(\theta) \frac{\partial \psi(\eta(\theta,\xi),\xi)}{\partial \xi_j} \frac{\partial \eta}{\partial \theta}\, d\theta \tag{4.10}$$

We recall that ψ and η are defined implicitly as functions of θ and ξ by (4.6). Let us agree that $\psi = \psi(\eta,\xi)$ is a function of η and ξ. Set $\Psi(\theta,\xi) = \psi(\eta(\theta,\xi),\xi)$. Implicit differentiation shows that, with the help of Lemmas 3.3 and 4.2,

$$\begin{aligned}
\begin{bmatrix} \frac{\partial \eta}{\partial \theta} & \frac{\partial \eta}{\partial \xi_1} & \frac{\partial \eta}{\partial \xi_2} \\[2ex] \frac{\partial \Psi}{\partial \theta} & \frac{\partial \Psi}{\partial \xi_1} & \frac{\partial \Psi}{\partial \xi_2} \end{bmatrix} &= - \begin{bmatrix} \sqrt{\rho^2+\Psi}\sin\eta & -\frac{\cos\eta}{2\sqrt{\rho^2+\Psi}} \\[2ex] -\sqrt{\rho^2+\Psi}\cos\eta & -\frac{\sin\eta}{2\sqrt{\rho^2+\Psi}} \end{bmatrix}^{-1} \\
&\times \begin{bmatrix} \frac{\cos\theta}{2\sqrt{\rho^2+\varphi}}\frac{\partial\varphi}{\partial\theta} - \sqrt{\rho^2+\varphi}\sin\theta & 1 + \frac{\cos\theta}{2\sqrt{\rho^2+\varphi}}\frac{\partial\varphi}{\partial\xi_1} & \frac{\cos\theta}{2\sqrt{\rho^2+\varphi}}\frac{\partial\varphi}{\partial\xi_2} \\[2ex] \frac{\sin\theta}{2\sqrt{\rho^2+\varphi}}\frac{\partial\varphi}{\partial\theta} + \sqrt{\rho^2+\varphi}\cos\theta & \frac{\sin\theta}{2\sqrt{\rho^2+\varphi}}\frac{\partial\varphi}{\partial\xi_1} & 1 + \frac{\sin\theta}{2\sqrt{\rho^2+\varphi}}\frac{\partial\varphi}{\partial\xi_2} \end{bmatrix} \\
&= 2 \begin{bmatrix} \frac{-\sin\eta}{2\sqrt{\rho^2+\Psi}} & \frac{\cos\eta}{2\sqrt{\rho^2+\Psi}} \\ \sqrt{\rho^2+\Psi}\cos\eta & \sqrt{\rho^2+\Psi}\sin\eta \end{bmatrix} \\
&\times \begin{bmatrix} -\sqrt{\rho^2+\varphi}\sin\theta + O(\gamma\rho^5) & 1+O(\gamma\rho^4) & O(\gamma\rho^4) \\ \sqrt{\rho^2+\varphi}\cos\theta + O(\gamma\rho^5) & O(\gamma\rho^4) & 1+O(\gamma\rho^4) \end{bmatrix}
\end{aligned}$$

At $\xi = \zeta$, $\eta = \theta$, $\Psi = \varphi$ and the above becomes

$$\begin{bmatrix} \frac{\partial \eta}{\partial \theta} & \frac{\partial \eta}{\partial \xi_1} & \frac{\partial \eta}{\partial \xi_2} \\[2ex] \frac{\partial \Psi}{\partial \theta} & \frac{\partial \Psi}{\partial \xi_1} & \frac{\partial \Psi}{\partial \xi_2} \end{bmatrix}_{\xi=\zeta} = \begin{bmatrix} 1+O(\gamma\rho^4) & -\frac{\sin\theta}{\sqrt{\rho^2+\varphi}} + O(\gamma\rho^3) & \frac{\cos\theta}{\sqrt{\rho^2+\varphi}} + O(\gamma\rho^3) \\[2ex] O(\gamma\rho^6) & 2\sqrt{\rho^2+\varphi}\cos\theta + O(\gamma\rho^5) & 2\sqrt{\rho^2+\varphi}\sin\theta + O(\gamma\rho^5) \end{bmatrix} \tag{4.11}$$

We have found that at $\xi = \zeta$,

$$\frac{\partial \Psi}{\partial \xi_1}|_{\xi=\zeta} = 2\rho\cos\theta + O(\gamma\rho^5), \quad \frac{\partial \Psi}{\partial \xi_2}|_{\xi=\zeta} = 2\rho\sin\theta + O(\gamma\rho^5). \tag{4.12}$$

To compute $\frac{\partial\psi}{\partial\xi_j}$, we invert $\eta = \eta(\xi, \theta)$ to express $\theta = \Theta(\eta, \xi)$. Then

$$\frac{\partial\psi}{\partial\xi_j} = \frac{\partial\Psi}{\partial\xi_j} + \frac{\partial\Psi}{\partial\theta}\frac{\partial\Theta}{\partial\xi_j}.$$

At $\xi = \zeta$, since

$$\frac{\partial\Psi}{\partial\theta}|_{\xi=\zeta} = O(\gamma\rho^6), \quad \frac{\partial\Theta}{\partial\xi_j}|_{\xi=\zeta} = -\frac{\frac{\partial\eta}{\partial\xi_j}}{\frac{\partial\eta}{\partial\theta}} = O(\frac{1}{\rho}), \tag{4.13}$$

we deduce that

$$\frac{\partial\psi}{\partial\xi_1}|_{\xi=\zeta} = 2\rho\cos\theta + O(\gamma\rho^5), \quad \frac{\partial\psi}{\partial\xi_2}|_{\xi=\zeta} = 2\rho\sin\theta + O(\gamma\rho^5). \tag{4.14}$$

Following (4.14) and the fact that $\frac{\partial\eta}{\partial\theta}|_{\xi=\zeta} = 1 + O(\rho^4\gamma)$ we find that (4.10) becomes

$$\begin{aligned}
\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial\xi_1}|_{\xi=\zeta} &= \frac{1}{2}\int_0^{2\pi} S_\zeta(\varphi)(2\rho\cos\theta + O(\gamma\rho^5))\,d\theta, \\
\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial\xi_2}|_{\xi=\zeta} &= \frac{1}{2}\int_0^{2\pi} S_\zeta(\varphi)(2\rho\sin\theta + O(\gamma\rho^5))\,d\theta,
\end{aligned} \tag{4.15}$$

Now we combine (3.1), (4.7) and (4.15) to derive that

$$\begin{aligned}
A_{1,\zeta}\int_0^{2\pi}\cos\theta(2\rho\cos\theta + O(\gamma\rho^5))\,d\theta + A_{2,\zeta}\int_0^{2\pi}\sin\theta(2\rho\cos\theta + O(\gamma\rho^5))\,d\theta &= 0 \\
A_{1,\zeta}\int_0^{2\pi}\cos\theta(2\rho\sin\theta + O(\gamma\rho^5))\,d\theta + A_{2,\zeta}\int_0^{2\pi}\sin\theta(2\rho\sin\theta + O(\gamma\rho^5))\,d\theta &= 0.
\end{aligned}$$

Writing the system in matrix form

$$\begin{bmatrix} 2\pi\rho + O(\gamma\rho^5) & O(\gamma\rho^5) \\ O(\gamma\rho^5) & 2\pi\rho + O(\gamma\rho^5) \end{bmatrix} \begin{bmatrix} A_{1,\zeta} \\ A_{2,\zeta} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{4.16}$$

we deduce, since (4.16) is non-singular when $\gamma\rho^4$ is small, $A_{1,\zeta} = A_{2,\zeta} = 0$, proving the lemma. $\square$

We have proved the existence part of Theorem 1.1. Because $\|\varphi(\cdot,\zeta)\|_{H^2} = O(\rho^6\gamma)$, the approximate radius of the perturbed disc $E_{\varphi(\cdot,\zeta)}$ is

$$\sqrt{\rho^2 + \varphi(\theta,\zeta)} = \rho + O(\gamma\rho^5), \quad \text{at each } \ \theta \in [0, 2\pi]. \tag{4.17}$$

The center of the disc is ζ which is close to a minimum of $\tilde{R}$.

In this theorem a solution is termed stable if it is a local minimizer of J in the space

$$U \times \{\phi: \ \phi \in H^1(S^1), \ \phi \perp 1, \ \cos\theta, \ \sin\theta\}. \tag{4.18}$$

Under the condition (1.8) Lemma 4.1, Part 2, shows that each $\varphi(\cdot,\xi)$ we found in Lemma 3.3 locally minimizes J, with fixed $\xi \in U$, in $\{\phi : \phi \in H^1(S^1), \ \phi \perp 1, \ \cos\theta, \ \sin\theta\}$. On the other hand $\varphi(\cdot,\zeta)$ minimizes $J(E_{\varphi(\cdot,\xi)})$ with respect to ξ. Hence $\varphi(\cdot,\zeta)$ is a local minimizer of J in (4.18).

If (1.8) does not hold and (1.5) is satisfied with

$$\epsilon n^2 < \gamma\rho^3 - 2n(n+1), \text{ and } \gamma\rho^3 - 2(n+1)(n+2) < -\epsilon(n+1)^2$$

for some $n \geq 2$, then the eigenvalue λ_n of the operator L_1 in the proof of Lemma 3.1 and its corresponding eigen function $\cos n\theta$ satisfy

$$\lambda_n < -\frac{C}{\rho^3}, \quad \langle L_1(\cos n\theta), \cos n\theta \rangle < -\frac{C}{\rho^3}.$$

By (3.17) and (3.19), the last inequality implies that

$$\langle L_\varsigma(\cos n\theta), \cos n\theta \rangle < -\frac{C}{\rho^3}.$$

Then by Lemma 3.2 and (4.2) in the proof of Lemma 4.1

$$\langle \tilde{L}_\varsigma(\cos n\theta), \cos n\theta \rangle < -\frac{C}{\rho^3}.$$

Therefore the solution is unstable.

5 Discussion

The functional (1.2) was derived from the Ohta-Kawasaki density functional theory for diblock copolymers in [31] as a Γ-limit. The density functional theory uses a function u on D to describe the density of A-monomers and $1-u$ to describe the density of B-monomers. The free energy of a diblock copolymer is

$$I(u) = \int_D [\frac{\epsilon^2}{2}|\nabla u|^2 + W(u) + \frac{\sigma}{2}|(-\Delta)^{-1/2}(u-a)|^2]\, dx \tag{5.1}$$

where u is in

$$\{u \in H^1(D) : \overline{u} = a\}. \tag{5.2}$$

The function W is a balanced double well potential such as $W(u) = \frac{1}{4}u^2(1-u)^2$. There are three positive parameters in (5.1): ϵ, σ, and a, where ϵ is small and a is in $(0,1)$.

If we take σ to be of order ϵ, i.e. by setting

$$\sigma = \epsilon\gamma \tag{5.3}$$

for some γ independent of ϵ. As ϵ tends to 0, the limiting problem of $\epsilon^{-1} I$ turns out to be

$$J(E) = \tau|D\chi_E|(D) + \frac{\gamma}{2}\int_D |(-\Delta)^{-1/2}(\chi_E - a)|^2\, dx \tag{5.4}$$

which is the same as the J in (1.2) except for the additional constant τ here. This constant is known as the surface tension and is given by

$$\tau = \int_0^1 \sqrt{2W(q)}\, dq. \tag{5.5}$$

The functional (5.4) is defined on the same admissible set Σ, (1.3).

The theory of Γ-convergence was developed by De Giorgi [10], Modica and Mortola [23], Modica [22], and Kohn and Sternberg [19]. It was proved that $\epsilon^{-1} I$ Γ-converges to J in the following sense.

Proposition 5.1 (Ren and Wei [31]) *1. For every family $\{u_\epsilon\}$ of functions in (5.2) satisfying $\lim_{\epsilon\to 0} u_\epsilon = \chi_E$ in $L^2(D)$,*

$$\liminf_{\epsilon\to 0} \epsilon^{-1} I(u_\epsilon) \geq J(E);$$

2. For every E in Σ, there exists a family $\{u_\epsilon\}$ of functions in (5.2) such that $\lim_{\epsilon\to 0} u_\epsilon = \chi_E$ in $L^2(D)$, and

$$\limsup_{\epsilon\to 0} \epsilon^{-1} I(u_\epsilon) \leq J(E).$$

The relationship between I and J becomes more clear when a result of Kohn and Sternberg [19] was used to show the following.

Proposition 5.2 (Ren and Wei [31]) *Let $\delta > 0$ and $E \in \Sigma$ be an isolated local minimzer in the sense that $J(E) < J(F)$ for all $\chi_F \in B_\delta(\chi_E)$ with $F \neq E$, where $B_\delta(\chi_E)$ is the open ball of radius δ centered at χ_E in $L^2(D)$. Then there exists $\epsilon_0 > 0$ such that for all $\epsilon < \epsilon_0$ there exists $u_\epsilon \in B_{\delta/2}(\chi_E)$ with $I(u_\epsilon) \leq I(u)$ for all $u \in B_{\delta/2}(\chi_E)$. In addition $\lim_{\epsilon\to 0} \|u_\epsilon - \chi_E\|_{L^2(D)} = 0$.*

Whether the existence of a stable solution $E_{\varphi(\cdot,\zeta)}$ to (1.1) in the sense of Theorem 1.1 implies the existence of a local minimizer, close to $\chi_{E_{\varphi(\cdot,\zeta)}}$ in $L^2(D)$, of I deserves further study. The stability concept used in this paper is weaker than in [19] and [31], because a stable solution here is defined as a local minimizer in a more restricted class of sets than in Proposition 5.2. Another problem is that the stable solution found in this paper is not always isolated. If we take D to be a ring: $\{x \in R^2 : 1 < |x| < 2\}$, then by rotating one droplet solution we obtain a connected family of droplet solutions, all having the same energy.

In Theorem 1.1 the center of the droplet is close to a global minimum of $\tilde{R}$. If η is a strict local minimum of $\tilde{R}$, i.e. there exists a neighborhood $\mathcal{N}$ of η such that $\tilde{R}(\eta) < \tilde{R}(\xi)$ for all $\xi \in \mathcal{N}$, then assuming the assumptions in Theorem 1.1, using the same reduction argument, we can show that there is a droplet solution whose center is close to η. Moreover if η is a strict local maximum of $\tilde{R}$, there is also a droplet solution whose center is close to η, although this droplet is always unstable.

In a forthcoming paper [30] we will show the existence of a multiple droplet pattern as a solution to (1.1) in a general two dimensional region. In addition to the difficulties encountered here, we must prevent a new phenomenon, pattern coarsening, from happening. Pattern coarsening means that some droplets become larger and others become smaller and disappear. Pattern coarsening is a central property in the Cahn-Hilliard problem, which is just (5.1) without the nonlocal term, i.e. $\sigma = 0$ in (5.1). See Alikakos and Fusco [2] and Alikakos, Fusco and Karali [3] for more studies of this phenomenon. We also point out that a single droplet solution also exists in the Cahn-Hilliard problem (see Alikakos and Fusco [1] and Wei and Winter [43]), although it is always unstable.

To prevent pattern coarsening in the diblock copolymer problem, in [30] we impose a lower bound on γ in addition to the conditions (1.5) and (1.12):

$$\gamma > \frac{1+\epsilon}{\rho^3 \log \frac{1}{\rho}}. \tag{5.6}$$

Here ρ is the average radius, i.e. $\rho = \sqrt{\frac{a|D|}{K\pi}}$ where $K \geq 2$ is the number of droplets. We see another difference between our approach and the one by Oshita. The parameter range used by Oshita will not yield a stable multiple droplet solution.

A Appendix 1

The derivative of $\mathcal{H}$ at 0 is given by straight forward calculations from (2.13):

$$\mathcal{H}'(0)(u) = -\frac{1}{\rho^3}(u'' + u). \tag{A.1}$$

The derivative of $\mathcal{A}$ at 0 has two terms according to (2.14). The first is

$$-\frac{\gamma}{8\pi}\int_0^{2\pi} u(\omega)\log(1-\cos(\theta-\omega))\,d\omega.$$

The second is

$$-\frac{\gamma u(\theta)}{4\pi}\int_{B_1(0)} \frac{(e^{i\theta}-y)\cdot e^{i\theta}}{|e^{i\theta}-y|^2}\,dy$$

for which we calculate the integral. Here $B_1(0)$ is the unit ball. Let $y = e^{i\theta}((1,0)-z)$, and $z = re^{i\beta}$. The disc $B_1(0)$ now becomes $B_1(1,0)$, the disc centered at $(1,0)$ of radius 1. Its boundary is parametrized in the polar coordinates by $r = 2\cos\beta$. Then we have

$$\int_{B_1(0)} \frac{(e^{i\theta}-y)\cdot e^{i\theta}}{|e^{i\theta}-y|^2}\,dy = \int_{B_1(1,0)} \frac{e^{i\theta}z\cdot e^{i\theta}}{|z|^2}\,dz = \int_{-\pi/2}^{\pi/2}\int_0^{2\cos\beta} \cos\beta\,drd\beta = \pi.$$

Then it follows that

$$\mathcal{A}'(0)(u) = -\frac{\gamma}{8\pi}\int_0^{2\pi} u(\omega)\log(1-\cos(\theta-\omega))\,d\omega - \frac{\gamma u}{4}. \tag{A.2}$$

B Appendix 2

We evaluate

$$\int_{B_1(0)} \frac{|e^{i\theta}-y|^2 - 2(1-e^{i\theta}\cdot y)^2}{|e^{i\theta}-y|^4}\,dy \tag{B.1}$$

where $B_1(0)$ is the unit disc. Let $y = e^{i\theta}((1,0)-z)$, and $z = re^{i\beta}$. The disc $B_1(0)$ now becomes $B_1(1,0)$, the disc centered at $(1,0)$ of radius 1. Its boundary is parametrized in the polar coordinates by $r = 2\cos\beta$. Then (B.1) becomes

$$\int_{B_1(1,0)} \frac{|z|^2 - 2(e^{i\theta}\cdot e^{i\theta}z)^2}{|z|^4}\,dz = \int_0^2\int_{-\arccos(r/2)}^{\arccos(r/2)} \frac{1-2\cos^2\beta}{r}\,d\beta dr = -\frac{\pi}{2} \tag{B.2}$$

Note that the last integral must be in the $d\beta dr$ order, otherwise it would be divergent.

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