

THE IMPACT OF THE DOMAIN BOUNDARY ON AN
INHIBITORY SYSTEM: INTERIOR DISCS AND BOUNDARY
HALF DISCS

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ABSTRACT. When the Ohta-Kawasaki theory for diblock copolymers is applied to a bounded domain with the Neumann boundary condition, one faces the possibility of micro-domain interfaces intersecting the system boundary. In a particular parameter range, there exist stationary assemblies, stable in some sense, that consist of both perturbed discs in the interior of the system and perturbed half discs attached to the boundary of the system. The circular arcs of the half discs meet the system boundary perpendicularly. The number of the interior discs and the number of the boundary half discs are arbitrarily prescribed and their radii are asymptotically the same. The locations of these discs and half discs are determined by the minimization of a function related to the Green's function of the Laplace operator with the Neumann boundary condition. Numerical calculations based on the theoretical findings show that boundary half discs help lower the energy of stationary assemblies.

1. Introduction. Morphological phases exist in multi-constituent physical or biological systems characterized by controlled growth. Common in these systems is that a deviation from homogeneity has a strong positive feedback on its further increase, and in the meantime a longer ranging confinement mechanism exists to limit increase and spreading. As a result, exquisitely structured patterns, known as morphological phases in materials science, arise in such systems as orderly outcomes of self-organization principles.

This study is to a large extent motivated by the diblock copolymer theory of Ohta and Kawasaki [8]. A diblock copolymer is a block copolymer whose molecular structure is a linear subchain of A-monomers grafted covalently to another sub-chain of B-monomers [2]. Because of the repulsion between the unlike monomers, the different type subchains tend to segregate, but as they are chemically bonded in chain molecules, segregation of subchains lead to local micro-phase separation: micro-domains rich in either A-monomers or B-monomers emerge as a result. These morphological structures determine the mechanical, optical, electrical, ionic, barrier and other physical properties.

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Here we consider an ideal situation where micro-domains are clearly separated from each other by interfaces with zero width [7, 10, 4]. Mathematically, let D be a bounded domain in \mathbb{R}^2 ; D is assumed to be of class C^5 , a condition necessary for many results in [9]. The energy functional is defined for every Lebesgue measurable subset Ω of D whose Lebesgue measure is fixed at $\omega|D|$:

$$|\Omega| = \omega|D|. \quad (1.1)$$

Here $\omega \in (0, 1)$ is one of the two parameters in this problem. We write $|\Omega|$ for the two dimensional Lebesgue measure of Ω and $|D|$ for the Lebesgue measure of D . The free energy of Ω is given by

$$\mathcal{J}(\Omega) = \mathcal{P}_D(\Omega) + \frac{\gamma}{2} \int_D |(-\Delta)^{-1/2}(\chi_\Omega - \omega)|^2 dx. \quad (1.2)$$

Here $\mathcal{P}_D(\Omega)$ is the perimeter of Ω in D . In the case that Ω is piecewise C^1 , it is the length of the part of the boundary of Ω that is inside D . For a general Ω , see [11, 9] for the definition of $\mathcal{P}_D(\Omega)$. The part of the boundary of Ω inside D is called the interface of Ω . It separates Ω from $D \setminus \Omega$.

To define the operator $(-\Delta)^{-1/2}$, let u be the solution of the following Poisson's equation with the Neumann boundary condition:

$$-\Delta u = f \text{ in } D, \quad \partial_\nu u = 0 \text{ on } \partial D, \quad \int_D u(x) dx = 0, \quad (1.3)$$

where $f \in L^2(D)$ and $\int_D f(x) dx = 0$. In (1.3) ∂_ν stands for the outward normal derivative at ∂D . Because the integral of f is 0, the partial differential equation with the boundary condition is solvable. The solution is unique up to an additive constant. The condition $\int_D u(x) dx = 0$ fixes this constant and gives us a unique solution. The map $f \rightarrow u$ from the space of $\{f \in L^2(D) : \int_D f(x) dx = 0\}$ to itself defines the operator $(-\Delta)^{-1}$. Since this operator is bounded and positive definite, it has a positive square root, which is $(-\Delta)^{-1/2}$ in (1.2). Like $(-\Delta)^{-1}$, $(-\Delta)^{-1/2}$ is a nonlocal operator. It acts on $\chi_\Omega - \omega$ where χ_Ω is the characteristic function of Ω ; $\chi_\Omega(x) = 1$ if $x \in \Omega$ and $\chi_\Omega(x) = 0$ if $x \in D \setminus \Omega$.

The notion of stationary sets in the most general sense is given in [9, (2.12)]. If the interface of Ω is C^2 , then Ω is stationary if and only if it satisfies the following Euler-Lagrange equation and the intersection condition:

$$K(\partial\Omega \cap D) + \gamma I(\Omega) = \lambda \text{ on } \partial\Omega \cap D, \quad (1.4)$$

$$\partial\Omega \cap D \perp \partial D \text{ at } \overline{\partial\Omega \cap D} \cap \partial D. \quad (1.5)$$

In (1.4), $K(\partial\Omega \cap D)$ is the curvature of the curve $\partial\Omega \cap D$ with respect to the normal vector inward towards Ω . The variable $I(\Omega)$ is called the inhibitor of Ω . It is the solution of the Poisson's equation (1.3) with $f = \chi_\Omega - \omega$:

$$-\Delta I(\Omega) = \chi_\Omega - \omega \text{ in } D, \quad \partial_\nu I(\Omega) = 0 \text{ on } \partial D, \quad \int_D I(\Omega)(x) dx = 0. \quad (1.6)$$

The equation (1.5) asserts that the interface of Ω is perpendicular to ∂D if the two meet.

One of the morphological phases observed in diblock copolymers is the cylindrical phase [2]. One monomer constituent is small in volume compared to the other monomer constituent. The minority monomers form many parallel cylinders in a system. Take D to be a cross section of the system. Then these cylinders give rise to an assembly Ω of discs.

In [11] Ren and Wei showed the existence of disc assemblies as stationary sets of the functional \mathcal{J} . In such a stationary assembly, Ω is a union of multiple components, each of which is a perturbed disc located inside the domain D . Their result require that the parameters ω and γ be in a particular range where ω is sufficiently small and γ is suitably large. Their proof also shows that these assemblies are stable in some sense. All the perturbed discs in their stationary assembly have approximately the same radius. If $\xi_{*,i}^1, \dots, \xi_{*,i}^{n_i}$ are the centers of the discs in a stationary assembly found in [11], then $(\xi_{*,i}^1, \dots, \xi_{*,i}^{n_i})$ is close to a minimum of a function F_i . This function is given by

$$F_i(\xi_i^1, \xi_i^2, \dots, \xi_i^{n_i}) = \sum_{j \leq n_i} R(\xi_i^j, \xi_i^j) + 2 \sum_{j < k \leq n_i} G(\xi_i^j, \xi_i^k). \quad (1.7)$$

Here n_i is the number of perturbed discs in the assembly, and $\xi_i^1, \dots, \xi_i^{n_i}$ are distinct points in D . The subscript i used here indicates that the points ξ_i^j are in the interior of D , not on the boundary of D . This point will become important later. The function G is the Green's function of $-\Delta$ on D with the Neumann boundary condition; namely it satisfies

$$-\Delta_x G(x, y) = \delta(x) - \frac{1}{|D|} \text{ in } D, \quad \partial_{\nu_x} G(x, y) = 0 \text{ on } \partial D, \quad \int_D G(x, y) dx = 0 \quad (1.8)$$

for all $y \in D$. One writes G as a sum of two parts:

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

where the first term is the fundamental solution of the $-\Delta$ operator, and the second term R , which appears in (1.7), is the regular part of G , a smooth function on $D \times D$.

One caveat in Ren and Wei's work is that the discs in their stationary assemblies do not touch the boundary of D . One can avoid the issue of the domain boundary by assuming that D is a rectangle and imposing the periodic boundary condition instead of the Neumann boundary condition; see [3, 6, 1, 5]. We prefer working with the more realistic Neumann boundary condition. In this case if the interface of a stationary set meets the domain boundary ∂D , (1.5) states that it does so perpendicularly.

Finding a stationary set whose interface meets the domain boundary is a difficult problem. The first non-trivial result came in our work [9]. When ω is sufficiently small and γ is suitably large, there exists a stationary set shaped like a perturbed half disc, stable in some sense, whose boundary inside D (a perturbed half circle) meets ∂D perpendicularly. A crucial quantity introduced in [9] is termed $R_b(\xi_b, \xi_b)$, $\xi_b \in \partial D$, given by

$$R_b(\xi_b, \xi_b) = \lim_{y \in D, y \rightarrow \xi_b} G(\xi_b, y) - \frac{1}{\pi} \log \frac{1}{|\xi_b - y|}, \quad \xi_b \in \partial D. \quad (1.10)$$

Note that the second term in 1.10 is twice the fundamental solution of $-\Delta$. If $\xi_{*,b} \in \partial D$ is the center of the perturbed half disc stationary set found in [9] and the parameters ω and γ are in the same range as in this paper specified in Theorem 1.1, then $\xi_{*,b}$ is close to a minimum of the function

$$\xi_b \rightarrow R_b(\xi_b, \xi_b), \quad \xi_b \in \partial D. \quad (1.11)$$

In this paper we construct stationary assemblies, stable in some sense, that contain both perturbed discs in the interior of D and perturbed half discs that are

attached to ∂D . The perturbed discs and perturbed half discs in a stationary assembly have approximately the same radius, and the locations of their centers are also determined asymptotically.

Let n_i and n_b be non-negative integers. We use the convention that the subscript i is attached to quantities related to the interior discs of an assembly, and the subscript b is attached to quantities related to the boundary half discs. For a stationary assembly of n_i perturbed discs inside D and n_b perturbed half discs attached to ∂D , it is convenient to introduce the average radius as a parameter in place of ω ; namely let $\rho > 0$ so that

$$\omega|D| = n_i\pi\rho^2 + \frac{n_b\pi\rho^2}{2}. \quad (1.12)$$

Now ρ and γ are the two parameters of our problem.

Theorem 1.1. *Let n_i , n_b be non-negative integers. There exists $\sigma > 0$ depending on n_i , n_b , and D , and for every $\epsilon > 0$ there exists $\delta > 0$ depending on ϵ , n_i , n_b , and D , such that if*

1. $\rho < \delta$,
2. $\frac{1+\epsilon}{\rho^3 \log \frac{1}{\rho}} < \gamma < \frac{\sigma}{\rho^3}$,

then \mathcal{J} admits a stationary assembly Ω_ of n_i perturbed interior discs and n_b perturbed boundary half discs, satisfying the constraint $|\Omega_*| = n_i\pi\rho^2 + \frac{n_b\pi\rho^2}{2}$.*

Define a function

$$\begin{aligned} F(\xi_i^1, \dots, \xi_i^{n_i}, \xi_b^1, \dots, \xi_b^{n_b}) &= \sum_{j \leq n_i} R(\xi_i^j, \xi_i^j) + \frac{1}{4} \sum_{j \leq n_b} R_b(\xi_b^j, \xi_b^j) + 2 \sum_{j < k \leq n_i} G(\xi_i^j, \xi_i^k) \\ &\quad + \frac{1}{2} \sum_{j < k \leq n_b} G(\xi_b^j, \xi_b^k) + \sum_{j \leq n_i, k \leq n_b} G(\xi_i^j, \xi_b^k) \end{aligned} \quad (1.13)$$

in the domain

$$\begin{aligned} \Xi = \left\{ \xi = (\xi_i^1, \dots, \xi_i^{n_i}, \xi_b^1, \dots, \xi_b^{n_b}) : \xi_i^j \in D \text{ for } j = 1, \dots, n_i, \xi_i^j \neq \xi_i^k \text{ if } j \neq k, \right. \\ \left. \xi_b^j \in \partial D \text{ for } j = 1, \dots, n_b, \xi_b^j \neq \xi_b^k \text{ if } j \neq k \right\}. \end{aligned} \quad (1.14)$$

Because $G(x, y) \rightarrow \infty$ if $|x - y| \rightarrow 0$ and $R(z, z) \rightarrow \infty$ if $z \rightarrow \partial D$, $F(\xi) \rightarrow \infty$ if $\xi \rightarrow \partial \Xi$. More precisely for every $M \in \mathbb{R}$ there exists a compact subset K of Ξ such that $F(\xi) > M$ whenever $\xi \in \Xi \setminus K$. In particular F admits a minimum in Ξ . The next theorem gives the sizes and the locations of the discs and half discs in the stationary assemblies.

Theorem 1.2. *Let $\xi_{*,i}^j \in D$ and $\xi_{*,b}^j \in \partial D$ be the centers and $r_{*,i}^j$ and $r_{*,b}^j$ be the radii of the perturbed discs and half discs in the stationary assembly Ω_* of Theorem 1.1.*

1. *As $\rho \rightarrow 0$, $\frac{r_{*,i}^j}{\rho} \rightarrow 1$ and $\frac{r_{*,b}^j}{\rho} \rightarrow 1$.*
2. *As $\rho \rightarrow 0$, every limit point of $(\xi_{*,i}^1, \dots, \xi_{*,i}^{n_i}, \xi_{*,b}^1, \dots, \xi_{*,b}^{n_b})$ along a subsequence is a minimum of F .*

This stationary assembly is stable in some sense.

These two theorems contain very detailed information about the stationary assemblies. Figure 1 shows several stationary assemblies when D is the unit disc. The range for n_i is the set of integers from, 0 to 10 and the range for n_b is the set of

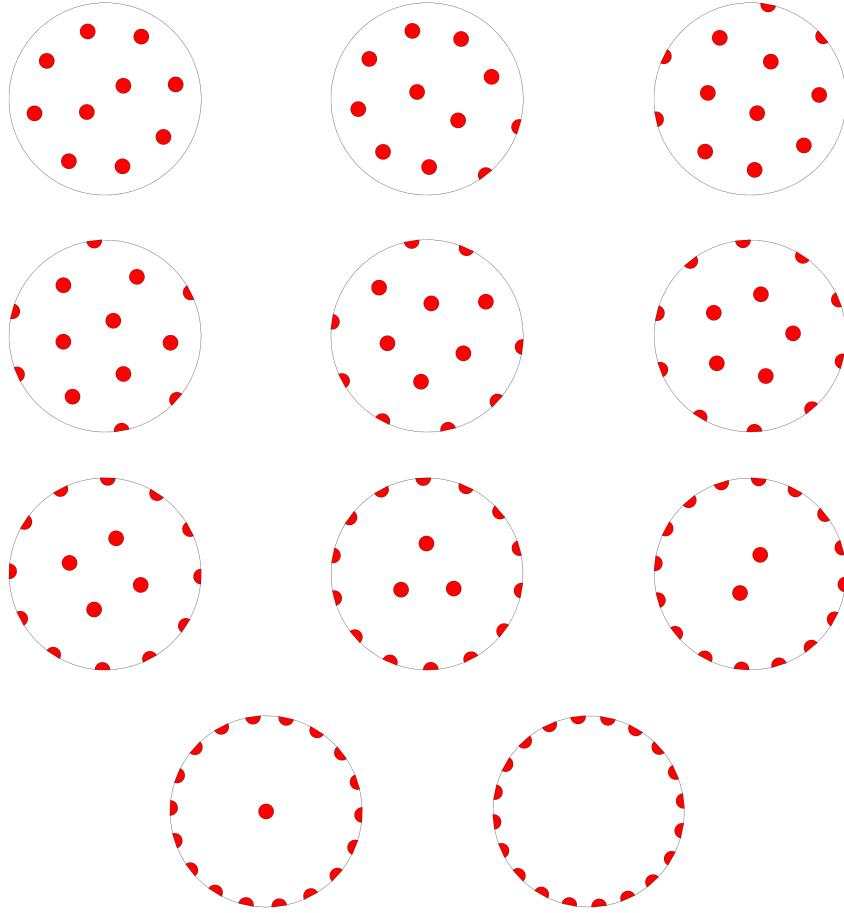


FIGURE 1. From the left of the first row with $n_i = 10$ and $n_b = 0$ to the right of the last row with $n_i = 0$ and $n_b = 20$, these assemblies, of $n_i + \frac{n_b}{2} = 10$, minimize F . Among them, the right one on the first row has the least F value. Here $\omega = 0.2$.

even integers from 0 to 20. In all these assemblies $n_i + \frac{n_b}{2} = 10$. The locations of the discs and half discs are determined by numerical minimization of F .

Probably the most important reason to study stationary assemblies with both interior discs and boundary half discs is to see whether one can lower the free energy of a stationary assembly of only interior discs by replacing some interior discs by some boundary half discs. In the proofs of the main theorems, one obtains detailed information on the stationary assemblies. This allows us to compare their energy. We present examples where stationary assemblies with only interior discs have higher energy than some stationary assemblies with both interior discs and boundary half discs.

The proofs of Theorems 1.1 and 1.2 are organized as follows. In section 2 one constructs approximately stationary assemblies of interior discs and boundary half discs. The centers and radii of the discs and half discs are to be determined. In

section 3 one formulates a problem $\mathcal{S}(\Phi) = 0$ in a Hilbert space. A solution to this problem solves the Euler-Lagrange equation (1.4) up to the constant λ . Namely that a solution of $\mathcal{S}(\Phi) = 0$ represents a set Ω of multiple components. On the boundary of each component, the equation (1.4) holds. However the constant λ varies from component to component.

To solve $\mathcal{S}(\Phi) = 0$, one actually solves a weaker problem in section 4: $\Pi\mathcal{S}(\Phi) = 0$ where Π is a projection operator. Here one uses a fixed point argument with the help of the invertibility of a linear operator. The resulting solutions are an improvement of the previously constructed approximately stationary assemblies. Finally in section 5 one chooses centers and radii properly so that the solution of $\Pi\mathcal{S}(\Phi) = 0$ is also a solution of $\mathcal{S}(\Phi) = 0$ and a solution of (1.4).

Section 6 is devoted to the question of the advantage of stationary assemblies with both interior discs and boundary half discs over stationary assemblies with just interior discs.

2. Approximately stationary assemblies. We start with a construction of an assembly of exact discs inside D and perturbed half discs attached to ∂D . Let $\alpha > 0$, $\beta \in (0, 1)$, and set

$$\Xi_\alpha = \{\xi = (\xi_i^1, \dots, \xi_i^{n_i}, \xi_b^1, \dots, \xi_b^{n_b}) : \xi_i^j \in D, \text{dist}(\xi_i^j, \partial D) \geq \alpha, |\xi_i^j - \xi_i^k| \geq 2\alpha \ \forall j \neq k, \xi_b^j \in \partial D, |\xi_b^j - \xi_b^k| \geq 2\alpha \ \forall j \neq k\} \quad (2.1)$$

$$W_\beta = \{r = (r_i^1, \dots, r_i^{n_i}, r_b^1, \dots, r_b^{n_b}) : r_i^j, r_b^j \in [(1 - \beta)\rho, (1 + \beta)\rho], \sum_{j \leq n_i} \pi(r_i^j)^2 + \sum_{j \leq n_b} \frac{\pi(r_b^j)^2}{2} = n_i \pi \rho^2 + \frac{n_b \pi \rho^2}{2}\}. \quad (2.2)$$

Note that we write ξ for $(\xi_i^1, \dots, \xi_i^{n_i}, \xi_b^1, \dots, \xi_b^{n_b})$ and r for $(r_i^1, \dots, r_i^{n_i}, r_b^1, \dots, r_b^{n_b})$ in this paper. The number α is small enough so that

$$\min_{\xi \in \Xi_\alpha} F(\xi) < \inf_{\xi \in \Xi \setminus \Xi_\alpha} F(\xi); \quad (2.3)$$

the number β is also small so that for all $t \in [(1 - \beta)^2, (1 + \beta)^2]$,

$$g''(t) > 0 \text{ where } g(t) = \frac{8\sqrt{t}}{1 + \epsilon} + t^2. \quad (2.4)$$

In (2.3) the set Ξ is the domain of F , given in (1.14); in (2.4) $\epsilon > 0$ is the number in the statement of Theorem 1.1. Note that, since $F(\xi) \rightarrow \infty$ if $\xi \rightarrow \partial \Xi$, (2.3) holds if α is sufficiently small. Also, since

$$g''(1) = -\frac{2}{1 + \epsilon} + 2 > 0,$$

a small β can be found so that (2.4) holds. The significance of the conditions (2.3) and (2.4) will emerge later in the paper. For now we only think of α and β as two small fixed numbers.

Let $\xi = (\xi_i^1, \dots, \xi_i^{n_i}, \xi_b^1, \dots, \xi_b^{n_b}) \in \Xi_\alpha$ and $r = (r_i^1, \dots, r_i^{n_i}, r_b^1, \dots, r_b^{n_b}) \in W_\beta$. We first make n_i discs centered at ξ_i^j of radius r_i^j :

$$E_i^j = \{x \in \mathbb{R}^2 : |x - \xi_i^j| < r_i^j\}. \quad (2.5)$$

Before making perturbed half discs attached to the domain boundary ∂D , one needs to set up coordinate frames on ∂D . Let

$$t \rightarrow \mathbf{r}(t) \quad (2.6)$$

be a parametrization of a part of ∂D . We sometimes identify t with $\mathbf{r}(t)$ if no confusion arises, and write $t \in \partial D$. Let $\mathbf{t}(t)$ and $\mathbf{n}(t)$ be the unit tangent and normal vectors of ∂D at t respectively. Assume that

1. $\mathbf{t}(t) = \frac{\mathbf{r}'(t)}{|\mathbf{r}'(t)|}$,
2. $\mathbf{n}(t) = i\mathbf{t}(t)$, i.e. $(\mathbf{t}(t), \mathbf{n}(t))$ is a right-handed coordinate system,
3. $\mathbf{n}(t)$ points inward with respect to D .

In this paper to simplify notation, \mathbb{R}^2 is identified with \mathbb{C} . Then $i\mathbf{t}(t)$, the counterclockwise 90 degree rotation of $\mathbf{t}(t)$, is just the complex product of i and $\mathbf{r}(t)$, the latter viewed as a complex number. The arc length variable s measured from a fixed point on ∂D is given by

$$\frac{ds}{dt} = |\mathbf{r}'(t)|. \quad (2.7)$$

The (signed) curvature κ of ∂D is defined with respect to the inward normal vector \mathbf{n} so that

$$\frac{d\mathbf{t}}{ds} = \kappa\mathbf{n}, \quad \frac{d\mathbf{n}}{ds} = -\kappa\mathbf{t}. \quad (2.8)$$

With $\mathbf{r}(t)$ being the center, $\mathbf{t}(t)$ and $\mathbf{n}(t)$ form a right-handed orthonormal frame so that any point x inside D or outside D can be described by

$$x = \mathbf{r}(t) + (\mathbf{t}(t), \mathbf{n}(t)) \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} \quad (2.9)$$

where p_1 and p_2 are the coordinates of x under this frame. The transformation T_t is defined to be

$$T_t : p = \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} \rightarrow \mathbf{r}(t) + (\mathbf{t}(t), \mathbf{n}(t)) \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}, \quad (2.10)$$

so that $x = T_t(p)$. We call x a point in the original space and p the coordinate vector of x under the $(\mathbf{t}(\xi), \mathbf{n}(\xi))$ frame.

Introduce a function f which is locally the graph of ∂D under the $(\mathbf{t}(t), \mathbf{n}(t))$ frame. More precisely, for τ near t there exist p_1 and p_2 such that $\mathbf{r}(\tau) = \mathbf{r}(t) + p_1\mathbf{t}(t) + p_2\mathbf{n}(t)$. The correspondence $p_1 \rightarrow p_2$ defines a function whose graph is ∂D near t under the $(\mathbf{t}(t), \mathbf{n}(t))$ frame. Since this function depends on the fixed point t , we treat it as a function of two variables, p_1 and t : $p_2 = f(p_1, t)$. With f we have

$$\mathbf{r}(\tau) = \mathbf{r}(t) + (\mathbf{t}(t), \mathbf{n}(t)) \begin{pmatrix} p_1 \\ f(p_1, t) \end{pmatrix}. \quad (2.11)$$

Note that

$$f(0, t) = D_1 f(0, t) = 0, \quad \text{for all } t \in \partial D. \quad (2.12)$$

In this paper we write $D_1 f$ for the first partial derivative of f with respect to its first argument, and $D_1^2 f$ for the second partial derivative of f with respect to its first argument, etc.

The function f also provides a way to locally flatten the domain D . Define a transformation Q_t by

$$Q_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 + f(u_1, t) \end{pmatrix}. \quad (2.13)$$

The derivative of Q_t is

$$\frac{DQ_t}{Du} = \begin{bmatrix} 1 & 0 \\ D_1 f(u_1, t) & 1 \end{bmatrix}, \quad \text{and} \quad \left. \frac{DQ_t}{Du} \right|_{u=\vec{0}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \quad (2.14)$$

The inverse of Q_t is

$$Q_t^{-1} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 - f(p_1, t) \end{pmatrix}. \quad (2.15)$$

Now we are ready to make perturbed half discs attached to ∂D . For each pair of ξ_b^j and r_b^j let

$$E_b^j = \{x = T_{\xi_b^j} \circ Q_{\xi_b^j}(u) : |u| < r_b^j, u = (u_1, u_2), u_2 > 0\}. \quad (2.16)$$

With these discs and perturbed half discs one obtains an assembly

$$E = \left(\bigcup_{j \leq n_i} E_i^j \right) \cup \left(\bigcup_{j \leq n_b} E_b^j \right). \quad (2.17)$$

The discs and half discs in E are non-overlapping if ρ is small because of the definition of Ξ_α . We use E as an approximate solution to the equations (1.4) and (1.5). The energy of E is estimated below. Its proof, which we omit, is a combination of [11, Lemma 3.2] and [9, Lemma 2.3].

Lemma 2.1.

$$\begin{aligned} \mathcal{J}(E) &= \sum_{j \leq n_i} 2\pi r_i^j + \sum_{j \leq n_b} \pi r_b^j + O(\rho^2) \\ &+ \frac{\gamma}{2} \left[\sum_{j \leq n_i} \left(\frac{\pi(r_i^j)^4}{2} \log \frac{1}{r_i^j} + \frac{\pi(r_i^j)^4}{8} + (\pi(r_i^j)^2)^2 R(\xi_i^j, \xi_i^j) \right) \right. \\ &+ \sum_{j \leq n_b} \left(\frac{\pi(r_b^j)^4}{4} \log \frac{1}{r_b^j} + \frac{\pi(r_b^j)^4}{16} + \left(\frac{\pi(r_b^j)^2}{2} \right)^2 R_b(\xi_b^j, \xi_b^j) \right) \\ &+ 2 \sum_{j < k \leq n_i} \pi^2 (r_i^j)^2 (r_i^k)^2 G(\xi_i^j, \xi_i^k) + 2 \sum_{j < k \leq n_b} \left(\frac{\pi(r_b^j)^2}{2} \right) \left(\frac{\pi(r_b^k)^2}{2} \right) G(\xi_b^j, \xi_b^k) \\ &\left. + 2 \sum_{j \leq n_i, k \leq n_b} \pi (r_i^j)^2 \left(\frac{\pi(r_b^k)^2}{2} \right) G(\xi_i^j, \xi_b^k) \right] + O(\gamma \rho^5). \end{aligned}$$

3. A Hilbert space. Lemma 3.1 below is a standard result on the variation of the length of a curve, and Lemma 3.2 gives a formula for the variation of an integral on a set. Following the two lemmas, the first variation of \mathcal{J} is derived in Lemma 3.3.

Suppose that $\mathbf{R}(\theta)$, $\theta \in [a, b]$, is a parametrized curve. The unit tangent vector of \mathbf{R} is \mathbf{T} given by

$$\mathbf{T}(\theta) = \frac{\mathbf{R}'(\theta)}{|\mathbf{R}'(\theta)|}. \quad (3.1)$$

Let \mathbf{N} be a unit normal vector to \mathbf{R} and K be the curvature of \mathbf{R} , so that $K\mathbf{N}$ is the curvature vector of \mathbf{R} . Moreover

$$\frac{d\mathbf{T}}{ds} = K\mathbf{N}, \quad (3.2)$$

where $ds = |\mathbf{R}'(\theta)|d\theta$ is the length element. A deformation of \mathbf{R} is a family of curves \mathbf{R}_ε , parametrized by ε in a neighborhood of 0, so that $\mathbf{R}_0 = \mathbf{R}$.

Lemma 3.1. *Let $\mathbf{R}(\theta)$, $\theta \in [a, b]$, be a curve and $\mathbf{R}_\varepsilon(\theta)$ be a deformation of $\mathbf{R}(\theta)$. Denote by \mathbf{X} the infinitesimal element of the deformation \mathbf{R}_ε : $\mathbf{X}(\theta) = \frac{\partial \mathbf{R}_\varepsilon(\theta)}{\partial \varepsilon}|_{\varepsilon=0}$. Then*

$$\frac{d}{d\varepsilon} \Big|_{\varepsilon=0} \int_a^b |\mathbf{R}'_\varepsilon| d\theta = \mathbf{T} \cdot \mathbf{X} \Big|_a^b - \int_a^b K\mathbf{N} \cdot \mathbf{X} ds,$$

where $\int_a^b |\mathbf{R}'_\varepsilon| d\theta$ is the length of \mathbf{R}_ε , and \mathbf{T} , \mathbf{N} , and K are the tangent, normal, and curvature of \mathbf{R} respectively.

Suppose that Ω is an open set with piecewise C^1 interface. A deformation Ω_ε is a family of open sets with piecewise C^1 boundary, parametrized by ε , such that $\partial\Omega_\varepsilon$ is a deformation of the curve $\partial\Omega$.

Lemma 3.2. *Suppose that a bounded domain Ω is enclosed by a curve $\partial\Omega$, and Ω_ε is a deformation of Ω . Let \mathbf{X} be the infinitesimal element of the deformation of $\partial\Omega$. Then*

$$\frac{d}{d\varepsilon} \Big|_{\varepsilon=0} \int_{\Omega_\varepsilon} f(x) dx = - \int_{\partial\Omega} f(x) \mathbf{N} \cdot \mathbf{X} ds$$

where \mathbf{N} is the inward unit normal vector on $\partial\Omega$.

Let us consider a set Ω with n_i components Ω_i^j inside D and n_b components Ω_b^j that touch the boundary of D . The first variation of this set is given by the following lemma.

Lemma 3.3. *Let Ω_ε be a deformation of a set Ω which consists of interior components Ω_i^j and boundary components Ω_b^j in D with piecewise C^1 interface parametrized by $\mathbf{R}_\mu^j(\theta)$, $\theta \in [a, b]$, $j = 1, \dots, n_\mu$, $\mu = i, b$. Then*

$$\begin{aligned} \frac{d\mathcal{J}(\Omega_\varepsilon)}{d\varepsilon} \Big|_{\varepsilon=0} &= - \sum_{j=1}^{n_i} \int_{\partial\Omega_i^j} (K(\partial\Omega \cap D) + \gamma I(\Omega)) \mathbf{N}_i^j \cdot \mathbf{X}_i^j ds \\ &\quad + \sum_{j=1}^{n_b} \left(\mathbf{T}_b^j \cdot \mathbf{X}_b^j \Big|_0^\pi - \int_{\partial\Omega_b^j \cap D} (K(\partial\Omega \cap D) + \gamma I(\Omega)) \mathbf{N}_b^j \cdot \mathbf{X}_b^j ds \right). \end{aligned}$$

Also

$$\frac{d|\Omega_\varepsilon|}{d\varepsilon} \Big|_{\varepsilon=0} = - \sum_{j \leq n_\mu, \mu=i,b} \int_{\partial\Omega_\mu^j \cap D} \mathbf{N}_\mu^j \cdot \mathbf{X}_\mu^j ds.$$

In this section we find a way to perturb the approximate solution E to a more general assembly Ω of perturbed discs and half discs. Such perturbations will be represented by elements in a Hilbert space.

To perturb an interior component E_i^j of E we need a 2π -periodic function ϕ_i^j and thus set

$$P_i^j = \left\{ t e^{i\theta} : \theta \in S^1, t \in [0, \sqrt{(r_i^j)^2 + 2\phi_i^j(\theta)}] \right\}. \quad (3.3)$$

The circle S^1 is used to denote the interval $[0, 2\pi]$ with identified end points. Shift P_i^j by ξ_i^j to

$$\Omega_i^j = \xi_i^j + P_i^j, \quad (3.4)$$

and this set is a perturbation of E_i^j . To perturb a boundary component E_b^j , let

$$P_b^j = \left\{ t e^{i\theta} : \theta \in (0, \pi), t \in [0, \sqrt{(r_b^j)^2 + 2\phi_b^j(\theta)}] \right\}, \quad (3.5)$$

and then map it to

$$\Omega_b^j = T_{\xi_b^j} \circ Q_{\xi_b^j}(P_b^j) \quad (3.6)$$

to yield a perturbation of E_b^j . Now set

$$\Omega = \left(\cup_{j \leq n_i} \Omega_i^j \right) \cup \left(\cup_{j \leq n_b} \Omega_b^j \right). \quad (3.7)$$

Obviously ϕ_i^j and ϕ_b^j need to be small compared to $(r_i^j)^2$ and $(r_b^j)^2$ respectively for the definitions (3.3) and (3.5) to be meaningful. We also need some smoothness for ϕ_i^j and ϕ_b^j for $\mathcal{J}(\Omega)$ to be defined. Let us start with a Hilbert space

$$\begin{aligned} \mathcal{Z} = & \left\{ \Phi = (\phi_i^1, \dots, \phi_i^{n_i}, (\phi_\pi^1, \phi_\pi^1, \phi_b^1), \dots, (\phi_0^{n_b}, \phi_\pi^{n_b}, \phi_b^{n_b})) : \right. \\ & \phi_i^j \in L^2(S^1), \int_0^{2\pi} \phi_i^j = 0, \quad j = 1, \dots, n_i, \\ & \phi_b^j \in L^2(0, \pi), \quad \phi_0^j, \phi_\pi^j \in \mathbb{R}, \quad \int_0^\pi \phi_b^j = 0, \quad j = 1, \dots, n_b \left. \right\}. \end{aligned} \quad (3.8)$$

The inner product in \mathcal{Z} is

$$\langle \Phi, \Psi \rangle = \sum_{j \in N_i} \int_0^{2\pi} \phi_i^j \psi_i^j + \sum_{j \in N_b} \left(\phi_0^j \psi_0^j + \phi_\pi^j \psi_\pi^j + \int_0^\pi \phi_b^j \psi_b^j \right). \quad (3.9)$$

The constraints

$$\int_0^{2\pi} \phi_i^j = 0, \quad j = 1, \dots, n_i, \quad \int_0^\pi \phi_b^j = 0, \quad j = 1, \dots, n_b \quad (3.10)$$

ensure that the area of Ω_i^j is fixed at $\pi(r_i^j)^2$ and the area of Ω_b^j is fixed at $\pi(r_b^j)^2/2$, since

$$\begin{aligned} |\Omega_i^j| &= \int_0^{2\pi} \int_0^{\sqrt{(r_i^j)^2 + 2\phi_i^j}} r dr d\theta = \pi(r_i^j)^2 + \int_0^{2\pi} \phi_i^j d\theta = \pi(r_i^j)^2 \\ |\Omega_b^j| &= \int_0^\pi \int_0^{\sqrt{(r_b^j)^2 + 2\phi_b^j}} r dr d\theta = \frac{\pi(r_b^j)^2}{2} + \int_0^\pi \phi_b^j d\theta = \frac{\pi(r_b^j)^2}{2}. \end{aligned}$$

Note that $|\Omega_b^j| = |P_b^j|$ since the Jacobian of $Q_{\xi_b^j}$ equals 1 by (2.14).

Next is a subspace \mathcal{Y} of \mathcal{Z} ,

$$\mathcal{Y} = \left\{ \Phi \in \mathcal{Z} : \phi_i^j \in H^1(S^1), \phi_b^j \in H^1(0, \pi), \phi_0^j = \phi_b^j(0), \phi_\pi^j = \phi_b^j(\pi) \right\}. \quad (3.11)$$

Let ξ and r be held fixed. Then the set Ω is represented by Φ and \mathcal{J} is viewed as a functional of Φ . In this setting, the domain of \mathcal{J} is a neighborhood of the 0 element in \mathcal{Y} :

$$Dom(\mathcal{J}) = \{ \Phi \in \mathcal{Y} : \|\Phi\|_{\mathcal{Y}} < b\rho^2 \}, \quad (3.12)$$

where b is a sufficiently small positive constant, independent of ρ , so that

$$(r_i^j)^2 + 2\phi_i^j(\theta) > 0, \quad \text{for all } \theta \in S^1, \quad (r_b^j)^2 + 2\phi_b^j(\theta) > 0, \quad \text{for all } \theta \in (0, \pi). \quad (3.13)$$

This makes (3.3) and (3.5) geometrically meaningful definitions of perturbed discs and half discs respectively.

It is easy to make a deformation in \mathcal{Y} . Let $\Phi \in Dom(\mathcal{J})$ and $\Psi \in \mathcal{Y}$. Then

$$\Phi \rightarrow \Phi + \varepsilon \Psi \quad (3.14)$$

defines a deformation of Φ . Consequently it gives rise to a deformation Ω_ε , represented by $\Phi + \varepsilon \Psi$, of the assembly Ω represented by Φ . This deformation leads to the first variation

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \mathcal{J}(\Phi + \varepsilon \Psi). \quad (3.15)$$

Another subspace \mathcal{X} of \mathcal{Z} is

$$\mathcal{X} = \left\{ \Phi \in \mathcal{Z} : \phi_i^j \in H^2(S^1), \phi_b^j \in H^2(0, \pi), \phi_0^j = \phi_b^j(0), \phi_\pi^j = \phi_b^j(\pi) \right\}. \quad (3.16)$$

The three spaces are nested: $\mathcal{X} \subset \mathcal{Y} \subset \mathcal{Z}$. In the case that $\Phi \in \mathcal{X}$, integration by parts yields

$$\frac{d}{d\varepsilon} \Big|_{\varepsilon=0} \mathcal{J}(\Phi + \varepsilon\Psi) = \langle \mathcal{S}(\Phi), \Psi \rangle. \quad (3.17)$$

In (3.17) \mathcal{S} is a nonlinear operator defined on

$$Dom(\mathcal{S}) = \{\Phi \in \mathcal{X} : \|\Phi\|_{\mathcal{X}} < b\rho^2\} \quad (3.18)$$

where b is the same as the one in (3.12). More specifically

$$\mathcal{S} = (\mathcal{S}_i^1, \dots, \mathcal{S}_i^{n_i}, (\mathcal{S}_0^1, \mathcal{S}_{\pi}^1, \mathcal{S}_b^1), \dots, (\mathcal{S}_0^{n_b}, \mathcal{S}_{\pi}^{n_b}, \mathcal{S}_b^{n_b})) \quad (3.19)$$

where

$$\mathcal{S}_i^j(\Phi) = K(\partial\Omega \cap D)(\mathbf{R}_i^j(\theta)) + I(\Omega)(\mathbf{R}_i^j(\theta)) - \lambda_i^j(\Phi) \quad (3.20)$$

$$\mathcal{S}_0^j(\Phi) = -\vec{T}^j(0) \cdot \frac{1}{\sqrt{(r_b^j)^2 + 2\phi_b^j(0)}} \left(\begin{array}{c} 1 \\ D_1 f(\sqrt{(r_b^j)^2 + 2\phi_b^j(0)}, \xi_b^j) \end{array} \right) \quad (3.21)$$

$$\mathcal{S}_{\pi}^j(\Phi) = \vec{T}^j(\pi) \cdot \frac{1}{\sqrt{(r_b^j)^2 + 2\phi_b^j(\pi)}} \left(\begin{array}{c} -1 \\ -D_1 f(-\sqrt{(r_b^j)^2 + 2\phi_b^j(\pi)}, \xi_b^j) \end{array} \right) \quad (3.22)$$

$$\mathcal{S}_b^j(\Phi) = K(\partial\Omega \cap D)(\mathbf{R}_b^j(\theta)) + I(\Omega)(\mathbf{R}_b^j(\theta)) - \lambda_b^j(\Phi). \quad (3.23)$$

The range of \mathcal{S} is a subspace of \mathcal{Z} .

Here Ω is the assembly represented by Φ . The interface of the component Ω_i^j (resp. Ω_b^j) is parametrized by \mathbf{R}_i^j (resp. \mathbf{R}_b^j):

$$\mathbf{R}_i^j(\theta) = \xi_i^j + \sqrt{(r_i^j)^2 + 2\phi_i^j(\theta)} e^{i\theta}, \quad j = 1, \dots, n_i \quad (3.24)$$

$$\mathbf{R}_b^j(\theta) = T_{\xi_b^j} \circ Q_{\xi_b^j}(\sqrt{(r_b^j)^2 + 2\phi_b^j(\theta)} e^{i\theta}), \quad j = 1, \dots, n_b. \quad (3.25)$$

The tangent and normal vectors of \mathbf{R}_{μ}^j are denoted \mathbf{T}_{μ}^j and \mathbf{N}_{μ}^j .

For \mathbf{R}_b^j , let \vec{R}_b^j be the parametrization under the $(\mathbf{t}(\xi_b^j), \mathbf{n}(\xi_b^j))$ frame so that

$$\vec{R}_b^j(\theta) = Q_{\xi_b^j}(\sqrt{(r_b^j)^2 + 2\phi_b^j(\theta)} e^{i\theta}), \quad \mathbf{R}_b^j(\theta) = T_{\xi_b^j}(\vec{R}_b^j(\theta)). \quad (3.26)$$

The tangent and normal vectors of \vec{R}_b^j are denoted \vec{T}_b^j and \vec{N}_b^j respectively.

In (3.20) and (3.23), $\lambda_{\mu}^j(\Phi)$ are numbers chosen such that

$$\int_0^{2\pi} \mathcal{S}_i^j(\Phi) d\theta = 0, \quad j = 1, \dots, n_i, \quad \int_0^{\pi} \mathcal{S}_b^j(\Phi) d\theta = 0, \quad j = 1, \dots, n_b. \quad (3.27)$$

If an assembly Ω represented by Φ is a solution of $\mathcal{S}(\Phi) = 0$, then Ω satisfies the equations

$$K(\partial\Omega_i^b) + \gamma I(\Omega) = \lambda_i^j \quad \text{on } \partial\Omega_i^j, \quad j = 1, \dots, n_i \quad (3.28)$$

$$K(\partial\Omega_b^b) + \gamma I(\Omega) = \lambda_b^j \quad \text{on } \partial\Omega_b^j \cap D, \quad j = 1, \dots, n_b \quad (3.29)$$

$$\mathbf{T}_b^j \perp \partial D \quad \text{on } \partial D, \quad j = 1, \dots, n_b. \quad (3.30)$$

Since the λ_{μ}^j 's vary from component to component, Ω is generally not a solution of (1.4).

If \mathbf{R}_{ε} is a deformation of \mathbf{R} such that $\mathbf{R}_0 = \mathbf{R}$, then the infinitesimal element is

$$\mathbf{X}_{\mu}^j = \frac{\partial \mathbf{R}_{\varepsilon, \mu}^j}{\partial \varepsilon} \Big|_{\varepsilon=0}, \quad \vec{X}_b^j = \frac{\partial \vec{R}_{\varepsilon}^j}{\partial \varepsilon} \Big|_{\varepsilon=0}$$

This deformation may be more general than the one considered in (3.14). Nevertheless the end points of each perturbed half disc can only move along the boundary of D in this deformation. Define X_0^j and X_π^j in \mathbb{R} by

$$\vec{X}_b^j(0) = \frac{X_0^j}{\sqrt{(r_b^j)^2 + 2\phi_b^j(0)}} \begin{pmatrix} 1 \\ D_1 f(\sqrt{(r_b^j)^2 + 2\phi_b^j(0)}, \xi_b^j) \end{pmatrix}, \quad (3.31)$$

$$\vec{X}_b^j(\pi) = \frac{X_\pi^j}{\sqrt{(r_b^j)^2 + 2\phi_b^j(\pi)}} \begin{pmatrix} 1 \\ -D_1 f(-\sqrt{(r_b^j)^2 + 2\phi_b^j(\pi)}, \xi_b^j) \end{pmatrix}. \quad (3.32)$$

The first variation formula in Lemma 3.3 can now be written as

$$\begin{aligned} \frac{\partial \mathcal{J}(\Phi)}{\partial \varepsilon} \Big|_{\varepsilon=0} &= - \sum_{j \leq n_i} \int_{\partial \Omega_i^j} (\mathcal{S}_i^j(\Phi) + \lambda_i^j(\Phi)) \mathbf{N}_i^j \cdot \mathbf{X}_i^j \, ds \\ &+ \sum_{j \leq n_b} \left(\mathcal{S}_0^j(\Phi) X_0^j + \mathcal{S}_\pi^j(\Phi) X_\pi^j - \int_{\partial \Omega_b^j \cap D} (\mathcal{S}_b^j(\Phi) + \lambda_b^j(\Phi)) \mathbf{N}_b^j \cdot \mathbf{X}_b^j \, ds \right). \end{aligned} \quad (3.33)$$

The next lemma gives an estimate of $\mathcal{S}(0)$, where the element 0 in \mathcal{X} represents the approximate assembly E . The proof of this lemma is a combination of [11, Lemma 3.1] and [9, Lemma 4.5].

Lemma 3.4.

$$\begin{aligned} \mathcal{S}_i^j(0) &= \frac{1}{r_i^j} + \gamma \left[\frac{(r_i^j)^2}{2} \log \frac{1}{r_i^j} + \pi(r_i^j)^2 R(\xi_i^j, \xi_i^j) + \sum_{k \leq n_i, k \neq j} \pi(r_i^k)^2 G(\xi_i^j, \xi_i^k) \right. \\ &\quad \left. + \sum_{k \leq n_b} \frac{\pi(r_b^k)^2}{2} G(\xi_i^j, \xi_b^k) + O(\rho^3) \right] - \lambda_i^j(0) \end{aligned} \quad (3.34)$$

$$\mathcal{S}_0^j(0) = O(1) \quad (3.35)$$

$$\mathcal{S}_\pi^j(0) = O(1) \quad (3.36)$$

$$\begin{aligned} \mathcal{S}_b^j(0) &= \frac{1}{r_b^j} + O(1) + \gamma \left[\frac{(r_b^j)^2}{2} \log \frac{1}{r_b^j} + \frac{\pi(r_b^j)^2}{2} R_b(\xi_b^j, \xi_b^j) + \sum_{k \leq n_b, k \neq j} \frac{\pi(r_b^k)^2}{2} G(\xi_b^j, \xi_b^k) \right. \\ &\quad \left. + \sum_{k \leq n_i} \pi(r_i^k)^2 G(\xi_b^j, \xi_i^k) + O(\rho^3) \right] - \lambda_b^j(0). \end{aligned} \quad (3.37)$$

Note that Lemma 3.4 implies the following.

Lemma 3.5. $\|\mathcal{S}(0)\|_{\mathcal{Z}} = O(1)$.

It is not realistic to solve the equation $\mathcal{S}(\Phi) = 0$ for any given ξ . Instead we will solve a weaker equation first. Let us define three more subspaces at this point.

$$\begin{aligned} \mathcal{Z}_b &= \left\{ \Phi \in \mathcal{Z} : \int_0^{2\pi} \phi_i^j \cos \theta = \int_0^{2\pi} \phi_i^j \sin \theta = 0, \, j = 1, \dots, n_i, \right. \\ &\quad \left. \phi_0^j - \phi_\pi^j + \int_0^\pi \phi_b^j \cos \theta = 0, \, j = 1, \dots, n_b \right\} \end{aligned} \quad (3.38)$$

$$\mathcal{Y}_b = \mathcal{Y} \cap \mathcal{Z}_b \quad (3.39)$$

$$\mathcal{X}_b = \mathcal{X} \cap \mathcal{Z}_b. \quad (3.40)$$

The projection from \mathcal{Z} to \mathcal{Z}_b is denoted Π , defined by the inner product (3.9). One first looks for an element in \mathcal{X}_b that solves $\Pi\mathcal{S}(\Phi) = 0$. Later one finds some special ξ for which $\mathcal{S}(\Phi) = 0$.

When $\mathcal{S}(\Phi) = 0$ is solved for all $r \in W_\beta$, one finds some special r such that in the equations (3.28-3.30) for the solution of $\mathcal{S}(\Phi) = 0$ associated with this particular r , all the λ_μ^j are the same and hence (1.4) holds.

Because of (3.10), if Ω is represented by $\Phi \in \mathcal{Z}$, the measure of Ω_i^j is $\pi(r_i^j)^2$ and the measure of Ω_b^j is $\frac{\pi(r_b^j)^2}{2}$. If in addition $\Phi \in \mathcal{Z}_b$, one interprets that ξ_i^j is the center of the perturbed disc Ω_i^j and that ξ_b^j is the center of the perturbed half disc Ω_b^j . The subspace \mathcal{Z}_b gives precise meanings of the center and radius of a perturbed disc or half disc. When $\Phi \in \mathcal{Z}_b$, we call the ξ_i^j 's and the ξ_b^j 's the centers of the perturbed discs and half discs in Φ and the r_i^j 's and the r_b^j 's their radii.

4. Solve $\Pi\mathcal{S}(\Phi) = 0$. Again consider \mathcal{J} as a functional on $\text{Dom}(\mathcal{J}) \subset \mathcal{Y}$. Let $\Phi \rightarrow \varepsilon_1\Psi + \varepsilon_2\Upsilon$ be a two parameter deformation. Then the second variation of \mathcal{J} can be written as

$$\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \Big|_{\varepsilon_1=\varepsilon_2=0} \mathcal{J}(\Phi + \varepsilon_1\Psi + \varepsilon_2\Upsilon) = \langle \mathcal{S}'(\Phi)(\Psi), \Upsilon \rangle. \quad (4.1)$$

Here \mathcal{S}' is the Fréchet derivative of \mathcal{S} . For each $\Phi \in \text{Dom}(\mathcal{S}) \subset \mathcal{X}$, $\mathcal{S}'(\Phi)$ is a linear operator from \mathcal{X} to \mathcal{Z} . Then $\langle \mathcal{S}'(\Phi)(\Psi), \Upsilon \rangle$ is defined for $\Phi \in \text{Dom}(\mathcal{S}) \subset \mathcal{X}$, $\Psi \in \mathcal{X}$, and $\Upsilon \in \mathcal{Z}$. The left side of (4.1) is also meaningful if $\Phi \in \text{Dom}(\mathcal{J}) \subset \mathcal{Y}$ and $\Psi, \Upsilon \in \mathcal{Y}$.

Lemma 4.1. 1. When ρ and $\gamma\rho^3$ are sufficiently small,

$$\|\Pi\mathcal{S}'(0)(\Psi)\|_{\mathcal{Z}} \geq \frac{1}{2\rho^3} \|\Psi\|_{\mathcal{X}} \quad (4.2)$$

holds for all $\Psi \in \mathcal{X}_b$. The linear map $\Pi\mathcal{S}'(0)$ is one-to-one and onto from \mathcal{X}_b to \mathcal{Z}_b , and whose inverse is bounded by $\|(\Pi\mathcal{S}'(0))^{-1}\| \leq 2\rho^3$.

2. When ρ and $\gamma\rho^3$ are small,

$$\langle \Pi\mathcal{S}'(0)(\Psi), \Psi \rangle \geq \frac{1}{2\rho^3} \|\Psi\|_{\mathcal{Y}}^2 \quad (4.3)$$

for all $\Psi \in \mathcal{Y}_b$.

Proof. The operator $\mathcal{S}'(0)$ is decomposed into

$$\mathcal{S}'(0) = \mathcal{H} + \mathcal{M}, \quad (4.4)$$

where \mathcal{H} is the major part and \mathcal{M} is the minor part. Let

$$\mathcal{H} = (\mathcal{H}_i^1, \dots, \mathcal{H}_i^{n_i}, (\mathcal{H}_0^1, \mathcal{H}_\pi^1, \mathcal{H}_b^1), \dots, (\mathcal{H}_0^{n_b}, \mathcal{H}_\pi^{n_b}, \mathcal{H}_b^{n_b})). \quad (4.5)$$

Then

$$\mathcal{H}_i^j(\Psi) = -\frac{1}{(r_i^j)^3} \left((\psi_i^j)'' + \psi_i^j \right) - h_i^j(\Psi) \quad (4.6)$$

$$\mathcal{H}_0^j(\Psi) = -\frac{1}{(r_b^j)^3} (\psi_b^j)'(0) \quad (4.7)$$

$$\mathcal{H}_\pi^j(\Psi) = \frac{1}{(r_b^j)^3} (\psi_b^j)'(\pi) \quad (4.8)$$

$$\mathcal{H}_b^j(\Psi) = -\frac{1}{(r_b^j)^3} \left((\psi_b^j)'' + \psi_b^j \right) - h_b^j(\Psi) \quad (4.9)$$

where the $h_\mu^j(\Psi)$'s are numbers chosen such that

$$\int_0^{2\pi} \mathcal{H}_i^j(\Psi) = 0, \quad j = 1, \dots, n_i, \quad \int_0^\pi \mathcal{H}_b^j(\Psi) = 0, \quad j = 1, \dots, n_b. \quad (4.10)$$

The operator \mathcal{H} has a non-trivial kernel which is the direct sum of

$$\mathcal{E}_{i,1}^j = \{\Psi : \psi_i^j = A_1 \cos \theta + A_2 \sin \theta, A_1, A_2 \in \mathbb{R}, \text{ other components of } \Psi \text{ are 0}\}, \quad (4.11)$$

$$\mathcal{E}_{b,0}^j = \{\Psi : (\psi_0^j, \psi_\pi^j, \psi_b^j) = B(1, -1, \cos \theta), B \in \mathbb{R}, \text{ other components of } \Psi \text{ are 0}\}. \quad (4.12)$$

In other words 0 is an eigenvalue of \mathcal{H} and the associated eigenspace is the direct sum of the $\mathcal{E}_{i,1}^j$'s and the $\mathcal{E}_{b,0}^j$'s. Denote this eigenvalue of multiplicity $2n_i + n_b$ by

$$\lambda_{i,1}^j = 0, \quad j = 1, \dots, n_i, \quad \lambda_{b,0}^j = 0, \quad j = 1, \dots, n_b. \quad (4.13)$$

The other eigenspaces of \mathcal{H} are

$$\mathcal{E}_{i,m}^j = \{\Psi : \psi_i^j = A_1 \cos m\theta + A_2 \sin m\theta, A_1, A_2 \in \mathbb{R}, \text{ other components of } \Psi \text{ are 0}\}, \quad m \geq 2 \quad (4.14)$$

$$\mathcal{E}_{b,m}^j = \{\Psi : (\psi_0^j, \psi_\pi^j, \psi_b^j) = B(\varphi_m(0), \varphi_m(\pi), \varphi_m), B \in \mathbb{R}, \text{ other components of } \Psi \text{ are 0}\}, \quad m \geq 1. \quad (4.15)$$

In (4.15), the functions φ_m are

$$\varphi_m = \begin{cases} \cos \mu_m \left(\theta - \frac{\pi}{2} \right) - \frac{2 \sin \frac{\pi \mu_m}{2}}{\pi \mu_m} & \text{if } m \geq 1 \text{ is odd} \\ \sin \mu_m \left(\theta - \frac{\pi}{2} \right) & \text{if } m \geq 1 \text{ is even} \end{cases}. \quad (4.16)$$

The μ_m 's in (4.16) are given as follows. Consider two algebraic equations

$$\frac{\pi \mu (\mu^2 - 1)}{2(\mu^2 - 1) - \pi \mu^2} = \tan \frac{\pi \mu}{2} \quad (4.17)$$

$$\frac{\mu}{\mu^2 - 1} = \tan \frac{\pi \mu}{2} \quad (4.18)$$

both considered for $\mu > 1$. The solutions to (4.17) are denoted $\mu_1, \mu_3, \mu_5, \dots$, and the solutions to (4.18) are denoted $\mu_2, \mu_4, \mu_6, \dots$. Moreover

$$1 < \mu_1 < 2 < \mu_2 < 3 < \mu_3 < 4 < \mu_4 < \dots < 2k-1 < \mu_{2k-1} < 2k < \mu_{2k} < 2k+1 \dots \quad (4.19)$$

and

$$\lim_{k \rightarrow \infty} (\mu_{2k-1} - (2k-1)) = 0, \quad \lim_{k \rightarrow \infty} (\mu_{2k} - 2k) = 0. \quad (4.20)$$

The eigenvalue of \mathcal{H} associated to $\mathcal{E}_{i,m}^j$ is clearly

$$\lambda_{i,m}^j = \frac{m^2 - 1}{(r_i^j)^3}. \quad (4.21)$$

It is shown in [9, Lemma 3.1] that the eigenvalue associated to $\mathcal{E}_{b,m}^j$ is

$$\lambda_{b,m}^j = \frac{\mu_m^2 - 1}{(r_b^j)^3}. \quad (4.22)$$

The space \mathcal{Z}_b is exactly the subspace of \mathcal{Z} that is perpendicular to all the kernel of \mathcal{H} , i.e. perpendicular to all $\mathcal{E}_{i,1}^j$, $j = 1, \dots, n_i$, and $\mathcal{E}_{b,0}^j$, $j = 1, \dots, n_b$. It can be written as a direct sum:

$$\mathcal{Z}_b = (\bigoplus_{j=1}^{n_i} \bigoplus_{m=2}^{\infty} \mathcal{E}_{i,m}^j) \oplus (\bigoplus_{j=1}^{n_b} \bigoplus_{m=1}^{\infty} \mathcal{E}_{b,m}^j). \quad (4.23)$$

The operator $\Pi\mathcal{H}$ restricted to \mathcal{X}_b maps from \mathcal{X}_b to \mathcal{Z}_b ; it is identical to \mathcal{H} restricted to \mathcal{X}_b . Moreover in expression (4.6) and (4.9) $h_{\mu}^j(\Psi) = 0$ when $\Psi \in \mathcal{X}_b$. The eigenvalues of $\Pi\mathcal{H}$,

$$\lambda_{i,m}^j, \quad j = 1, 2, \dots, n_i, \quad m = 2, 3, 4, \dots, \quad \lambda_{b,m}^j, \quad j = 1, 2, \dots, n_b, \quad m = 1, 2, 3, \dots, \quad (4.24)$$

are all positive. Let us denote a pair of orthonormal eigenfunctions associated to the eigenspace $\mathcal{E}_{i,m}^j$ by $e_{i,m,1}^j$ and $e_{i,m,2}^j$ and a normalized eigenfunction associated to $\mathcal{E}_{b,m}^j$ by $e_{b,m}^j$. For any $\Psi \in \mathcal{Z}_b$, one can expand

$$\Psi = \sum_{j=1}^{n_i} \sum_{m=2}^{\infty} \sum_{p=1}^2 C_{i,m,p}^j e_{i,m,p}^j + \sum_{j=1}^{n_b} \sum_{m=1}^{\infty} C_{b,m}^j e_{b,m}^j. \quad (4.25)$$

The norms in \mathcal{Z}_b , \mathcal{Y}_b and \mathcal{X}_b are taken to be

$$\|\Psi\|_{\mathcal{Z}}^2 = \sum_{j=1}^{n_i} \sum_{m=2}^{\infty} \sum_{p=1}^2 |C_{i,m,p}^j|^2 + \sum_{j=1}^{n_b} \sum_{m=1}^{\infty} |C_{b,m}^j|^2, \quad \text{if } \Psi \in \mathcal{Z}_b, \quad (4.26)$$

$$\|\Psi\|_{\mathcal{Y}}^2 = \sum_{j=1}^{n_i} \sum_{m=2}^{\infty} \sum_{p=1}^2 |C_{i,m,p}^j|^2 (m^2 - 1) + \sum_{j=1}^{n_b} \sum_{m=1}^{\infty} |C_{b,m}^j|^2 (\mu_m^2 - 1), \quad \text{if } \Psi \in \mathcal{Y}_b, \quad (4.27)$$

$$\|\Psi\|_{\mathcal{X}}^2 = \sum_{j=1}^{n_i} \sum_{m=2}^{\infty} \sum_{p=1}^2 |C_{i,m,p}^j|^2 (m^2 - 1)^2 + \sum_{j=1}^{n_b} \sum_{m=1}^{\infty} |C_{b,m}^j|^2 (\mu_m^2 - 1)^2, \quad \text{if } \Psi \in \mathcal{X}_b. \quad (4.28)$$

It is shown in [9, Lemma 3.2] that the $\|\cdot\|_{\mathcal{Y}}$ norm is equivalent to the usual H^1 norm of a Sobolev space and the $\|\cdot\|_{\mathcal{X}}$ norm is equivalent to the H^2 norm.

Since for $\Psi \in \mathcal{Y}_b$

$$\langle \Pi\mathcal{H}\Psi, \Psi \rangle = \sum_{j=1}^{n_i} \sum_{m=2}^{\infty} \sum_{p=1}^2 |C_{i,m,p}^j|^2 \lambda_{i,m}^j + \sum_{j=1}^{n_b} \sum_{m=1}^{\infty} |C_{b,m}^j|^2 \lambda_{b,m}^j, \quad (4.29)$$

we deduce from (4.27) and (4.28) that

$$\|\Pi\mathcal{H}\Psi\|_{\mathcal{Z}} \geq \frac{1}{1.5\rho^3} \|\Psi\|_{\mathcal{X}}, \quad \forall \Psi \in \mathcal{X}_b, \quad (4.30)$$

$$\langle \Pi\mathcal{H}\Psi, \Psi \rangle \geq \frac{1}{1.5\rho^3} \|\Psi\|_{\mathcal{Y}}^2, \quad \forall \Psi \in \mathcal{Y}_b, \quad (4.31)$$

if β in (2.2) is so small that r_i^j and r_b^j are sufficiently close to ρ .

Regarding the minor part \mathcal{M} , one has

$$\|\mathcal{M}(\Psi)\|_{\mathcal{Z}} \leq C\left(\frac{1}{\rho^2} + \gamma\right)\|\Psi\|_{\mathcal{X}} \quad (4.32)$$

$$|\langle \mathcal{M}(\Psi), \Psi \rangle| \leq C\left(\frac{1}{\rho^2} + \gamma\right)\|\Psi\|_{\mathcal{Y}}^2. \quad (4.33)$$

The details of these estimates are found in the proofs of [11, Lemma 5.2] and [9, Lemma 5.1]. Then (4.2) follows from (4.30) and (4.32), and (4.3) follows from (4.31) and (4.33).

Finally to show that $\Pi\mathcal{S}'(0)$ is from \mathcal{X}_b onto \mathcal{Z}_b , note that $\Pi\mathcal{S}'(0)$ is an unbounded self-adjoint operator on \mathcal{Z}_b with the domain $\mathcal{X}_b \subset \mathcal{Z}_b$. If $\Upsilon \in \mathcal{Z}_b$ is perpendicular to the range of $\Pi\mathcal{S}'(0)$, i.e. $\langle \Pi\mathcal{S}'(0)(\Psi), \Upsilon \rangle = 0$ for all $\Psi \in \mathcal{X}_b$, then the self-adjointness of $\Pi\mathcal{S}'(0)$ implies that $\Upsilon \in \mathcal{X}_b$ and $\Pi\mathcal{S}'(0)(\Upsilon) = 0$. By the estimate in part 1, $\Upsilon = 0$. Hence, the range of $\Pi\mathcal{S}'(0)$ is dense in \mathcal{Z}_b . The estimate in part 1 also implies that the range of $\Pi\mathcal{S}'(0)$ is a closed subspace of \mathcal{Z}_b . Therefore $\Pi\mathcal{S}'(0)$ is onto. \square

Lemma 4.2. *When ρ and $\gamma\rho^3$ are sufficiently small, for each $\xi \in \Xi_\alpha$ and $r \in W_\beta$, the equation $\Pi\mathcal{S}(\Phi) = 0$ admits a solution $\Phi_* \in \text{Dom}(\mathcal{S}) \cap \mathcal{X}_b$ satisfying $\|\Phi_*\|_{\mathcal{X}} = O(\rho^3)$.*

The proof of this lemma uses a fixed point argument. It makes use of Lemmas 3.5 and 4.1. See the proof of [9, Lemma 6.1] for more details.

The first part of the next lemma shows that Φ_* is non-degenerate; the second part asserts that Φ_* is locally energy minimizing among assemblies of perturbed discs and half discs of prescribed centers and radii. The proof of the lemma is the same as the one of [9, Lemma 6.2].

Lemma 4.3. 1. For all $\Psi \in \mathcal{X}_b$

$$\|\Pi\mathcal{S}'(\Phi_*)(\Psi)\|_{\mathcal{Z}} \geq \frac{1}{4\rho^3}\|\Psi\|_{\mathcal{X}}.$$

2. For all $\Psi \in \mathcal{Y}$

$$\langle \Pi\mathcal{S}'(\Phi_*)(\Psi), \Psi \rangle \geq \frac{1}{4\rho^3}\|\Psi\|_{\mathcal{Y}}^2.$$

The energy of Φ_* turns out to be very close to the energy of the approximate assembly E , as stated in the following lemma. The proof is similar to that of [9, Lemma 6.3].

Lemma 4.4. *It holds uniformly with respect to $\xi \in \Xi_\alpha$ and $r \in W_\beta$ that*

$$\begin{aligned} \mathcal{J}(\Phi_*) &= \sum_{j \leq n_i} 2\pi r_i^j + \sum_{j \leq n_b} \pi r_b^j \\ &+ \frac{\gamma}{2} \left[\sum_{j \leq n_i} \left(\frac{\pi(r_i^j)^4}{2} \log \frac{1}{r_i^j} + \frac{\pi(r_i^j)^4}{8} + (\pi(r_i^j)^2)^2 R(\xi_i^j, \xi_i^j) \right) \right. \\ &+ \sum_{j \leq n_b} \left(\frac{\pi(r_b^j)^4}{4} \log \frac{1}{r_b^j} + \frac{\pi(r_b^j)^4}{16} + \left(\frac{\pi(r_b^j)^2}{2} \right)^2 R_b(\xi_b^j, \xi_b^j) \right) \\ &+ 2 \sum_{j < k \leq n_i} \pi^2(r_i^j)^2(r_i^k)^2 G(\xi_i^j, \xi_i^k) + 2 \sum_{j < k \leq n_b} \left(\frac{\pi(r_b^j)^2}{2} \right) \left(\frac{\pi(r_b^k)^2}{2} \right) G(\xi_b^j, \xi_b^k) \end{aligned}$$

$n_i + \frac{n_b}{2}$	n_i	n_b	Minimum F
1	1	0	-0.0796
1	0	2	-0.0307
1.5	1	1	-0.1365
1.5	0	3	-0.1131
2	2	0	-0.2221
2	1	2	-0.2333
2	0	4	-0.2025
2.5	2	1	-0.3440
2.5	1	3	-0.3374
2.5	0	5	-0.2922
3	3	0	-0.4619
3	2	2	-0.4706
3	1	4	-0.4421
3	0	6	-0.3780
3.5	3	1	-0.5955
3.5	2	3	-0.5890
3.5	1	5	-0.5707
3.5	0	7	-0.4573
4	4	0	-0.7301
4	3	2	-0.7287
4	2	4	-0.6783
4	1	6	-0.6963
4	0	8	-0.5280

TABLE 1. Stationary assemblies with $n_i + \frac{n_b}{2}$ less than or equal to 4.

$$+ 2 \sum_{j \leq n_i, k \leq n_b} \pi(r_i^j)^2 \left(\frac{\pi(r_b^k)^2}{2} \right) G(\xi_i^j, \xi_b^k) \Big] + O(\rho^2).$$

5. Find the right ξ and r . Now we emphasize that Φ_* , the solution of $\Pi\mathcal{S}(\Phi_*) = 0$ found in Lemma 4.2, depends on ξ and r , and we denote it by $\Phi_*(\xi, r)$. The energy of $\Phi_*(\xi, r)$ can be viewed as a function of ξ and r , and thus denoted by $J(\xi, r)$:

$$J(\xi, r) = \mathcal{J}(\Phi_*(\xi, r)), \quad (\xi, r) \in \Xi_\alpha \times W_\beta. \quad (5.1)$$

This function is estimated in Lemma 4.4.

Lemma 5.1. 1. Let $r \in W_\beta$ be fixed. If ξ_* is a critical point of the function $\xi \rightarrow J(\xi, r)$ from Ξ_α to \mathbb{R} , then $\mathcal{S}(\Phi_*(\xi_*, r)) = 0$.
2. If (ξ_*, r_*) is a critical point of the function $(\xi, r) \rightarrow J(\xi, r)$ from $\Xi_\alpha \times W_\beta$ to \mathbb{R} , then $\Phi_*(\xi_*, r_*)$ is a stationary assembly of \mathcal{J} .

Proof. Denote the parametrization of the boundary of the perturbed discs in $\Phi_*(\xi, r)$ by $\mathbf{R}_i^1, \mathbf{R}_i^2, \dots, \mathbf{R}_i^{n_i}$ where

$$\mathbf{R}_i^j(\theta) = \xi_i^j + \sqrt{(r_i^j)^2 + 2\phi_{*,i}^j(\theta)} e^{i\theta}. \quad (5.2)$$

The unit tangent and normal vectors of \mathbf{R}_i^j are

$$\mathbf{T}_i^j(\theta) = \frac{\frac{\partial \mathbf{R}_i^j(\theta)}{\partial \theta}}{\left| \frac{\partial \mathbf{R}_i^j(\theta)}{\partial \theta} \right|}, \quad \mathbf{N}_i^j(\theta) = i \mathbf{T}_i^j(\theta), \quad (5.3)$$

respectively. Note that $\mathbf{N}_i^k(\theta, \beta, \xi)$ is inward pointing.

For the perturbed half discs in Φ_* , denote by $\mathbf{R}_b^j(\theta)$, $\mathbf{T}_b^j(\theta)$, and $\mathbf{N}_b^j(\theta)$, $j = 1, \dots, n_b$, the parametrization of the boundary, the unit tangent vector, and the unit normal vector respectively. The corresponding quantities under the $(\mathbf{t}(\xi_b^j), \mathbf{n}(\xi_b^j))$ frame are $\vec{R}_b^j(\theta)$, $\vec{T}_b^j(\theta)$, and $\vec{N}_b^j(\theta)$. Let us denote the rotation matrix

$$\mathbf{M}(\xi_b^j) = (\mathbf{t}(\xi_b^j), \mathbf{n}(\xi_b^j)). \quad (5.4)$$

Then

$$\mathbf{R}_b^j(\theta) = \mathbf{r}(\xi_b^j) + \mathbf{M}(\xi_b^j)\vec{R}_b^j(\theta) \quad (5.5)$$

where

$$\vec{R}_b^j(\theta) = \begin{pmatrix} \sqrt{(r_b^j)^2 + 2\phi_{*,b}^j(\theta)} \cos \theta \\ \sqrt{(r_b^j)^2 + 2\phi_{*,b}^j(\theta)} \sin \theta + f(\sqrt{(r_b^j)^2 + 2\phi_{*,b}^j(\theta)} \cos \theta, \xi) \end{pmatrix}. \quad (5.6)$$

Fix r and vary each $\xi_{i,q}^k$, $k = 1, \dots, n_i$, $q = 1, 2$. This leads to a deformation of Φ_* and a variation along the path

$$\begin{aligned} \frac{\partial J(\xi, r)}{\partial \xi_{i,q}^k} = & - \sum_{j \leq n_i} \int_{\partial \Omega_i^j} (\mathcal{S}_i^j(\Phi_*) + \lambda_i^j(\Phi_*)) \mathbf{N}_i^j \cdot \mathbf{X}_i^j(k, q) \, ds \\ & + \sum_{j \leq n_b} \left(\mathcal{S}_0^j(\Phi_*) X_0^j(k, q) + \mathcal{S}_\pi^j(\Phi_*) X_\pi^j(k, q) \right. \\ & \left. - \int_{\partial \Omega_b^j} (\mathcal{S}_b^j(\Phi_*) + \lambda_b^j(\Phi_*)) \mathbf{N}_b^j \cdot \mathbf{X}_b^j(k, q) \, ds \right) \end{aligned} \quad (5.7)$$

by (3.33). Here $\mathbf{X}(k, q)$ is the infinitesimal element of the deformation:

$$\mathbf{X}_\mu^j(k, q) = \frac{\partial \mathbf{R}_\mu^j}{\partial \xi_{i,q}^k}, \quad j = 1, \dots, n_\mu, \quad \mu = i, b, \quad k = 1, \dots, n_i, \quad q = 1, 2, \quad (5.8)$$

and $X_0^j(k, q)$ and $X_\pi^j(k, q)$ are given by (3.31) and (3.32) respectively. Similarly one varies each ξ_b^k to obtain

$$\begin{aligned} \frac{\partial J(\xi, r)}{\partial \xi_b^k} = & - \sum_{j \leq n_i} \int_{\partial \Omega_i^j} (\mathcal{S}_i^j(\Phi_*) + \lambda_i^j(\Phi_*)) \mathbf{N}_i^j \cdot \mathbf{X}_i^j(k) \, ds \\ & + \sum_{j \leq n_b} \left(\mathcal{S}_0^j(\Phi_*) X_0^j(k) + \mathcal{S}_\pi^j(\Phi_*) X_\pi^j(k) \right. \\ & \left. - \int_{\partial \Omega_b^j} (\mathcal{S}_b^j(\Phi_*) + \lambda_b^j(\Phi_*)) \mathbf{N}_b^j \cdot \mathbf{X}_b^j(k) \, ds \right) \end{aligned} \quad (5.9)$$

where $\mathbf{X}(k)$ is the infinitesimal element of the deformation:

$$\mathbf{X}_\mu^j(k) = \frac{\partial \mathbf{R}_\mu^j}{\partial \xi_b^k}, \quad j = 1, \dots, n_\mu, \quad \mu = i, b, \quad k = 1, \dots, n_b. \quad (5.10)$$

Since $\Pi \mathcal{S}(\Phi_*(\xi, r)) = 0$, there exist $A_p^j(\xi, r)$, $p = 1, 2$, and $B^j(\xi, r)$ in \mathbb{R} such that

$$\mathcal{S}_i^j(\Phi(\xi, r)) = A_1^j \cos \theta + A_2^j \sin \theta, \quad j = 1, \dots, n_i \quad (5.11)$$

$$\mathcal{S}_0^j(\Phi(\xi, r)) = B^j, \quad j = 1, \dots, n_b \quad (5.12)$$

$$\mathcal{S}_\pi^j(\Phi(\xi, r)) = -B^j, \quad j = 1, \dots, n_b \quad (5.13)$$

$$\mathcal{S}_b^j(\Phi(\xi, r)) = B^j \cos \theta, \quad j = 1, \dots, n_b. \quad (5.14)$$

Since the deformations $\mathbf{X}(k, q)$ and $\mathbf{X}(k)$ preserve the area of each component,

$$\int_{\partial\Omega_i^j} \mathbf{N}_i^j \cdot \mathbf{X}_i^j(k, q) ds = 0, \quad j = 1, \dots, n_i \quad (5.15)$$

$$\int_{\partial\Omega_b^j} \mathbf{N}_b^j \cdot \mathbf{X}_b^j(k, q) ds = 0, \quad j = 1, \dots, n_b \quad (5.16)$$

$$\int_{\partial\Omega_i^j} \mathbf{N}_i^j \cdot \mathbf{X}_i^j(k) ds = 0, \quad j = 1, \dots, n_i \quad (5.17)$$

$$\int_{\partial\Omega_b^j} \mathbf{N}_b^j \cdot \mathbf{X}_b^j(k) ds = 0, \quad j = 1, \dots, n_b. \quad (5.18)$$

One can drop the $\lambda_\mu^j(\Phi_*)$ terms in (5.7) and (5.9) and arrive at

$$\begin{aligned} \frac{\partial J(\xi, r)}{\partial \xi_{i,q}^k} = & - \sum_{j \leq n_i} \int_0^{2\pi} (A_1^j \cos \theta + A_2^j \sin \theta) \mathbf{N}_i^j \cdot \mathbf{X}_i^j(k, q) d\theta \\ & + \sum_{j \leq n_b} \left(B^j X_0^j(k, q) - B^j X_\pi^j(k, q) - \int_0^\pi B^j \cos \theta \vec{N}_b^j \cdot \vec{X}_b^j(k, q) d\theta \right) \end{aligned} \quad (5.19)$$

$$\begin{aligned} \frac{\partial J(\xi, r)}{\partial \xi_b^k} = & - \sum_{j \leq n_i} \int_0^{2\pi} (A_1^j \cos \theta + A_2^j \sin \theta) \mathbf{N}_i^j \cdot \mathbf{X}_i^j(k) d\theta \\ & + \sum_{j \leq n_b} \left(B^j X_0^j(k) - B^j X_\pi^j(k) - \int_0^\pi B^j \cos \theta \vec{N}_b^j \cdot \vec{X}_b^j(k) d\theta \right) \end{aligned} \quad (5.20)$$

At a critical point ξ_* of $\xi \rightarrow J(\xi, r)$, the left sides of (5.19) and (5.20) vanish and one obtains a linear homogeneous system for A_p^j and B^j . One can show, as in the proof of [9, Lemma 8.1], that this system is non-singular and hence

$$A_p^j(\xi_*, r) = 0, \quad j = 1, \dots, n_i, \quad p = 1, 2, \quad B^j(\xi_*, r) = 0, \quad j = 1, \dots, n_b \quad (5.21)$$

proving the first part of the lemma.

For the second part of the lemma, we replace r by a more convenient variable m :

$$m_i^j = \pi(r_i^j)^2, \quad m_b^j = \pi(r_b^j)^2 \quad (5.22)$$

One varies each m_ν^k to obtain another deformation of Φ_* . Since $A_p^j(\xi_*, m_*) = 0$ and $B^j(\xi_*, m_*) = 0$, the first variation formula (3.33) yields

$$\begin{aligned} \frac{\partial J(\xi, m)}{\partial m_\nu^k} \Big|_{(\xi, m) = (\xi_*, m_*)} = & - \sum_{j \leq n_i} \int_{\partial\Omega_i^j} \lambda_i^j(\xi_*, m_*) \mathbf{N}_i^j \cdot \mathbf{X}_i^j(\nu, k) ds \\ & - \sum_{j \leq n_b} \int_{\partial\Omega_b^j} \lambda_b^j(\xi_*, m_*) \mathbf{N}_b^j \cdot \mathbf{X}_b^j(\nu, k) ds \\ = & - \sum_{j \leq n_i} \lambda_i^j(\xi_*, m_*) \frac{\partial |\Omega_i^j|}{\partial m_\nu^k} - \sum_{j \leq n_b} \lambda_b^j(\xi_*, m_*) \frac{\partial |\Omega_b^j|}{\partial m_\nu^k} \\ = & - \sum_{j \leq n_i} \lambda_i^j(\xi_*, m_*) \frac{\partial m_i^j}{\partial m_\nu^k} - \sum_{j \leq n_b} \lambda_b^j(\xi_*, m_*) \frac{\partial (\frac{m_b^j}{2})}{\partial m_\nu^k} \end{aligned}$$

$$= \begin{cases} -\lambda_i^k(\xi_*, m_*) & \text{if } \nu = i \\ -\frac{\lambda_b^k(\xi_*, m_*)}{2} & \text{if } \nu = b \end{cases}. \quad (5.23)$$

Here $\mathbf{X}(\nu, k)$ is the infinitesimal element of the deformation. Note that the area of the component Ω_ν^k is not preserved in this deformation. Because m_μ^j are constrained by

$$\sum_{j \leq n_i} m_i^j + \sum_{j \leq n_b} \frac{m_b^j}{2} = \omega |D|, \quad (5.24)$$

there exists a Lagrange multiplier $\lambda \in \mathbb{R}$ such that

$$\frac{\partial J(\xi, m)}{\partial m_i^k} \Big|_{(\xi, m) = (\xi_*, m_*)} + \lambda = 0, \quad \frac{\partial J(\xi, m)}{\partial m_b^k} \Big|_{(\xi, m) = (\xi_*, m_*)} + \frac{\lambda}{2} = 0. \quad (5.25)$$

It follows from (5.23) and (5.25) that

$$\lambda_\nu^k(\xi_*, m_*) = \lambda, \quad k = 1, \dots, n_\nu, \quad \nu = i, b. \quad (5.26)$$

This proves the second part of the lemma. \square

Proof of Theorem 1.1. Consider J in the domain $\Xi_\alpha \times W_\beta$ where Ξ_α and W_β are given in (2.1) and (2.2) respectively. One views Ξ_α as a compact $2n_i + n_b$ dimensional manifold with boundary and W_β as a compact $n_i + n_b - 1$ dimensional manifold with boundary. Then $\Xi_\alpha \times W_\beta$ is a compact $3n_i + 2n_b - 1$ dimensional manifold with boundary. For each $(\xi, r) \in \Xi_\alpha \times W_\beta$ there is $\Phi_*(\xi, r)$ that solves $\Pi\mathcal{S}(\Phi_*(\xi, r)) = 0$ by Lemma 4.2. Since $\Xi_\alpha \times W_\beta$ is compact, there exists $(\xi_*, r_*) \in \Xi_\alpha \times W_\beta$ that minimizes J in $\Xi_\alpha \times W_\beta$. It suffices to show that (ξ_*, r_*) is in the interior of $\Xi_\alpha \times W_\beta$.

First prove

$$\frac{r_{*,i}^j}{\rho} \rightarrow 1 \text{ and } \frac{r_{*,b}^j}{\rho} \rightarrow 1, \text{ as } \rho \rightarrow 0. \quad (5.27)$$

Let $R_i^j = \frac{r_i^j}{\rho}$ and $R_b^j = \frac{r_b^j}{\rho}$, so $R = (R_i^1, \dots, R_i^{n_i}, R_b^1, \dots, R_b^{n_b})$ is a scaled version of r . By Lemma 4.4 we write

$$J(\xi, r) = J(\xi, R) = \left(\gamma \rho^4 \log \frac{1}{\rho} \right) J_1(R) + \gamma \rho^4 J_2(\xi, R) + O(\rho^2) \quad (5.28)$$

where

$$\begin{aligned} J_1(R) &= \frac{1}{\gamma \rho^3 \log \frac{1}{\rho}} \left(\sum_{j \leq n_i} 2\pi R_i^j + \sum_{j \leq n_b} \pi R_b^j \right) \\ &\quad + \frac{1}{2} \left[\sum_{j \leq n_i} \frac{\pi (R_i^j)^4}{2} + \sum_{j \leq n_b} \frac{\pi (R_b^j)^4}{4} \right] \\ J_2(\xi, R) &= \frac{1}{2} \left[\sum_{j \leq n_i} \left(\frac{\pi (R_i^j)^4}{2} \log \frac{1}{R_i^j} + \frac{\pi (R_i^j)^4}{8} + (\pi (R_i^j)^2)^2 R(\xi_i^j, \xi_i^j) \right) \right. \\ &\quad \left. + \sum_{j \leq n_b} \left(\frac{\pi (R_b^j)^4}{4} \log \frac{1}{R_b^j} + \frac{\pi (R_b^j)^4}{16} + \left(\frac{\pi (R_b^j)^2}{2} \right)^2 R_b(\xi_b^j, \xi_b^j) \right) \right] \end{aligned} \quad (5.29)$$

$$\begin{aligned}
& +2 \sum_{j < k \leq n_i} \pi^2 (R_i^j)^2 (R_i^k)^2 G(\xi_i^j, \xi_i^k) \\
& +2 \sum_{j < k \leq n_b} \left(\frac{\pi(R_b^j)^2}{2} \right) \left(\frac{\pi(R_b^k)^2}{2} \right) G(\xi_b^j, \xi_b^k) \\
& +2 \sum_{j \leq n_i, k \leq n_b} \pi(R_i^j)^2 \left(\frac{\pi(R_b^k)^2}{2} \right) G(\xi_i^j, \xi_b^k).
\end{aligned} \tag{5.30}$$

Because of the lower bound $\frac{1+\epsilon}{\rho^3 \log \frac{1}{\rho}} < \gamma$ for γ in this theorem, the term $O(\rho^2)$ in (5.28) is much smaller than the other two terms in (5.28). By (2.4), the condition $\frac{1}{\gamma \rho^3 \log \frac{1}{\rho}} < \frac{1}{1+\epsilon}$ in the theorem, the range $R_i^j, R_b^j \in [1-\beta, 1+\beta]$, and the constraint

$$\sum_{j \in N_i} (R_i^j)^2 + \sum_{j \in N_b} \frac{(R_b^j)^2}{2} = n_i + \frac{n_b}{2}, \tag{5.31}$$

one derives that J_1 is minimized at $R_i^j = R_b^j = 1$. The corresponding $r_i^j = r_b^j = \rho$ is a point in the interior of W_β . Since (5.28) implies that

$$\frac{1}{\gamma \rho^4 \log \frac{1}{\rho^3 \log \frac{1}{\rho}}} J(\xi, R) \rightarrow J_1(R), \text{ as } \rho \rightarrow 0, \tag{5.32}$$

uniformly with respect to ξ and R , $R_* = \frac{r_*}{\rho}$ must converge to the minimum of J_1 , i.e.

$$R_* \rightarrow (1, \dots, 1, 1, \dots, 1) \text{ as } \rho \rightarrow 0, \tag{5.33}$$

so (5.27) follows. Next consider $J(\xi, r_*)$ where $\xi \in \Xi_\alpha$ but r is taken to be r_* and correspondingly $R = R_*$. By (5.28) and (5.33),

$$\begin{aligned}
& \lim_{\rho \rightarrow 0} \frac{1}{\gamma \rho^4} \left(J(\xi, R_*) - \left(\gamma \rho^4 \log \frac{1}{\rho} \right) J_1(R_*) \right) \\
& = \lim_{\rho \rightarrow 0} J_2(\xi, R_*) \\
& = \frac{1}{2} \left(\frac{n_i \pi}{8} + \frac{n_b \pi}{16} + \pi^2 F(\xi) \right)
\end{aligned} \tag{5.34}$$

uniformly with respect to ξ . Consequently, since J_1 does not depend on ξ , every limit point of ξ_* along a subsequence must be a minimum of F in Ξ_α . But (2.3) says that a minimum of F in Ξ_α is also a minimum of F in Ξ and it is not on the boundary of Ξ_α .

The last assertion and (5.27) imply that when ρ is small, (ξ_*, r_*) is in the interior of $\Xi_\alpha \times W_\beta$. Therefore (ξ_*, r_*) is a critical point of J , and the theorem follows from Lemma 5.1.2. \square

Proof of Theorem 1.2. The first part is proved in (5.27) and the second part is proved after (5.34). Our assertion that $\Phi_*(\xi_*, r_*)$ is a stable assembly is based on the fact that this stationary point is obtained in successive (local) minimization procedures. In section 4 for each (ξ, r) in $\Xi_\alpha \times W_\beta$, $\Phi_*(\xi, r)$ was found as a fixed point. Because of Lemma 4.3.2, $\Phi_*(\xi, r)$ is locally minimizing in \mathcal{X}_b , i.e. locally minimizing in the class of assemblies whose discs are centered at ξ_μ^j and of radii r_μ^j . Then in the proof of Theorem 1.1, (ξ_*, r_*) is taken to be the minimum of $\mathcal{J}(\Phi_*(\xi, r))$ with respect to (ξ, r) in $\Xi_\alpha \times W_\beta$. \square

$n_i + \frac{n_b}{2}$	n_i	n_b	Minimum F
10	10	0	-2.5781
10	9	2	-2.5819
10	8	4	-2.5885
10	7	6	-2.5793
10	6	8	-2.5644
10	5	10	-2.5433
10	4	12	-2.4791
10	3	14	-2.2864
10	2	16	-1.9222
10	1	18	-1.3549
10	0	20	-0.3911

TABLE 2. Stationary assemblies with $n_i + \frac{n_b}{2} = 10$.

6. Boundary half discs lower energy. Let $\Phi_*(\xi_*, r_*)$ be an stationary assembly found in Theorem 1.1. Since the $r_{*,i}^j$ and $r_{*,b}^j$ are all close to ρ according to Theorem 1.2, by Lemma 4.4 $\mathcal{J}(\Omega_*)$ is approximately equal to

$$\begin{aligned} \mathcal{J}(\Omega_*) \approx & 2\pi\left(n_i + \frac{n_b}{2}\right)\rho + \frac{\pi\gamma\rho^4 \log \frac{1}{\rho} \left(n_i + \frac{n_b}{2}\right)}{4} \\ & + \frac{\pi\gamma\rho^4 \left(n_i + \frac{n_b}{2}\right)}{16} + \frac{\pi^2\gamma\rho^4}{2}F(\xi_*). \end{aligned} \quad (6.1)$$

Assume that γ and ω are in a specific parameter range such that

$$\gamma = \frac{\mu}{\omega^{3/2} \log \frac{1}{\omega}} = \frac{\mu}{\left(\frac{\left(n_i + \frac{n_b}{2}\right)\pi}{|D|}\right)^{3/2} \rho^3 \log \frac{|D|}{\left(n_i + \frac{n_b}{2}\right)\pi\rho^2}} \quad (6.2)$$

for a fixed $\mu > 0$. The leading order of the free energy calculated from (6.1) is

$$\begin{aligned} 2\pi\left(n_i + \frac{n_b}{2}\right)\rho + \frac{\pi\gamma\rho^4 \left(n_i + \frac{n_b}{2}\right) \log \frac{1}{\rho}}{4} &= 2\sqrt{\omega|D|\pi} \sqrt{n_i + \frac{n_b}{2}} \\ &+ \frac{\sqrt{\omega}|D|^2\mu}{8\pi} \frac{1}{n_i + \frac{n_b}{2}} \\ &+ \text{smaller term.} \end{aligned} \quad (6.3)$$

With respect to $n_i + \frac{n_b}{2}$ the last quantity is minimized at

$$n_i + \frac{n_b}{2} \approx \frac{|D|\mu^{2/3}}{4\pi}. \quad (6.4)$$

This gives the optimal number of discs in a stationary assembly. Note that under (6.2) and (6.4), the corresponding ρ and γ fall into the range specified in Theorem 1.1.

One should compare the energy of stationary assemblies of the same area, i.e. the same ω , and the same number of discs, i.e. the same $n_i + \frac{n_b}{2}$. In particular one can compare stationary assemblies of the same area and of the optimal number of discs. Then all disc radii are approximately equal to the same ρ . One must look at the higher order term to distinguish the energy of these assemblies. By (6.1), the

energy in the higher order is determined by $F(\xi_*)$. This leads to the minimization of F .

Let the domain D be the unit disc $\{x \in \mathbb{R}^2 : |x| < 1\}$ so that the Green's function of $-\Delta$ is explicitly known:

$$G(x, y) = \frac{1}{2\pi} \log \frac{1}{|x - y|} + \frac{1}{2\pi} \left(\frac{|x|^2}{2} + \frac{|y|^2}{2} + \log \frac{1}{|x\bar{y} - 1|} \right) - \frac{3}{8\pi}. \quad (6.5)$$

Table 1 lists the numerical minimum value of F together with $n_i + \frac{n_b}{2}$, n_i , and n_b . A row with highlighted minimum F value is the stationary assembly with the lowest energy among all stationary assemblies of the same ω and the same $n_i + \frac{n_b}{2}$. For instance, when $n_i + \frac{n_b}{2} = 3$ the stationary assembly with the lowest energy has 2 interior discs and 2 boundary half discs.

One has a more realistic scenario when $n_i + \frac{n_b}{2}$ is a large number. Table 2 lists stationary assemblies with $n_i + \frac{n_b}{2} = 10$. Here the assemblies with 9, 8, 7 interior discs respectively have lower energy than the one with interior discs only. The assembly of the lowest energy has 8 interior discs and 4 boundary half discs.

As one finds the minimum of F numerically, the centers of the interior discs and the boundary half discs of a stationary assembly are determined. Figure 1 shows these stationary assemblies based on the numerical minimum of F for all the cases with $n_i + \frac{n_b}{2} = 10$.

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