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SPHERICAL SOLUTIONS TO A NONLOCAL FREE BOUNDARY PROBLEM FROM DIBLOCK COPOLYMER MORPHOLOGY*

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Abstract. The Γ-limit of the Ohta–Kawasaki density functional theory of diblock copolymers is a nonlocal free boundary problem. For some values of block composition and the nonlocal interaction, an equilibrium pattern of many spheres exists in a three-dimensional domain. A subrange of the parameters is found where the multiple sphere pattern is stable. This stable pattern models the spherical phase in the diblock copolymer morphology. The spheres are approximately round. They satisfy an equation that involves their mean curvature and a quantity that depends nonlocally on the whole pattern. The locations of the spheres are determined via a Green's function of the domain.

Key words. spherical phase, diblock copolymer morphology, sphere coarsening, interface oscillation

AMS subject classifications. 35R35, 82B24, 82D60

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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 subchain of A-monomers grafted covalently to another subchain of B-monomers. 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 cannot lead to a macroscopic phase separation. Only a local microphase separation occurs: microdomains rich in A-monomers and microdomains rich in B-monomers emerge as a result. These microdomains form patterns that are known as morphology phases. Various phases, including lamellar, cylindrical, spherical, and gyroid, have been observed in experiments. See Bates and Fredrickson [1] for more on block copolymers.

This paper deals with the spherical phase of the block copolymer morphology (Figure 1.1, Plot 1). Let $a \in (0,1)$ be the block composition fraction which is the number of the A-monomers divided by the number of all the A- and B-monomers in a chain molecule. The spherical phase occurs when a is relatively close to 0 (or close to 1), and the A-monomers (or B-monomers, respectively) form small balls in space.

The model we use here is a nonlocal free boundary problem derived from the Ohta–Kawasaki density functional theory of diblock copolymers [18]. Let D be a bounded and sufficiently smooth domain in R^3 occupied by a diblock copolymer melt in the spherical phase. Let E be a subset of D where A-monomers concentrate. Then $D \backslash E$ is the subset where B-monomers concentrate. Denote the part of the boundary of E that is in D by $\partial_D E$ which is the set of the interfaces separating the A-rich microdomains from the B-rich microdomains. Denote the Lebesgue measure of E by $|E|$. Given a block composition fraction $a \in (0,1)$, one has $|E| = a|D|$.

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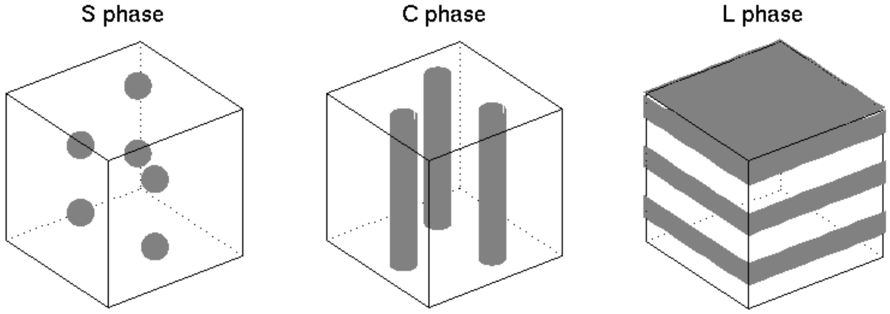

FIG. 1.1. *The spherical, cylindrical, and lamellar morphology phases commonly observed in diblock copolymer melts. The dark color indicates the concentration of type A monomers, and the white color indicates the concentration of type B monomers.*

Moreover, there exists a number λ such that 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 mean curvature of $\partial_D E$ viewed from E, γ is a positive parameter, and χ_E is the characteristic function of E, i.e. $\chi_E(x) = 1$ if $x \in E$, and $\chi_E(x) = 0$ if $x \in D \backslash E$. The expression $(-\Delta)^{-1}(\chi_E - a)$ is the solution v of the problem

$$-\Delta v = \chi_E - a \text{ in } D, \qquad \partial_\nu v = 0 \text{ on } \partial D, \qquad \overline{v} = 0,$$

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 defined from $\{q \in L^2(D) : \overline{q} = 0\}$ to itself, the free boundary problem (1.1) is nonlocal.

Equation (1.1) is the Euler–Lagrange equation of the free energy J of the system. The functional J is given by

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

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. In (1.2), $|D\chi_E|(D)$ is the perimeter of E. When ∂E is smooth, this is merely the surface area of $\partial_D E$. For a more general E, χ_E is a BV-function and $D\chi_E$ is a vector valued finite measure. We denote the magnitude of this measure by $|D\chi_E|$ which is a positive, finite measure. The perimeter of E is defined to be the size of D under this measure. The operator $(-\Delta)^{-1/2}$ is the positive square root of $(-\Delta)^{-1}$.

The main difficulty in (1.1) stems from the nonlocal term. Without it, i.e., if $\gamma = 0$, (1.1) would just be the equation of constant mean curvature. However with the nonlocal term the curvature of a solution in general is not constant. One exception occurs in the study of the lamellar phase (Figure 1.1, Plot 3) where interfaces are parallel planes (Ren and Wei [20, 23]). The solution we are looking for in this paper is a union of a number of disconnected sets each of which is close to a small round ball. The solution is hence termed a spherical solution.

Nishiura and Ohnishi [16] 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 [20] 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 mathematically to these problems. The lamellar phase (Figure 1.1, Plot 3) is studied by Ren and Wei [20, 22, 23, 27, 28], Fife and Hilhorst [9], Choksi and Ren [4], Chen and Oshita [2], and Choksi and Sternberg [6]. The result obtained by Müller [15] is related to the lamellar phase in the case $a = 1/2$, as observed in [16]. Radially symmetric bubble and ring patterns are studied by Ren and Wei [21, 26, 29]. The gyroid phase is numerically studied by Teramoto and Nishiura [33]. Triblock copolymers are studied by Ren and Wei [24, 25]. A diblock copolymer/homopolymer blend is studied by Choksi and Ren [5]. Also, see Ohnishi et al. [17] and Choksi [3].

The cylindrical phase (Figure 1.1, Plot 2) is studied by Ren and Wei [31, 30], in which a variant of the Lyapunov–Schmidt reduction procedure is developed to study a cross section of Figure 1.1, Plot 2. A pattern with a number of approximate small discs is found which satisfies the two-dimensional version of (1.1). In two dimensions, $\partial_D E$ is a union of curves and $H(\partial_D E)$ is the curvature of the curves.

In this paper we adapt the Lyapunov–Schmidt reduction procedure to three dimensions to construct spherical solutions. These solutions look like Figure 1.1, Plot 1. They model the spherical phase of diblock copolymer morphology.

The main results are presented in section 2. Our strategy to prove them consists of setting up a first approximation (section 3) and through linearization (sections 4 and 5) and fixed point argument (sections 6 and 7) solving a projected version of the full problem (up to spherical harmonics of order 0 and 1 corresponding to translations and changes in volume). This reduces the infinite dimensional variational problem to a finite dimensional minimization problem in centers and radii. After finding a minimum of the finite dimensional problem, we show that it is indeed an exact solution of the full problem, using a tricky reparametrization argument (section 8).

Our construction yields, in addition, information on the spectra of linearization, interpreted as forms of stability-instability.

Compared to the two-dimensional case, the study of the linearized problem is more involved here. In two dimensions the corresponding linearized problem is analyzed by the Fourier series method. Here in three dimensions we use spherical harmonics to diagonalize the linearized operator (see Lemma 5.1). More differences between the two-dimensional and the three-dimensional cases are given in section 9.

2. Main results.

The Green's function of $-\Delta$ is denoted by G. It is a sum of two parts:

$$G(x,y) = \frac{1}{4\pi|x-y|} + R(x,y). \tag{2.1}$$

The first part on the right-hand side of (2.1) is the fundamental solution in three dimensions. The second part is the regular part of $G(x,y)$, denoted by $R(x,y)$. The

Green's function satisfies

(2.2)
$$-\Delta_x G(x,y) = \delta(x-y) - \frac{1}{|D|} \text{ in } D, \quad \partial_{\nu(x)} G(x,y) = 0 \text{ on } \partial D, \quad \overline{G(\cdot,y)} = 0 \ \forall y \in D.$$

Here Δ_x is the Laplacian with respect to the x-variable of G, and $\nu(x)$ is the outward normal direction at $x \in \partial D$. We set

$$F(\xi_1, \xi_2, \dots, \xi_K) = \sum_{k=1}^{K} R(\xi_k, \xi_k) + \sum_{k=1}^{K} \sum_{l=1, l\neq k}^{K} G(\xi_k, \xi_l), \tag{2.3}$$

for $\xi_k \in D$ and $\xi_k \neq \xi_l$ if $k \neq l$. Because $G(x,y) \to \infty$ if $|x-y| \to 0$ and $R(x,x) \to \infty$ if $x \to \partial D$, F admits at least one global minimum.

The average sphere radius is

$$\rho = \left(\frac{3a|D|}{4\pi K} \right)^{1/3}. \tag{2.4}$$

The main result of this paper is the following existence theorem.

THEOREM 2.1. *Let $K \geq 2$ be an integer.*

1. *For every $\epsilon > 0$ there exists $\delta > 0$, depending on ϵ, K, and D only, such that if*

$$\gamma \rho^3 > 3 + \epsilon, \tag{2.5}$$

$$\left| \gamma\rho^3 - \frac{3(n+2)(2n+1)}{2} \right| > \epsilon n^2 \ \forall \ n = 2, 3, 4, \dots, \tag{2.6}$$

and

$$\rho < \delta, \tag{2.7}$$

then there exists a solution E of (1.1).

2. *The solution E is a union of K approximate balls. The radius of each ball is close to ρ.*
3. *Let the centers of these balls be $\zeta_1, \zeta_2, \dots, \zeta_K$. Then $\zeta = (\zeta_1, \zeta_2, \dots, \zeta_K)$ is close to a global minimum of the function F.*

The precise meaning that each component of E is close to a ball of radius ρ is given in (8.18). As ρ (or a) tends to 0, ζ converges to a global minimum of F, possibly along a subsequence.

We have opted for a rather general existence theorem. The solution found in the theorem is not necessarily stable. The stability of the solution depends on how (2.6) is satisfied.

THEOREM 2.2. *If* (2.6) *is satisfied because*

$$\gamma\rho^3 - \frac{3(n+2)(2n+1)}{2} < -\epsilon n^2 \ \forall \ n \geq 2, \tag{2.8}$$

then the spherical solution is stable. Otherwise if (2.6) *is satisfied but*

$$\epsilon n^2 < \gamma\rho^3 - \frac{3(n+2)(2n+1)}{2}, \text{ and } \gamma\rho^3 - \frac{3(n+3)(2n+3)}{2} < -\epsilon(n+1)^2 \tag{2.9}$$

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

When we delete intervals around $\frac{3(n+2)(2n+1)}{2}$, $n = 2, 3, \ldots$, in (2.6), 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 $\frac{3(n+2)(2n+1)}{2}$. When this happens, $\gamma\rho^3$ cannot be placed above such $\frac{3(n+2)(2n+1)}{2}$. This implies that there exists $C(\epsilon) > 0$ depending on ϵ such that

$$\gamma < \frac{C(\epsilon)}{\rho^3}. \tag{2.10}$$

A little computation shows that $C(\epsilon)$ is

$$C(\epsilon) = \frac{3}{2}\left(\frac{6+\sqrt{36+18\epsilon}}{2\epsilon} + 2\right)\left(\frac{6+\sqrt{36+18\epsilon}}{\epsilon} + 1\right).$$

Combining (2.10) with (2.5) we see that ρ and γ are in a somewhat narrow parameter range

$$\rho < \delta, \quad \frac{3+\epsilon}{\rho^3} < \gamma < \frac{C(\epsilon)}{\rho^3}, \tag{2.11}$$

and $\gamma\rho^3$ must stay away from the sequence $\frac{3(n+2)(2n+1)}{2}$, $n = 2, 3, \ldots$, in the sense of (2.6). From (2.11) one sees that ρ must be small and γ be appropriately large.

We may assign a negative gradient flow to J and consider a dynamic counterpart of (1.1) (see [16]). The condition (2.5) prevents coarsening in such a dynamic process. By coarsening we mean that some balls become larger and other balls shrink and disappear.

The gap condition (2.6) controls interface oscillation. Interface oscillation refers to a phenomenon that oscillations appear on the boundary of a ball. The gap condition also suggests bifurcations to oscillating solutions. Elsewhere gap conditions have appeared in constructing layered solutions for singularly perturbed problems. See Malchiodi and Montenegro [12], del Pino, Kowalczyk, and Wei [8], Pacard and Ritoré [19], and the references therein.

The solution found in Theorem 2.1 may be unstable because of interface oscillation. The condition (2.8) in Theorem 2.2 eliminates this possibility. Under (2.8), ϵ must be no greater than 3, and ρ and γ must satisfy a more stringent requirement

$$\rho < \delta, \quad \frac{3+\epsilon}{\rho^3} < \gamma < \frac{30-4\epsilon}{\rho^3}. \tag{2.12}$$

This means that $\gamma\rho^3$ must stay to the left of the sequence $\frac{3(n+2)(2n+1)}{2}$, $n = 2, 3, \ldots$. If (2.9) holds, then we have an unstable mode that tends to bring oscillations to the spheres.

The spheres in the solution we construct are approximately round, with the same approximate radius. Theorem 2.1, part 3 asserts that the sphere centers must minimize F approximately.

We can even determine the optimal number of balls in a spherical pattern. Because of (2.11), we write

$$\gamma = \frac{\mu}{a} = \frac{\mu}{\left(\frac{4\pi K}{3|D|}\right)\rho^3}. \tag{2.13}$$

Now a and μ are the parameters of the problem. We hold μ fixed and make a and hence ρ small.

With (2.13) and (2.4) the leading order of the free energy is calculated from the formula in Lemma 8.1,

$$4\pi\rho^2 K + \frac{\gamma}{2}\left(\frac{8\pi\rho^5 K}{15}\right) = 4\pi K^{1/3}\left(\frac{3a|D|}{4\pi}\right)^{2/3} + \frac{\mu 4\pi}{15a}\left(\frac{3a|D|}{4\pi}\right)^{5/3} K^{-2/3}. \tag{2.14}$$

With respect to K the last quantity is minimized at

$$K = \frac{|D|\mu}{10\pi}. \tag{2.15}$$

Note that the choice (2.15) of K does not violate the condition (2.12), since, with this K,

$$\gamma = \frac{\mu}{a} = \mu\frac{3|D|}{K4\pi\rho^3} = \mu\frac{3|D|}{4\pi\rho^3}\frac{10\pi}{\mu|D|} = \frac{30}{4\rho^3}. \tag{2.16}$$

Equation (2.15) gives the optimal number of spheres in a spherical pattern.

3. Approximate solutions.

Throughout the rest of this paper we are given $\epsilon > 0$, and γ and ρ satisfy (2.5) and (2.6).

Let U_1 be a small neighborhood in D^K of the set $\{\eta :\ F(\eta) = \min_{\xi\in D^K} F(\xi)\}$, and U_2 be the set

$$U_2 = \Big\{(r_1, r_2, \dots, r_K) \in R^K :\ r_k \in ((1-\delta_2)\rho, (1+\delta_2)\rho),$$
$$k = 1, 2, \dots, K,\quad \sum_{k=1}^{K} \frac{4\pi r_k^3}{3} = a|D|\Big\}. \tag{3.1}$$

The constant δ_2 is positive, small, and depends on ϵ. It will be fixed later in the proofs of Lemmas 5.3 and 8.2. Define

$$U = U_1 \times U_2. \tag{3.2}$$

Let $\xi_1, \xi_2, \dots, \xi_K$ be K distinct points in D such that $\xi = (\xi_1, \xi_2, \dots, \xi_K)$ is in U_1, and $r = (r_1, r_2, \dots, r_K)$ is in U_2. Denote the ball centered at ξ_k of radius r_k by B_k. The union of the B_k's is B:

$$B = \bigcup_{k=1}^{K} B_k = \bigcup_{k=1}^{K} \{x \in R^3 : |x - \xi_k| < r_k\}. \tag{3.3}$$

With U_1 close to $\{\eta :\ F(\eta) = \min_{\kappa\in D^K} F(\kappa)\}$ and ρ sufficiently small, the B_k's are all inside D and disjoint.

LEMMA 3.1. *When E is B, the left-hand side of* (1.1) *is*

$$\frac{1}{r_k} + \gamma\left[\frac{r_k^2}{3} + \frac{4\pi r_k^3}{3}R(\xi_k, \xi_k) + \sum_{l\neq k}\frac{4\pi r_l^3}{3}G(\xi_k, \xi_l)\right] + O(\rho)$$

at each $\xi_k + r_k\theta_k$, where $\theta_k \in S^2$ and S^2 is the unit sphere.

Proof. At a boundary point $\xi_k + r_k\theta_k$ of B_k, the curvature is $\frac{1}{r_k}$.

We compute $v_k = (-\Delta)^{-1}(\chi_{B_k} - \frac{4\pi r_k^3}{3|D|})$. Define

$$P_k(x) = \begin{cases} -\frac{|x-\xi_k|^2}{6} + \frac{r_k^2}{2} & \text{if } |x-\xi_k| < r_k \\ \frac{r_k^3}{3|x-\xi_k|}, & \text{if } |x-\xi_k| \geq r_k. \end{cases}$$

Then $-\Delta P_k = \chi_{B_k}$. Write $v_k(x) = P_k(x) + Q_k(x,\xi_k)$. Clearly

$$-\Delta Q_k(x,\xi_k) = -\frac{4\pi r_k^3}{3|D|},\ \partial_{\nu(x)} Q_k(x,\xi_k) = -\partial_\nu \frac{4\pi r_k^3}{3}\frac{1}{4\pi|x-\xi_k|}$$
$$\text{on } \partial D,\ \overline{Q_k(\cdot,\xi_k)} = -\overline{P_k}.$$

From (2.2) we see that $Q_k(x,\xi_k)$ and $\frac{4\pi r_k^3}{3}R(x,\xi_k)$ satisfy the same equation and the same boundary condition, where R is the regular part of the Green's function G. Therefore they can differ only by a constant. This constant is $\overline{Q_k(\cdot,\xi_k)} - \frac{4\pi r_k^3}{3}\overline{R(\cdot,\xi_k)}$. But $\overline{v_k} = \overline{G(\cdot,\xi_k)} = 0$ implies that this constant is

$$-\overline{P_k} + \frac{4\pi r_k^3}{3}\overline{\frac{1}{4\pi|x-\xi_k|}} = \frac{4\pi r_k^5}{3}\frac{1}{10|D|}$$

by direct calculation. Hence

$$Q_k(x,\xi_k) = \frac{4\pi r_k^3}{3}R(x,\xi_k) + \frac{4\pi}{3}\frac{r_k^5}{10|D|}$$

and

$$v_k(x) = P_k(x) + \frac{4\pi r_k^3}{3}R(x,\xi_k) + \frac{4\pi}{3}\frac{r_k^5}{10|D|}. \tag{3.4}$$

Let $v = (-\Delta)^{-1}(\chi_B - a) = \sum_l v_l$. Then at $\xi_k + r_k\theta_k$

$$\begin{aligned} v(\xi_k + r_k\theta_k) &= \frac{r_k^2}{3} + \frac{4\pi r_k^3}{3}R(\xi_k + r_k\theta_k,\xi_k) + \sum_{l\neq k}\frac{4\pi r_l^3}{3}G(\xi_k + r_k\theta_k,\xi_l) \\ &\quad + \sum_{l=1}^{K}\frac{4\pi}{3}\frac{r_l^5}{10|D|} \\ &= \frac{r_k^2}{3} + \frac{4\pi r_k^3}{3}R(\xi_k,\xi_k) + \sum_{l\neq k}\frac{4\pi r_l^3}{3}G(\xi_k,\xi_l) + O(\rho^4). \end{aligned} \tag{3.5}$$

The lemma follows from (2.10). ☐

LEMMA 3.2. *The free energy of B is*

$$\begin{aligned} J(B) = \sum_{k=1}^{K} 4\pi r_k^2 + \frac{\gamma}{2}\Bigg\{ &\sum_{k=1}^{K}\left[\frac{8\pi r_k^5}{15} + \left(\frac{4\pi}{3}\right)^2 r_k^6 R(\xi_k,\xi_k)\right] \\ &+ \sum_{k=1}^{K}\sum_{l=1,l\neq k}^{K}\left(\frac{4\pi}{3}\right)^2 r_k^3 r_l^3 G(\xi_k,\xi_l) + \sum_{k=1}^{K}\sum_{l=1}^{K}\left(\frac{4\pi}{3}\right)^2\left(\frac{r_k^3 r_l^5}{10|D|} + \frac{r_k^5 r_l^3}{10|D|}\right)\Bigg\}. \end{aligned}$$

Proof. The local part of the free energy is just $\sum_{k=1}^K 4\pi r_k^2$.

The nonlocal part of the free energy is

$$\begin{aligned}
&\int_D |(-\Delta)^{-1/2}(\chi_B - a)|^2\,dx\\
&\quad = \int_D (\chi_B - a)v(x)\,dx \; = \; \sum_{l=1}^K \int_{B_l} v(x)\,dx\\
&\quad = \sum_{l=1}^K \sum_{k=1}^K \int_{B_l} v_k(x)\,dx \; = \; \sum_{l=1}^K \sum_{k=1}^K \left[\int_{B_l} P_k(x)\,dx + \int_{B_l} Q_k(x,\xi_k)\,dx \right].
\end{aligned}$$

There are two possibilities. When $l = k$, from the definition of P_k we find

$$\int_{B_k} P_k(x)\,dx = \frac{8\pi r_k^5}{15}. \tag{3.6}$$

For the integral of Q_k, we have

$$\int_{B_k} Q_k(x,\xi_k)\,dx = \frac{4\pi r_k^3}{3} \int_{B_k} R(x,\xi_k)\,dx + \left(\frac{4\pi}{3}\right)^2 \frac{r_k^8}{10|D|}.$$

Since $R(x,\xi_k) - \frac{1}{6|D|}|x-\xi_k|^2$ is harmonic in x, by the mean value theorem for harmonic functions

$$\begin{aligned}
\int_{B_k} R(x,\xi_k)\,dx &= \int_{B_k} \left(R(x,\xi_k) - \frac{1}{6|D|}|x-\xi_k|^2 \right) dx + \int_{B_k} \frac{1}{6|D|}|x-\xi_k|^2\,dx\\
&= \frac{4\pi r_k^3}{3} R(\xi_k,\xi_k) + \frac{4\pi}{3}\frac{r_k^5}{10|D|}. \qquad (3.7)
\end{aligned}$$

Hence

$$\int_{B_k} v_k\,dx = \frac{8\pi r_k^5}{15} + \left(\frac{4\pi}{3}\right)^2 r_k^6 R(\xi_k,\xi_k) + \left(\frac{4\pi}{3}\right)^2 \frac{r_k^8}{5|D|}.$$

When $l \neq k$, for $x \in B_l$, since P_k is harmonic,

$$\begin{aligned}
\int_{B_l} v_k\,dx &= \int_{B_l} P_k\,dx + \frac{4\pi r_k^3}{3} \int_{B_l} R(x,\xi_k)\,dx + \left(\frac{4\pi}{3}\right)^2 \frac{r_k^5 r_l^3}{10|D|}\\
&= \frac{4\pi}{3} r_l^3 \frac{r_k^3}{3|\xi_k-\xi_l|} + \frac{4\pi r_k^3}{3} \left[\int_{B_l} \left(R(x,\xi_k) - \frac{1}{6|D|}|x-\xi_l|^2 \right) dx \right.\\
&\quad \left. + \int_{B_l} \frac{1}{6|D|}|x-\xi_l|^2\,dx \right] + \left(\frac{4\pi}{3}\right)^2 \frac{r_k^5 r_l^3}{10|D|}\\
&= \left(\frac{4\pi}{3}\right)^2 \frac{r_k^3 r_l^3}{4\pi|\xi_k-\xi_l|} + \left(\frac{4\pi}{3}\right)^2 r_k^3 r_l^3 R(\xi_k,\xi_l) + \left(\frac{4\pi}{3}\right)^2 \left(\frac{r_k^3 r_l^5}{10|D|} + \frac{r_k^5 r_l^3}{10|D|} \right).
\end{aligned}$$

Finally the nonlocal part of the free energy is

$$\begin{aligned}\int_D (\chi_B - a) v\, dx = {} & \sum_{k=1}^K \left[\frac{8\pi r_k^5}{15} + \left(\frac{4\pi}{3}\right)^2 r_k^6 R(\xi_k, \xi_k) \right] \\ & + \sum_{k=1}^K \sum_{l=1, l\neq k}^K \left[\left(\frac{4\pi}{3}\right)^2 \frac{r_k^3 r_l^3}{4\pi|\xi_k - \xi_l|} + \left(\frac{4\pi}{3}\right)^2 r_k^3 r_l^3 R(\xi_k, \xi_l) \right] \\ & + \sum_{k=1}^K \sum_{l=1}^K \left(\frac{4\pi}{3}\right)^2 \left(\frac{r_k^3 r_l^5}{10|D|} + \frac{r_k^5 r_l^3}{10|D|} \right). \end{aligned} \tag{3.8}$$

The lemma now follows. ◻

4. Perturbed spheres.

We perturb each ball B_k considered in the last section. A perturbed ball denoted by E_{ϕ_k} is described by a function $\phi_k = \phi_k(\theta_k)$, $\theta_k \in S^2$:

$$E_{\phi_k} = \{\xi_k + t\theta_k : \ \theta_k \in S^2, \ t \in [0, (r_k^3 + \phi_k(\theta_k))^{1/3}]\}. \tag{4.1}$$

Each ϕ_k is small compared to r_k^3 so that $r_k^3 + \phi_k(\theta_k)$ is positive. Each θ_k is identified by its longitude and latitude $(\theta_{k,1}, \theta_{k,2})$, namely

$$\theta_k = (\cos\theta_{k,1} \sin\theta_{k,2}, \ \sin\theta_{k,1}\sin\theta_{k,2}, \ \cos\theta_{k,2}). \tag{4.2}$$

The ϕ_k's satisfy

$$\sum_{k=1}^K \int_{S^2} \phi_k(\theta_k)\, d\theta_k = 0. \tag{4.3}$$

Here the integral is a surface integral over S^2 and

$$d\theta_k = \sin\theta_{k,2}\, d\theta_{k,1} d\theta_{k,2} \tag{4.4}$$

is the surface element on S^2. Hence the total volume inside the perturbed spheres remains fixed:

$$\begin{aligned}\sum_{k=1}^K |E_{\phi_k}| &= \sum_k \int_{S^2} \int_0^{(r_k^3 + \phi_k(\theta_k))^{1/3}} t^2\, dt d\theta_k \\ &= \sum_k \int_{S^2} \left(\frac{r_k^3}{3} + \frac{\phi_k(\theta_k)}{3} \right) d\theta_k = \sum_k \frac{4\pi r_k^3}{3} = a|D|.\end{aligned}$$

The union of the E_{ϕ_k}'s is E_ϕ:

$$E_\phi = \bigcup_{k=1}^K E_{\phi_k}. \tag{4.5}$$

With these notations $B = E_0$.

We let $\theta = (\theta_1, \theta_2, \dots, \theta_K)$ and $\phi(\theta) = (\phi_1(\theta_1), \phi_2(\theta_2), \dots \phi_K(\theta_K))$. To express surface area in terms of ϕ_k, first define

$$L(s, p, q, \beta) = s^{-1/3} \sqrt{\frac{p^2}{9\sin^2\beta} + \frac{q^2}{9} + s^2}, \tag{4.6}$$

and then define

$$L_k\left(\phi_k, \frac{\partial\phi_k}{\partial\theta_{k,1}}, \frac{\partial\phi_k}{\partial\theta_{k,2}}, \theta_{k,2}\right) = r_k^2 L\left(1+\frac{\phi_k}{r_k^3}, \frac{1}{r_k^3}\frac{\partial\phi_k}{\partial\theta_{k,1}}, \frac{1}{r_k^3}\frac{\partial\phi_k}{\partial\theta_{k,2}}, \theta_{k,2}\right). \tag{4.7}$$

The surface area of $\partial_D E_\phi$ can be expressed as

$$\sum_{k=1}^K |D\chi_{E_{\phi_k}}|(D) = \sum_{k=1}^K \int_{S^2} L_k\left(\phi_k, \frac{\partial\phi_k}{\partial\theta_{k,1}}, \frac{\partial\phi_k}{\partial\theta_{k,2}}, \theta_{k,2}\right) d\theta_k. \tag{4.8}$$

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

$$\frac{\gamma}{2}\int_D |(-\Delta)^{-1/2}(\chi_{E_\phi}-a)|^2\,dx = \frac{\gamma}{2}\int_{E_\phi}\int_{E_\phi} G(x,y)\,dxdy. \tag{4.9}$$

The first variation of J can now be written as

$$J'(E_\phi)(w) = \sum_{k=1}^K \int_{S^2}\left[\frac{\partial L_k}{\partial\phi_k}w_k + \frac{\partial L_k}{\partial\phi_{k,1}}w_{k,1} + \frac{\partial L_k}{\partial\phi_{k,2}}w_{k,2}\right] d\theta_k \tag{4.10}$$

$$+ \sum_{k=1}^K \int_{S^2} w_k(\theta_k)\left[\sum_{l=1}^K \frac{\gamma}{3}\int_{E_{\phi_l}} G(\xi_k + (r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, y)\,dy\right] d\theta_k. \tag{4.11}$$

Here we have used shorthand notations $\phi_{k,1} = \frac{\partial\phi_k}{\partial\theta_{k,1}}$ and $\phi_{k,2} = \frac{\partial\phi_k}{\partial\theta_{k,2}}$, and so on. From (4.10) we define a second order, quasilinear elliptic operator

$$\mathcal{H}_k(\phi_k)(\theta_k) = \frac{1}{\sin\theta_{k,2}}\left[\frac{\partial L_k}{\partial\phi_k}\sin\theta_{k,2} - \frac{\partial}{\partial\theta_{k,1}}\left(\frac{\partial L_k}{\partial\phi_{k,1}}\sin\theta_{k,2}\right) - \frac{\partial}{\partial\theta_{k,2}}\left(\frac{\partial L_k}{\partial\phi_{k,2}}\sin\theta_{k,2}\right)\right]. \tag{4.12}$$

This is just the mean curvature of the perturbed sphere ∂E_{ϕ_k} at $\xi_k+(r_k^3+\phi_k(\theta_k))^{1/3}\theta_k$, multiplied by $\frac{1}{3}$. The second part (4.11) of the first variation of J gives rise to a nonlocal operator

$$\phi \to \sum_{l=1}^K \frac{\gamma}{3}\int_{E_{\phi_l}} G(\xi_k + (r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, y)\,dy. \tag{4.13}$$

This is just

$$\frac{\gamma}{3}(-\Delta)^{-1}(\chi_{E_\phi}-a)(\xi_k + (r_k^3+\theta_k)^{1/3}\theta_k),$$

the nonlocal part of (1.1) at $\xi_k + (r_k^3+\phi_k(\theta_k))^{1/3}\theta_k$ multiplied by $\frac{1}{3}$.

There are two cases in the sum over l in (4.13); when $l = k$ we write

$$\frac{\gamma}{3}\int_{E_{\phi_k}} G(\xi_k + (r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, y)\,dy$$
$$= \frac{\gamma}{3}\int_{E_{\phi_k}} \frac{dy}{4\pi|\xi_k + (r_k^3+\phi_k(\theta_k))^{1/3}\theta_k - y|} + \frac{\gamma}{3}\int_{E_{\phi_k}} R(\xi_k + (r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, y)\,dy.$$

We denote the last two terms by

$$\mathcal{A}_k(\phi_k)(\theta_k) = \frac{\gamma}{3}\int_{E_{\phi_k}} \frac{dy}{4\pi|\xi_k + (r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k - y|}, \tag{4.14}$$

$$\mathcal{B}_k(\phi_k)(\theta_k) = \frac{\gamma}{3}\int_{E_{\phi_k}} R(\xi_k + (r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k, y)\, dy. \tag{4.15}$$

When $l \neq k$ in (4.13) we let

$$\mathcal{C}_{kl}(\phi_k, \phi_l)(\theta_k) = \frac{\gamma}{3}\int_{E_{\phi_l}} G(\xi_k + (r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k, y)\, dy. \tag{4.16}$$

The left-hand side of (1.1) (multiplied by $\frac{1}{3}$) now becomes

$$\mathcal{H}_k(\phi_k)(\theta_k) + \mathcal{A}_k(\phi_k)(\theta_k) + \mathcal{B}_k(\phi_k)(\theta_k) + \sum_{l\neq k}\mathcal{C}_{kl}(\phi_k, \phi_l)(\theta_k)$$

at $\xi_k + (r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k$. Let us define

$$\mathcal{S} = (\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_K), \tag{4.17}$$

where

$$\mathcal{S}_k(\phi)(\theta_k) = \mathcal{H}_k(\phi_k)(\theta_k) + \mathcal{A}_k(\phi_k)(\theta_k) + \mathcal{B}_k(\phi_k)(\theta_k) + \sum_{l\neq k}\mathcal{C}_{kl}(\phi_k, \phi_l)(\theta_k) + \lambda(\phi). \tag{4.18}$$

Here $\lambda(\phi)$ is a number, independent of k. It is given by

$$\lambda(\phi) = -\frac{1}{K}\sum_{k=1}^{K}\overline{\left[\mathcal{H}_k(\phi_k) + \mathcal{A}_k(\phi_k) + \mathcal{B}_k(\phi_k) + \sum_{l\neq k}\mathcal{C}_{kl}(\phi_k, \phi_l)\right]}. \tag{4.19}$$

The bar over the quantity here stands for the average of the quantity over S^2. With this definition of λ,

$$\sum_{k=1}^{K}\overline{\mathcal{S}_k(\phi_k)} = 0. \tag{4.20}$$

The operator $\mathcal{S}$ maps from

$$\mathcal{X} = \left\{\phi = (\phi_1, \phi_2, \dots, \phi_K):\ \phi_k \in W^{2,p}(S^2),\ k = 1, 2, \dots, K,\ \sum_{k=1}^{K}\overline{\phi_k} = 0\right\} \tag{4.21}$$

to

$$\mathcal{Y} = \left\{q = (q_1, q_2, \dots, q_K):\ q_k \in L^p(S^2),\ k = 1, 2, \dots, K,\ \sum_{k=1}^{K}\overline{q_k} = 0\right\}. \tag{4.22}$$

For technical reasons p is assumed to be in the range

$$2 < p < \infty. \tag{4.23}$$

This guarantees that $D\phi_k$ is continuous, a fact needed in the proof of Lemma 6.1. Equation (1.1) now becomes

$$\mathcal{S}(\phi) = 0. \tag{4.24}$$

By defining

$$\mathcal{C} = (\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_K), \text{ where } \mathcal{C}_k(\phi_1, \phi_2, \dots, \phi_K) = \sum_{l \neq k} \mathcal{C}_{kl}(\phi_k, \phi_l), \tag{4.25}$$

we write

$$\mathcal{S} = \mathcal{H} + \mathcal{A} + \mathcal{B} + \mathcal{C} + \lambda. \tag{4.26}$$

In the map $\mathcal{S}$ the inputs $\phi_1, \phi_2, \dots, \phi_k$ interact only in $\mathcal{C}$ and λ. The other operators can be written in the block matrix form

$$\mathcal{H} = \begin{bmatrix} \mathcal{H}_1 & 0 & \dots & 0 \\ 0 & \mathcal{H}_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \mathcal{H}_K \end{bmatrix}, \ \mathcal{A} = \begin{bmatrix} \mathcal{A}_1 & 0 & \dots & 0 \\ 0 & \mathcal{A}_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \mathcal{A}_K \end{bmatrix}, \ \mathcal{B} = \begin{bmatrix} \mathcal{B}_1 & 0 & \dots & 0 \\ 0 & \mathcal{B}_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \mathcal{B}_K \end{bmatrix}, \tag{4.27}$$

where each entry in a matrix is an operator from $W^{2,p}(S^2)$ to $L^p(S^2)$. The scalar operator λ gives the projection $-(\lambda(\phi), \lambda(\phi), \dots, \lambda(\phi))$ of $\mathcal{H}(\phi) + \mathcal{A}(\phi) + \mathcal{B}(\phi) + \mathcal{C}(\phi)$ to the one-dimensional space spanned by $(1, 1, \dots, 1)$.

Let us write the first Fréchet derivatives of these operators. For simplicity we write

$$\phi_{k,i} = \frac{\partial \phi_k}{\partial \theta_{k,i}}, \ \phi_{k,ij} = \frac{\partial^2 \phi_k}{\partial \theta_{k,ij}}, \ u_{k,i} = \frac{\partial u_k}{\partial \theta_{k,i}}, \ u_{k,ij} = \frac{\partial^2 u_k}{\partial \theta_{k,ij}}.$$

Calculations show that

$$\mathcal{H}_k'(\phi_k)(u_k) = \frac{\partial \mathcal{H}_k}{\partial \phi_k} u_k + \sum_{i=1}^{2} \frac{\partial \mathcal{H}_k}{\partial \phi_{k,i}} u_{k,i} + \sum_{i,j=1}^{2} \frac{\mathcal{H}_k}{\partial \phi_{k,ij}} u_{k,ij}, \tag{4.28}$$

$$\begin{aligned} \mathcal{A}_k'(\phi_k)(u_k)(\theta_k) = {} & \frac{\gamma}{9} \int_{S^2} \frac{u_k(\omega_k)\, d\omega_k}{4\pi |(r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k - (r_k^3 + \phi_k(\omega_k))^{1/3}\omega_k|} \\ & - \frac{\gamma u_k(\theta_k)}{9(r_k^3 + \phi_k(\theta_k))^{2/3}} \int_{\tilde{E}_{\phi_k}} \frac{((r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k - y) \cdot \theta_k}{4\pi |(r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k - y|^3}\, dy. \end{aligned} \tag{4.29}$$

$$\begin{aligned} & \mathcal{B}_k'(\phi_k)(u_k)(\theta_k) \\ & \quad = \frac{\gamma}{9} \int_{S^2} u_k(\omega_k) R(\xi_k + (r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k, \xi_k + (r_k^3 + \phi_k(\omega_k))^{1/3}\omega_k)\, d\omega_k \\ & \quad + \frac{\gamma u_k(\theta_k)}{9(r_k^3 + \phi_k(\theta_k))^{2/3}} \int_{E_{\phi_k}} \nabla R(\xi_k + (r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k, y) \cdot \theta_k\, dy. \end{aligned} \tag{4.30}$$

$$\begin{aligned} & \mathcal{C}_{kl}'(\phi_k, \phi_l)(u_k, u_l)(\theta_k) \\ & \quad = \frac{\gamma}{9} \int_{S^2} u_l(\omega_l) G(\xi_k + (r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k, \xi_l + (r_l^3 + \phi_l(\omega_l))^{1/3}\omega_l)\, d\omega_l \\ & \quad + \frac{\gamma u_k(\theta_k)}{9(r_k^3 + \phi_k(\theta_k))^{2/3}} \int_{E_{\phi_l}} \nabla G(\xi_k + (r_k^3 + \phi_k(\theta_k))^{1/3}\theta_k, y) \cdot \theta_k\, dy. \end{aligned} \tag{4.31}$$

In $\mathcal{A}_k'$, $\tilde{E}_{\phi_k} = E_{\phi_k} - \xi_k$ is a shift of E_{ϕ_k}. The center of $\tilde{E}_{\phi_k}$ is 0. The derivative

$$\lambda'(\phi_1, \phi_2, \dots, \phi_K)(u_1, u_2, \dots, u_K) \tag{4.32}$$

is so chosen that

$$\sum_{k=1}^{K} \overline{\mathcal{S}_k'(u)} = 0. \tag{4.33}$$

5. A linear operator.

Let $\mathcal{L}$ be the linearized operator of $\mathcal{S}$ at $\phi = 0$, i.e.,

$$\mathcal{L} = \mathcal{S}'(0). \tag{5.1}$$

Going back to (4.28), (4.29), (4.30), and (4.31) we find that

$$\begin{aligned}
\mathcal{H}_k'(0)(u_k) &= -\frac{1}{9r_k^4}\left[\frac{1}{\sin^2\theta_{k,2}}\frac{\partial^2 u_k}{\partial\theta_{k,1}^2} + \frac{\partial^2 u_k}{\partial\theta_{k,2}^2} + \cot\theta_{k,2}\frac{\partial u_k}{\partial\theta_{k,2}}\right] - \frac{2}{9r_k^4}u,\\
\mathcal{A}_k'(0)(u_k)(\theta_k) &= \frac{\gamma}{9r_k}\int_{S^2}\frac{u_k(\omega_k)\,d\omega_k}{4\pi|\theta_k - \omega_k|} - \frac{\gamma u_k(\theta_k)}{27r_k},\\
\mathcal{B}_k'(0)(u_k)(\theta_k) &= \frac{\gamma}{9}\int_{S^2} u_k(\omega_k)R(\xi_k + r_k\theta_k, \xi_k + r_k\omega_k)\,d\omega_k\\
&\quad + \frac{\gamma u_k(\theta_k)}{9r_k^2}\int_{B_k}\nabla R(\xi_k + r_k\theta_k, y)\cdot\theta_k\,dy,\\
\mathcal{C}_{kl}'(0,0)(u_k, u_l)(\theta_k) &= \frac{\gamma}{9}\int_{S^2} u_l(\omega_l)G(\xi_k + r_k\theta_k, \xi_l + r_l\omega_l)\,d\omega_l\\
&\quad + \frac{\gamma u_k(\theta_k)}{9r_k^2}\int_{B_l}\nabla G(\xi_k + r_k\theta_k, y)\cdot\theta_k\,dy.
\end{aligned}$$

The derivation of $\mathcal{A}_k'(0)$ is explained in more detail in Appendix A.

Let us separate $\mathcal{L}$ to a dominant part $\mathcal{L}_1$ and a minor part $\mathcal{L}_2$. We define $\mathcal{L}_{1,k}$, the kth component of $\mathcal{L}_1$, to be

$$\mathcal{L}_{1,k}(u)(\theta_k) = \mathcal{H}_k'(0)(u_k)(\theta_k) + \mathcal{A}_k'(0)(u_k)(\theta_k) + l_1(u).$$

The real valued linear operator l_1 is independent of k. It is so chosen that $\mathcal{L}_1$ maps from $\mathcal{X}$ to $\mathcal{Y}$. The rest of $\mathcal{L}$ is denoted by $\mathcal{L}_2$.

We are more interested in the operators $\Pi\mathcal{L}$ and $\Pi\mathcal{L}_1$, where Π is the orthogonal projection operator from $\mathcal{Y}$ to

$$\mathcal{Y}_* = \{q = (q_1, \dots, q_K) \in \mathcal{Y} :\ q_k \perp H_1,\ q_k \perp 1,\ k = 1, \dots, K\}. \tag{5.2}$$

Here H_1 is the space of spherical harmonics of degree 1. See, for instance, [10] for more on spherical harmonics. The operator $\Pi\mathcal{L}$ is defined on

$$\mathcal{X}_* = \{\phi = (\phi_1, \dots, \phi_K) \in \mathcal{X} :\ \phi_k \perp H_1,\ \phi_k \perp 1,\ k = 1, \dots, K\}. \tag{5.3}$$

We use the same Π to denote the orthogonal projection from

$$L^2(S^2) \text{ to } \{q_k \in L^2(S^2) : q_k \perp H_1,\ q_k \perp 1\}. \tag{5.4}$$

Lemma 5.1. *Consider* $\Pi\mathcal{L}_1$ *as an operator from* $\mathcal{X}_*$ *to* $\mathcal{Y}_*$*. The eigenvalues of* $\Pi\mathcal{L}_1$ *are*

$$\lambda_{k,n} = \frac{(n-1)(n+2)}{9r_k^4} - \frac{\gamma}{9r_k}\left[\frac{2(n-1)}{3(2n+1)}\right], \quad k = 1, 2, \ldots, K, \ n = 2, 3, 4, \ldots \tag{5.5}$$

whose multiplicity is $2n+1$*. The corresponding eigenvectors are the spherical harmonics of degree* n*; i.e.,* H_n *is the eigenspace associated with* $\lambda_{k,n}$*.*

Proof. In $\mathcal{X}_*$, $\mathcal{L}_1$ is simplified to

$$\mathcal{L}_{1,k}(u) = -\frac{1}{9r_k^4}\left[\frac{1}{\sin^2\theta_{k,2}}\frac{\partial^2 u_k}{\partial\theta_{k,1}^2} + \frac{\partial^2 u_k}{\partial\theta_{k,2}^2} + \cot\theta_{k,2}\frac{\partial u_k}{\partial\theta_{k,2}}\right] - \frac{2u_k}{9r_k^4}$$
$$+ \frac{\gamma}{9r_k}\int_{S^2}\frac{u_k(\omega_k)\,d\omega_k}{4\pi|\theta_k-\omega_k|} - \frac{\gamma u_k(\theta_k)}{27r_k},$$

for each k. This is a diagonalized operator. Note that in $\mathcal{X}_*$, $\Pi\mathcal{L}_1 = \mathcal{L}_1$. To find the spectrum of $\mathcal{L}_1$ in $\mathcal{X}_*$ we consider the effect of $\mathcal{L}_1$ on the spherical harmonics $h \in H_n$ of degree n. Since

$$\frac{1}{\sin^2\theta_{k,2}}\frac{\partial^2}{\partial\theta_{k,1}^2} + \frac{\partial^2}{\partial\theta_{k,2}^2} + \cot\theta_2\frac{\partial}{\partial\theta_{k,2}} := \Delta_{S^2} \tag{5.6}$$

is the Laplacian–Beltrami operator on the unit sphere,

$$-\left[\frac{1}{\sin^2\theta_{k,2}}\frac{\partial^2 h}{\partial\theta_{k,1}^2} + \frac{\partial^2 h}{\partial\theta_{k,2}^2} + \cot\theta_2\frac{\partial h}{\partial\theta_{k,2}}\right] = n(n+1)h. \tag{5.7}$$

In Appendix B we find that

$$\int_{S^2}\frac{h(\omega)\,d\omega}{4\pi|\theta-\omega|} = \frac{h(\theta)}{2n+1}. \tag{5.8}$$

Following (5.7) and (5.8) one deduces that

$$\mathcal{L}_{1,k}(h) = \left[\frac{n(n+1)-2}{9r_k^4} + \frac{\gamma}{9r_k}\left(\frac{1}{2n+1} - \frac{1}{3}\right)\right]h. \tag{5.9}$$

This proves the lemma. ☐

The second part of $\mathcal{L}$ is minor.

Lemma 5.2. *There exists* $C > 0$ *independent of* ξ*,* r*,* ρ*, and* γ *such that*

$$\|\mathcal{L}_2(u)\|_{L^p} \le \frac{C}{\rho^2}\|u\|_{L^p}$$

for all $u \in \mathcal{Y}_*$*. A similar estimate holds if the two* p*'s above are replaced by* 2*.*

Proof. Let $\mathcal{L}_{2,k}$ be the kth component of $\mathcal{L}_2$. Then

$$\begin{aligned}\mathcal{L}_{2,k}(u)(\theta_k) = {} & \frac{\gamma}{9}\int_{S^2} u_k(\omega_k)(R(\xi_k + r_k\theta_k, \xi_k + r_k\omega_k) - R(\xi_k,\xi_k))\,d\omega_k \\ & + \frac{\gamma u_k(\theta_k)}{9r_k^2}\int_{B_k} \nabla R(\xi_k + r_k\theta_k, y)\cdot\theta_k\,dy \\ & + \sum_{l\neq k}\frac{\gamma}{9}\int_{S^2} u_l(\omega_l)(G(\xi_k + r_k\theta_k, \xi_l + r_l\omega_l) - G(\xi_k,\xi_l))\,d\omega_l \\ & + \sum_{l\neq k}\frac{\gamma u_k(\theta_k)}{9r_k^2}\int_{B_l}\nabla G(\xi_k + r_k\theta_k, y)\cdot\theta_k\,dy \\ & + l_2(u),\end{aligned}$$

where $l_2(u)$ is real valued and independent of k. It is included so that $\mathcal{L}_2(u)$ is in $\mathcal{Y}$.

Because

$$\begin{aligned} R(\xi_k + r_k\theta_k, \xi_k + r_k\omega_k) - R(\xi_k,\xi_k) &= O(\rho), \\ G(\xi_k + r_k\theta_k, \xi_l + r_l\omega_l) - G(\xi_k,\xi_l) &= O(\rho),\end{aligned}$$

we obtain that

$$\begin{aligned}\left\|\frac{\gamma}{9}\int_{S^2} u_k(\omega_k)(R(\xi_k + r_k\theta_k, \xi_k + r_k\omega_k) - R(\xi_k,\xi_k))\,d\omega_k\right\|_{L^p} &\le C\gamma\rho\|u\|_{L^p} \\ \left\|\frac{\gamma}{9}\int_{S^2} u_l(\omega_l)(G(\xi_k + r_k\theta_k, \xi_l + r_l\omega_l) - G(\xi_k,\xi_l))\,d\omega_l\right\|_{L^p} &\le C\gamma\rho\|u_k\|_{L^p}.\end{aligned}$$

Since the volume of B_k is $\frac{4\pi r_k^3}{3}$,

$$\begin{aligned}\left\|\frac{\gamma u_k(\theta_k)}{9r_k^2}\int_{B_k}\nabla R(\xi_k + r_k\theta_k, y)\cdot\theta_k\,dy\right\|_{L^p} &\le C\gamma\rho\|u_k\|_{L^p} \\ \left\|\frac{\gamma u_k(\theta_k)}{9r_k^3}\int_{B_l}\nabla G(\xi_k + r_k\theta_k, y)\cdot\theta_k\,dy\right\|_{L^p} &\le C\gamma\rho\|u_k\|_{L^p}.\end{aligned}$$

The condition

$$\sum_{k=1}^{K}\overline{\mathcal{L}_{2,k}(u)(\theta_k)} = 0$$

implies that

$$|l_2(u)| \le C\gamma\rho\|u\|_{L^p}.$$

The lemma then follows, with the help of (2.10). □

LEMMA 5.3.

1. *For* $u \in \mathcal{X}_*$

$$\|u\|_{W^{2,p}} \le C\rho^4\|\Pi\mathcal{L}u\|_{L^p}.$$

2. *The operator* $\Pi\mathcal{L}$ *is invertible from* $\mathcal{X}_*$ *to* $\mathcal{Y}_*$.
3. *If* (2.8) *holds,*

$$\|u\|_{W^{1,2}}^2 \le C\rho^4\langle\Pi\mathcal{L}u, u\rangle.$$

Proof. From Lemma 5.1 we have

$$\frac{|\lambda_{k,n}|}{n^2} = \frac{n-1}{9r_k^4 n}\left|\frac{n+2}{n} - \frac{2\gamma r_k^3}{3(2n+1)n}\right| > \frac{n-1}{18r_k^4 n}\left|\frac{n+2}{n} - \frac{2\gamma\rho^3}{3(2n+1)n}\right|$$

if δ_2 in the definition (3.1) of U_2 is small enough. Then (2.6) implies that

$$\frac{|\lambda_{k,n}|}{n^2} > \frac{(n-1)}{18r_k^4 n}\frac{2\epsilon n}{3(2n+1)} \geq \frac{C}{\rho^4}, \quad n = 2, 3, \dots.$$

If we expand u_k by spherical harmonics

$$u_k = \sum_{n=2}^{\infty}\sum_{l=1}^{2n+1} c_{n,l}h_{n,l},$$

where $h_{n,l}$, $l = 1, \dots, 2n+1$, form an orthonormal basis in H_n, then

$$-\Delta_{S^2}u_k = \sum_{n=2}^{\infty}\sum_{l=1}^{2n+1} n(n+1)c_{n,l}h_{n,l}, \ \mathcal{L}_{1,k}u_k = \sum_{n=2}^{\infty}\sum_{l=1}^{2n+1} \lambda_{k,n}c_{n,l}h_{n,l}.$$

Our estimate on $|\lambda_{k,n}|$ shows that

$$\|\Delta_{S^2}u_k\|_{L^2}^2 = \sum_{n=2}^{\infty}\sum_{l=1}^{2n+1} n^2(n+1)^2c_{n,l}^2 \leq C\rho^8\sum_{n=2}^{\infty}\sum_{l=1}^{2n+1} \lambda_{k,n}^2 c_{n,l}^2 = C\rho^8\|\mathcal{L}_{1,k}u_k\|_{L^2}^2.$$

The standard elliptic theory implies that

$$\|u\|_{W^{2,2}} \leq C\|\Delta_{S^2}u\|_{L^2} \leq C\rho^4\|\Pi\mathcal{L}_1(u)\|_{L^2}. \tag{5.10}$$

To prove part 1 of Lemma 5.3, we divide $\Pi\mathcal{L}_1$ into

$$\Pi\mathcal{L}_{1,k} = -\frac{1}{9r_k^4}\Delta_{S^2} + \mathcal{M}_k, \tag{5.11}$$

where Δ_{S^2} is defined in (5.6), and $\mathcal{M} = (\mathcal{M}_1, \mathcal{M}_2, \dots, \mathcal{M}_K)$ is defined by (5.11). The standard elliptic estimate asserts that

$$\|u_k\|_{W^{2,p}} \leq C\|\Delta_{S^2}u_k\|_{L^p},$$

which by (5.11) is turned to

$$\begin{aligned}\|u_k\|_{W^{2,p}} &\leq C\|9r_k^4\mathcal{M}_k u - 9r_k^4\Pi\mathcal{L}_{1,k}u\|_{L^p}\\ &\leq C\rho^4(\|\mathcal{M}_k u\|_{L^p} + \|\Pi\mathcal{L}_{1,k}u\|_{L^p}).\end{aligned}$$

One observes that

$$\|\mathcal{M}u\|_{L^p} \leq \frac{C}{\rho^4}\|u\|_{L^p} \leq \frac{C}{\rho^4}\|u\|_{W^{2,2}},$$

where the last inequality comes from the Sobolev embedding $W^{2,2}(S^2) \to W^{1,p}(S^2) \subset L^p(S^2)$ for any $p \geq 1$. Hence when $p > 2$, by (5.10) we deduce that

$$\begin{aligned}\|u_k\|_{W^{2,p}} &\leq C\rho^4(\rho^{-4}\|u\|_{W^{2,2}} + \|\Pi\mathcal{L}_{1,k}u\|_{L^p})\\ &\leq C\rho^4(\|\Pi\mathcal{L}_{1,k}u\|_{L^2} + \|\Pi\mathcal{L}_{1,k}u\|_{L^p})\\ &\leq C\rho^4\|\Pi\mathcal{L}_{1,k}u\|_{L^p}.\end{aligned}$$

Lemma 5.2 implies that

$$\|\Pi\mathcal{L}u\|_{L^p} \geq \|\Pi\mathcal{L}_1 u\|_{L^p} - \|\Pi\mathcal{L}_2 u\|_{L^p} \geq \frac{C}{\rho^4}\|u\|_{W^{2,p}} - \frac{C}{\rho^2}\|u\|_{L^p} \geq \frac{C}{\rho^4}\|u\|_{W^{2,p}}$$

for small ρ. This proves part 1 of Lemma 5.3.

Part 2 of Lemma 5.3 follows from the Fredholm alternative.

When (2.8) holds,

$$\frac{\lambda_{k,n}}{n^2} = \frac{n-1}{9r_k^4 n}\left(\frac{n+2}{n} - \frac{2\gamma r_k^3}{3(2n+1)n}\right) > \frac{n-1}{18r_k^4 n}\frac{2\epsilon n}{3(2n+1)} \geq \frac{C}{\rho^4}, \quad n = 2, 3, \ldots,$$

if δ_2 in (3.1) is small. This implies that, with the help of expansion by spherical harmonics,

$$\begin{aligned}\langle \Pi\mathcal{L}_{1,k}(u_k), u_k\rangle &= \sum_{n=2}^{\infty}\sum_{l=1}^{2n+1}\lambda_{k,n}c_{n,l}^2 \ \geq\ \frac{C}{\rho^4}\sum_{n=2}^{\infty}\sum_{l=1}^{2n+1} n(n+1)c_{n,l}^2 \\ &= \frac{C}{\rho^4}\langle -\Delta_{S^2}u_k, u_k\rangle \ =\ \frac{C}{\rho^4}\langle \nabla u_k, \nabla u_k\rangle \ \geq\ \frac{C}{\rho^4}\|u\|_{W^{1,2}}^2.\end{aligned}$$

Using the estimate of Lemma 5.2 with p replaced by 2, we find that

$$\langle \Pi\mathcal{L}(u), u\rangle = \langle \Pi\mathcal{L}_1(u), u\rangle + \langle \Pi\mathcal{L}_2(u), u\rangle \geq \frac{C}{\rho^4}\|u\|_{W^{1,2}}^2 - \frac{C}{\rho^2}\|u\|_{L^2}^2 \geq \frac{C}{\rho^4}\|u\|_{W^{1,2}}^2.$$

This proves part 3 of Lemma 5.3. □

6. The second Fréchet derivative.

LEMMA 6.1. *Suppose that $\|\phi\|_{W^{2,p}} \leq c\rho^3$, where c is sufficiently small. The following estimates hold:*

1. $\|\mathcal{H}_k''(\phi_k)(u_k, v_k)\|_{L^p} \leq \frac{C}{\rho^7}\|u_k\|_{W^{2,p}}\|v_k\|_{W^{2,p}}$.
2. $\|\mathcal{A}_k''(\phi_k)(u_k, v_k)\|_{L^p} \leq \frac{C}{\rho^7}\|u_k\|_{W^{1,p}}\|v_k\|_{W^{1,p}}$.
3. $\|\mathcal{B}_k''(\phi_k)(u_k, v_k)\|_{L^p} \leq \frac{C}{\rho^5}\|u_k\|_{W^{1,p}}\|v_k\|_{W^{1,p}}$.
4. $\|\mathcal{C}_{kl}''(\phi_k, \phi_l)(u_k, u_l)(v_k, v_l)\|_{L^p} \leq \frac{C}{\rho^5}(\|u_k\|_{W^{1,p}}+\|u_l\|_{W^{1,p}})(\|v_k\|_{W^{1,p}}+\|v_l\|_{W^{1,p}})$.
5. $|\lambda''(\phi)(u, v)| \leq \frac{C}{\rho^7}\|u\|_{W^{2,p}}\|v\|_{W^{2,p}}$.

Proof. Note that by taking c small, we keep $r_k^3 + \phi_k$ positive, so ∂E_{ϕ_k} is a perturbed sphere.

The mean curvature operator $\mathcal{H}_k$ is elliptic and quasilinear. Its second Fréchet derivative is calculated from (4.28):

$$\begin{aligned}&\mathcal{H}_k''(\phi_k, D\phi_k, D^2\phi_k)(u_k, v_k) \\ &= \frac{\partial^2\mathcal{H}_k}{\partial\phi_k^2}u_k v_k + \sum_{i=1}^{2}\frac{\partial^2\mathcal{H}_k}{\partial\phi_k\partial\phi_{k,i}}(u_k v_{k,i} + u_{k,i}v_k) + \sum_{i,j=1}^{2}\frac{\partial^2\mathcal{H}_k}{\partial\phi_{k,i}\partial\phi_{k,j}}(u_{k,i}v_{k,j} + u_{k,j}v_{k,i}) \\ &\quad + \sum_{l,m=1}^{2}\frac{\partial^2\mathcal{H}_k}{\partial\phi_k\partial\phi_{k,lm}}(u_k v_{k,lm} + u_{k,lm}v_k) + \sum_{i,l,m=1}^{2}\frac{\partial^2\mathcal{H}_k}{\partial\phi_{k,i}\partial\phi_{k,lm}}(u_{k,i}v_{k,lm} + u_{k,lm}v_{k,i}).\end{aligned}$$

It is important to note that because $\mathcal{H}_k$ is quasilinear, i.e., it is linear in $D^2\phi_k$, the term

$$\sum_{i,j,l,m=1}^{2} \frac{\partial^2 \mathcal{H}_k}{\partial \phi_{k,ij} \partial \phi_{k,lm}} (u_{k,ij} v_{k,lm} + u_{k,lm} v_{k,ij})$$

is 0 and hence absent in $\mathcal{H}_k''$. The Sobolev embedding $W^{1,p} \to L^\infty$ and $\|\phi_k\|_{W^{2,p}} \le c\rho^3$ for a small c implies that $|\phi_k| \le C\rho^3$ and $|D\phi_k| \le C\rho^3$. From the definition (4.12) of $\mathcal{H}_k$ we have the pointwise estimate

$$\begin{aligned} &|\mathcal{H}_k''(\phi_k, D\phi_k, D^2\phi_k)(u_k, v_k)| \\ &\le \frac{C}{\rho^7} \left(\left| \frac{D^2\phi_k}{r_k^3} \right| |u_k|\,|v_k| + \left| \frac{D^2\phi_k}{r_k^3} \right| |u_k|\,|Dv_k| + \left| \frac{D^2\phi_k}{r_k^3} \right| |Du_k|\,|v_k| \right. \\ &\quad \left. + \left| \frac{D^2\phi_k}{r_k^3} \right| |Du_k|\,|Dv_k| + |u_k|\,|D^2 v_k| + |D^2 u_k|\,|v_k| + |Du_k|\,|D^2 v_k| + |D^2 u_k|\,|Dv_k| \right), \end{aligned}$$

when θ_k is some distance away from the two poles (where $\theta_{k,2} = 0$ or π) of S^2. Near the two poles one can use a different parametrization of S^2 so that the same pointwise estimate holds. The same Sobolev embedding implies that

$$\|\mathcal{H}_k''(\phi)(u_k, v_k)\|_{L^p} \le \frac{C}{\rho^7} \|u_k\|_{W^{2,p}} \|v_k\|_{W^{2,p}}. \tag{6.1}$$

This proves part 1 of Lemma 6.1.

We now turn to part 2 of Lemma 6.1. In our estimation of $\mathcal{A}_k''$ and $\mathcal{B}_k''$ we drop the subscript k in most quantities. The second Fréchet derivative of $\mathcal{A}_k$ is calculated from (4.29):

$$\mathcal{A}_k''(\phi)(u,v) = A_1(\phi)(u,v) + A_2(\phi)(u,v) + A_3(\phi)(u,v) + A_4(\phi)(u,v) + A_5(\phi)(u,v), \tag{6.2}$$

where

$$\begin{aligned} A_1(\phi)(u,v) &= -\frac{\gamma v(\theta)\theta}{108\pi (r^3 + \phi(\theta))^{2/3}} \cdot \int_{S^2} K(\theta,\omega) u(\omega)\, d\omega, \\ A_2(\phi)(u,v) &= -\frac{\gamma u(\theta)\theta}{108\pi (r^3 + \phi(\theta))^{2/3}} \cdot \int_{S^2} K(\theta,\omega) v(\omega)\, d\omega, \\ A_3(\phi)(u,v) &= \frac{\gamma}{108\pi} \int_{S^2} K(\theta,\omega) \cdot \omega \frac{u(\omega)v(\omega)}{(r^3 + \phi(\omega))^{2/3}}\, d\omega, \\ A_4(\phi)(u,v) &= -\frac{\gamma u(\theta) v(\theta)}{108\pi (r^3 + \phi(\theta))^{4/3}} \\ &\quad \times \int_{\tilde{E}_{\phi_k}} \frac{|(r^3 + \phi(\theta))^{1/3}\theta - y|^2 - 3((r^3 + \phi(\theta))^{1/3} - \theta \cdot y)^2}{|(r^3 + \phi(\theta))^{1/3}\theta - y|^5}\, dy, \\ A_5(\phi)(u,v) &= \frac{2\gamma u(\theta) v(\theta)}{108\pi (r^3 + \phi(\theta))^{5/3}} \int_{\tilde{E}_{\phi_k}} \frac{((r^3 + \phi(\theta))^{1/3}\theta - y) \cdot \theta}{|(r^3 + \phi(\theta))^{1/3}\theta - y|^3} dy. \end{aligned}$$

Recall that $\tilde{E}_{\phi_k}$ in A_4 and A_5 is $E_{\phi_k} - \xi_k$. The kernel K is

$$K(\theta,\omega) = \frac{(r^3 + \phi(\theta))^{1/3}\theta - (r^3 + \phi(\omega))^{1/3}\omega}{|(r^3 + \phi(\theta))^{1/3}\theta - (r^3 + \phi(\omega))^{1/3}\omega|^3}. \tag{6.3}$$

Here we encounter a singular integral operator

$$\mathcal{K}(u)(\theta) = \int_{S^2} K(\theta,\omega)u(\omega)\,d\omega. \tag{6.4}$$

A variant of the Calderon–Zygmund estimate [32, Theorem 1] is applicable to this operator:

$$\|\mathcal{K}(u)\|_q \le \frac{C}{\rho^2}\|u\|_{L^q}$$

for any $q \in (1,\infty)$. In [32] the kernel takes the form $K(x-y)$. To meet this requirement, we can transform (6.4) to an integral on the perturbed sphere ∂E_{ϕ_k}, then $K(\theta,\omega)$ becomes $\frac{x-y}{|x-y|^3}$, where $x, y \in \partial E_{\phi_k}$.

For $\|\phi\|_{W^{2,p}} \le c\rho^3$ with a small c, we consider

$$\|\mathcal{A}_k''(\phi)(u,v)\|_{L^p} \le \sum_{i=1}^{5} \|A_i(\phi)(u,v)\|_{L^p}.$$

For sufficiently large q

$$\|A_1(\phi)(u,v)\|_{L^p} \le \frac{C}{\rho^7}\|v_k\|_{L^q}\|\mathcal{K}(u_k)\|_{L^q} \le \frac{C}{\rho^7}\|v_k\|_{L^q}\|u_k\|_{L^q} \le \frac{C}{\rho^7}\|u_k\|_{W^{1,p}}\|v_k\|_{W^{1,p}}.$$

Similarly

$$\|A_2(\phi)(u,v)\|_{L^p} \le \frac{C}{\rho^7}\|u\|_{W^{1,p}}\|v_k\|_{W^{1,p}}.$$

Regarding A_3 we have, using the Calderon–Zygmund estimate in L^p and the Sobolev embedding theory,

$$\|A_3(\phi)(u,v)\|_{L^p} \le \frac{C}{\rho^7}\|uv\|_{L^p} \le \frac{C}{\rho^7}\|u\|_{W^{1,p}}\|v\|_{W^{1,p}}.$$

For A_4, the integral

$$\int_{\tilde{E}_{\phi_k}} \frac{|(r^3+\phi(\theta))^{1/3}\theta - y|^2 - 3((r^3+\phi(\theta))^{1/3} - \theta\cdot y)^2}{|(r^3+\phi(\theta))^{1/3}\theta - y|^5}\,dy$$

is a convergent improper integral defined by its principal part. It is of order 1 and uniformly bounded with respect to θ. In the case of ϕ equal to 0, it may be explicitly computed. (See Appendix C.) Therefore

$$\|A_4(\phi)(u,v)\|_{L^p} \le \frac{C}{\rho^7}\|uv\|_{L^p} \le \frac{C}{\rho^7}\|u\|_{W^{1,p}}\|v\|_{W^{1,p}}.$$

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

$$\|A_5(\phi)(u,v)\|_{L^p} \le \frac{C}{\rho^7}\|u\|_{W^{1,p}}\|v\|_{W^{1,p}}.$$

Now we have

$$\|\mathcal{A}_k''(\phi)(u_k,v_k)\|_{L^p} \le \frac{C}{\rho^7}\|u_k\|_{W^{1,p}}\|v_k\|_{W^{1,p}}.$$

This proves part 2 of Lemma 6.1.

The kernel R in $\mathcal{B}_k$ is a smooth function. Calculations from (4.30) show that

$$\begin{aligned}
&\mathcal{B}_k''(\phi)(u,v)(\theta)\\
&\quad= \frac{\gamma v(\theta)}{27(r^3+\phi(\theta))^{2/3}} \int_{S^2} u(\omega) D_1 R(\xi+(r^3+\phi(\theta))^{1/3}\theta, \xi+(r^3+\phi(\omega))^{1/3}\omega)\cdot\theta \, d\omega\\
&\quad\ \frac{\gamma u(\theta)}{27(r^3+\phi(\theta))^{2/3}} \int_{S^2} v(\omega) D_1 R(\xi+(r^3+\phi(\theta))^{1/3}\theta, \xi+(r^3+\phi(\omega))^{1/3}\omega)\cdot\theta \, d\omega\\
&\quad+ \frac{\gamma}{27} \int_{S^2} \frac{u(\omega)v(\omega)}{(r^3+\phi(\omega))^{2/3}} D_2 R(\xi+(r^3+\phi(\theta))^{1/3}\theta, \xi+(r^3+\phi(\omega))^{1/3}\omega)\cdot\theta \, d\omega\\
&\quad+ \frac{\gamma u(\theta)v(\theta)}{27(r^3+\phi(\theta))^{4/3}} \int_{E_{\phi_k}} D_1^2 R(\xi+(r^3+\phi(\theta))^{1/3}\theta, y)\theta\cdot\theta \, dy\\
&\quad- \frac{2\gamma u(\theta)v(\theta)}{27(r^3+\phi(\theta))^{5/3}} \int_{E_{\phi_k}} D_1 R(\xi+(r^3+\phi(\theta))^{1/3}\theta, y)\cdot\theta \, dy,
\end{aligned}$$

where D_1 and D_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 of Lemma 6.1 is now proved easily.

The function G is also smooth in $\mathcal{C}$. We restore subscripts in the rest of this section. Similar to $\mathcal{B}_k''$, we find from (4.31) that

$$\begin{aligned}
&\mathcal{C}_{kl}''(\phi_k,\phi_l)(u_k,u_l)(v_k,v_l)(\theta_k)\\
&\quad= \frac{\gamma v_k(\theta_k)}{27(r_k^3+\phi_k(\theta_k))^{2/3}} \int_{S^2} u_l(\omega_l) D_1 G(\xi_k+(r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, \xi_l\\
&\quad+ (r_l^3+\phi_l(\omega_l))^{1/3}\omega_l)\cdot\theta_k \, d\omega_l\\
&\quad+ \frac{\gamma u_k(\theta_k)}{27(r_k^3+\phi_k(\theta_k))^{2/3}} \int_{S^2} v_l(\omega_l) D_1 G(\xi_k+(r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, \xi_l\\
&\quad+ (r_l^3+\phi_l(\omega_l))^{1/3}\omega_l)\cdot\theta_k \, d\omega_l\\
&\quad+ \frac{\gamma}{27} \int_{S^2} \frac{u_l(\omega_l)v_l(\omega_l)}{(r_l^3+\phi_l(\omega_l))^{2/3}} D_2 G(\xi_k+(r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, \xi_l\\
&\quad+ (r_l^3+\phi_l(\omega_l))^{1/3}\omega_l)\cdot\omega_l \, d\omega_l\\
&\quad+ \frac{\gamma u_k(\theta_k)v_k(\theta_k)}{27(r_k^3+\phi_k(\theta_k))^{4/3}} \int_{E_{\phi_l}} D_1^2 G(\xi_k+(r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, y)\theta_k\cdot\theta_k \, dy\\
&\quad- \frac{2\gamma u_k(\theta_k)v_k(\theta_k)}{27(r_k^3+\phi_k(\theta_k))^{5/2}} \int_{E_{\phi_l}} D_1 G(\xi_k+(r_k^3+\phi_k(\theta_k))^{1/3}\theta_k, y)\cdot\theta_k \, dy.
\end{aligned}$$

Part 4 of Lemma 6.1 then follows.

Part 5 of Lemma 6.1 follows from parts 1–4 and the fact that

$$\begin{aligned}
0 &= \sum_k \overline{S_k''(\phi)(u,v)}\\
&= \sum_k \overline{\mathcal{H}_k''(\phi_k)(u_k,v_k)} + \sum_k \overline{\mathcal{A}_k''(\phi_k)(u_k,v_k)} + \sum_k \overline{\mathcal{B}_k''(\phi_k)(u_k,v_k)}\\
&\quad+ \sum_k \overline{\mathcal{C}_k''(\phi)(u)} + K\lambda''(\phi)(u,v). \qquad \square
\end{aligned}$$

7. Reduction to $4K-1$ dimensions.

We view $\mathcal{S}$ as a nonlinear operator from $\mathcal{X}$ to $\mathcal{Y}$. In this section it will be proved that, for each $(\xi, r) \in U$, a $\varphi(\cdot, \xi, r)$ exists such that $\varphi(\cdot, \xi, r) \in \mathcal{X}_*$ and

$$\mathcal{S}_k(\varphi)(\theta_k) = A_{k,1} \cos\theta_{k,1} \sin\theta_{k,2} + A_{k,2} \sin\theta_k \sin\theta_{k,2} + A_{k,3} \cos\theta_{k,2} + A_k, \quad k = 1, 2, \ldots, K \tag{7.1}$$

for some numbers $A_{k,1}, A_{k,2}, A_{k,3}, A_k$. Note that φ is sought in $\mathcal{X}_*$. Each $\phi \in \mathcal{X}_*$ satisfies

$$\int_{S^2} \phi_k(\theta_k)\, d\theta_k = 0, \quad k = 1, 2, \ldots, K, \tag{7.2}$$

$$\int_{S^2} \phi_k(\theta_k) \cos\theta_{k,1} \sin\theta_{k,2}\, d\theta_k = 0, \quad k = 1, 2, \ldots, K, \tag{7.3}$$

$$\int_{S^2} \phi_k(\theta_k) \sin\theta_{k,1} \sin\theta_{k,2}\, d\theta_k = 0, \quad k = 1, 2, \ldots, K, \tag{7.4}$$

$$\int_{S^2} \phi_k(\theta_k) \cos\theta_{k,2}\, d\theta_k = 0, \quad k = 1, 2, \ldots, K. \tag{7.5}$$

The condition (7.2) means that $\phi_k \perp H_0$, the space of spherical harmonics of degree 0, and the conditions (7.3–7.5) state that $\phi_k \perp H_1$.

Write (7.1) as

$$\Pi \mathcal{S}(\varphi) = 0, \tag{7.6}$$

where Π is the orthogonal projection operator from $\mathcal{Y}$ to $\mathcal{Y}_*$. In the next section we will find a particular (ξ, r), say (ζ, s) at which $A_{k,1} = A_{k,2} = A_{k,3} = A_k = 0$, i.e., $\mathcal{S}(\varphi(\cdot, \zeta, s)) = 0$. This means that by finding φ we reduce the original problem (1.1) to a problem of finding a (ζ, s) in a $4K-1$ dimensional set U.

Recall $\mathcal{L}$, the linearized operator of $\mathcal{S}$ at $\phi = 0$. Expand $\mathcal{S}(\phi)$ as

$$\mathcal{S}(\phi) = \mathcal{S}(0) + \mathcal{L}(\phi) + \mathcal{N}(\phi), \tag{7.7}$$

where $\mathcal{N}$ is a higher order term defined by (7.7). Turn (7.6) to a fixed point form

$$\phi = -(\Pi\mathcal{L})^{-1}(\Pi\mathcal{S}(0) + \Pi\mathcal{N}(\phi)). \tag{7.8}$$

Lemma 7.1. *There exists $\varphi = \varphi(\theta, \xi, r)$ such that for every $(\xi, r) \in U$, $\varphi(\cdot, \xi, r) \in \mathcal{X}_*$ solves* (7.8) *and $\|\varphi\|_{W^{2,p}} \leq c\rho^5$, where c is a sufficiently large constant independent of ξ, r, ρ, and γ.*

Proof. To use the contraction mapping principle, let

$$\mathcal{T}(\phi) = -(\Pi\mathcal{L})^{-1}(\Pi\mathcal{S}(0) + \Pi\mathcal{N}(\phi)) \tag{7.9}$$

be an operator defined on

$$D(\mathcal{T}) = \{\phi \in \mathcal{X}_* : \|\phi\|_{W^{2,p}} \leq c\rho^5\}, \tag{7.10}$$

where the constant c is sufficiently large and will be determined shortly.

Lemma 3.1 shows that

$$\mathcal{S}_k(0)(\theta_k) - \lambda(0) = \frac{1}{3r_k} + \frac{\gamma}{3}\left[\frac{r_k^2}{3} + \frac{4\pi r_k^3}{3} R(\xi_k, \xi_k) + \sum_{l \neq k} \frac{4\pi r_l^3}{3} G(\xi_k, \xi_l)\right] + O(\rho).$$

Each $\mathcal{S}_k(0)$ is sum of a number independent of θ_k and a quantity of order $O(\rho)$. After we apply the projection operator Π the number vanishes and

$$\|\Pi\mathcal{S}(0)\|_{L^p} = O(\rho). \tag{7.11}$$

By Lemma 5.3 we find

$$\|(\Pi\mathcal{L})^{-1}\Pi\mathcal{S}(0)\|_{W^{2,p}} \le C\rho^5. \tag{7.12}$$

For $\mathcal{N}(\phi)$ we decompose it into three parts. The first is $\mathcal{N}_1$ whose kth component is

$$\mathcal{N}_{1,k}(\phi_k) = \mathcal{H}_k(\phi_k) - \mathcal{H}_k(0) - \mathcal{H}_k'(0)(\phi_k) \tag{7.13}$$

which is $\mathcal{H}_k(\phi)$ minus its linear approximation at 0. Lemma 6.1, part 1, shows that

$$\|\mathcal{N}_1(\phi)\|_{L^p} \le \frac{C}{\rho^7}\|\phi\|^2_{W^{2,p}}. \tag{7.14}$$

The second part of $\mathcal{N}$, denoted by $\mathcal{N}_2$, is $\mathcal{A}(\phi)+\mathcal{B}(\phi)+\mathcal{C}(\phi)$ minus its linear approximation, i.e.,

$$\mathcal{N}_2(\phi) = \mathcal{A}(\phi)-\mathcal{A}(0)-\mathcal{A}'(0)(\phi)+\mathcal{B}(\phi)-\mathcal{B}(0)-\mathcal{B}'(0)(\phi)+\mathcal{C}(\phi)-\mathcal{C}(0)-\mathcal{C}'(0)(\phi). \tag{7.15}$$

Lemma 6.1, parts 2, 3, and 4, implies that

$$\|\mathcal{N}_2(\phi)\|_{L^p} \le \frac{C}{\rho^7}\|\phi\|^2_{W^{1,p}}. \tag{7.16}$$

The third part of $\mathcal{N}$, which is denoted by $\mathcal{N}_3$, merely gives a constant so that

$$\sum_k \overline{\mathcal{N}_k(\phi)} = \sum_k \overline{\mathcal{N}_{1,k}(\phi)} + \sum_k \overline{\mathcal{N}_{2,k}(\phi)} + K\mathcal{N}_3(\phi) = 0.$$

It follows that

$$|\mathcal{N}_3(\phi)| \le \frac{C}{\rho^7}\|\phi\|^2_{W^{2,p}}. \tag{7.17}$$

Therefore we deduce, from (7.14), (7.16), (7.17), and with the help of Lemma 5.3, that

$$\|\mathcal{N}(\phi)\|_{L^p} \le \frac{C}{\rho^7}\|\phi\|^2_{W^{2,p}}, \tag{7.18}$$

$$\|(\Pi\mathcal{L})^{-1}\Pi\mathcal{N}(\phi)\|_{W^{2,p}} \le \frac{C}{\rho^3}\|\phi\|^2_{W^{2,p}}. \tag{7.19}$$

Using (2.10), (7.12), (7.10), and (7.19) we find

$$\|\mathcal{T}(\phi)\|_{W^{2,p}} \le C\rho^5 + Cc^2\rho^7 \le c\rho^5$$

if c is sufficiently large and ρ sufficiently small. Therefore $\mathcal{T}$ is a map from $D(\mathcal{T})$ into itself.

Next we show that $\mathcal{T}$ is a contraction. For $\mathcal{N}_1$ we note that

$$\mathcal{N}_1(\phi_1) - \mathcal{N}_1(\phi_2) = \mathcal{H}(\phi_1) - \mathcal{H}(\phi_2) - \mathcal{H}'(0)(\phi_1 - \phi_2).$$

Therefore using Lemma 6.1, part 1, we obtain

$$\begin{aligned}&\|\mathcal{H}(\phi_1)-\mathcal{H}(\phi_2)-\mathcal{H}'(0)(\phi_1-\phi_2)\|_{L^p}\\ &\quad\le \|\mathcal{H}'(\phi_2)(\phi_1-\phi_2)-\mathcal{H}'(0)(\phi_1-\phi_2)\|_{L^p}+\frac{C}{\rho^7}\|\phi_1-\phi_2\|^2_{W^{2,p}}\\ &\quad\le \frac{C}{\rho^7}\|\phi_2\|_{W^{2,p}}\|\phi_1-\phi_2\|_{W^{2,p}}+\frac{C}{\rho^7}\|\phi_1-\phi_2\|^2_{W^{2,p}}\\ &\quad\le \frac{C}{\rho^7}(\|\phi_1\|_{W^{2,p}}+\|\phi_2\|_{W^{2,p}})\|\phi_1-\phi_2\|_{W^{2,p}}.\end{aligned}$$

This shows that

$$\|\mathcal{N}_1(\phi_1)-\mathcal{N}_2(\phi_2)\|_{L^p}\le \frac{C}{\rho^2}\|\phi_1-\phi_2\|_{W^{2,p}}. \tag{7.20}$$

For $\mathcal{N}_2$ we note that

$$\begin{aligned}\mathcal{N}_2(\phi_1)-\mathcal{N}_2(\phi_2)&=\mathcal{A}(\phi_1)-\mathcal{A}(\phi_2)-\mathcal{A}'(0)(\phi_1-\phi_2)+\mathcal{B}(\phi_1)-\mathcal{B}(\phi_2)\\ &\quad-\mathcal{B}'(0)(\phi_1-\phi_2)+\mathcal{C}(\phi_1)-\mathcal{C}(\phi_2)-\mathcal{C}'(0)(\phi_1-\phi_2).\end{aligned}\tag{7.21}$$

Therefore using Lemma 6.1, part 2, we obtain

$$\begin{aligned}&\|\mathcal{A}(\phi_1)-\mathcal{A}(\phi_2)-\mathcal{A}'(0)(\phi_1-\phi_2)\|_{L^p}\\ &\quad\le \|\mathcal{A}'(\phi_2)(\phi_1-\phi_2)-\mathcal{A}'(0)(\phi_1-\phi_2)\|_{L^p}+\frac{C}{\rho^7}\|\phi_1-\phi_2\|^2_{W^{1,p}}\\ &\quad\le \frac{C}{\rho^7}\|\phi_2\|_{W^{1,p}}\|\phi_1-\phi_2\|_{W^{1,p}}+\frac{C}{\rho^7}\|\phi_1-\phi_2\|^2_{W^{1,p}}\\ &\quad\le \frac{C}{\rho^7}(\|\phi_1\|_{W^{1,p}}+\|\phi_2\|_{W^{1,p}})\|\phi_1-\phi_2\|_{W^{1,p}}.\end{aligned}$$

Similarly using Lemma 6.1, parts 3 and 4, we deduce

$$\begin{aligned}\|\mathcal{B}(\phi_1)-\mathcal{B}(\phi_2)-\mathcal{B}'(0)(\phi_1-\phi_2)\|_{L^p}&\le \frac{C}{\rho^5}(\|\phi_1\|_{W^{1,p}}+\|\phi_2\|_{W^{1,p}})\|\phi_1-\phi_2\|_{W^{1,p}}\\ \|\mathcal{C}(\phi_1)-\mathcal{C}(\phi_2)-\mathcal{C}'(0)(\phi_1-\phi_2)\|_{L^p}&\le \frac{C}{\rho^5}(\|\phi_1\|_{W^{1,p}}+\|\phi_2\|_{W^{1,p}})\|\phi_1-\phi_2\|_{W^{1,p}}.\end{aligned}$$

From (7.21) we conclude that

$$\begin{aligned}\|\mathcal{N}_2(\phi_1)-\mathcal{N}_2(\phi_2)\|_{L^p}&\le \frac{C}{\rho^7}(\|\phi_1\|_{W^{1,p}}+\|\phi_2\|_{W^{1,p}})\|\phi_1-\phi_2\|_{W^{1,p}}\\ &\le \frac{C}{\rho^2}\|\phi_1-\phi_2\|_{W^{1,p}}.\end{aligned}\tag{7.22}$$

We also have

$$\|\mathcal{N}_3(\phi_1)-\mathcal{N}_3(\phi_2)\|_{L^p}\le \frac{C}{\rho^2}\|\phi_1-\phi_2\|_{W^{2,p}}. \tag{7.23}$$

Hence, following (7.20), (7.22), and (7.23), we find that

$$\begin{aligned}&\|\mathcal{T}(\phi_1)-\mathcal{T}(\phi_2)\|_{W^{2,p}}\\ &\quad=\|(\Pi\mathcal{L})^{-1}\Pi\mathcal{N}(\phi_1)-(\Pi\mathcal{L})^{-1}\Pi\mathcal{N}(\phi_2)\|_{W^{2,p}}\le C\rho^2\|\phi_1-\phi_2\|_{W^{2,p}},\end{aligned}\tag{7.24}$$

i.e., that $\mathcal{T}$ is a contraction map if ρ is sufficiently small. A fixed point φ exists. ☐

Since φ satisfies $\|\phi\|_{W^{2,p}} \le c\rho^5$, by taking ρ small we see that $r_k^3 + \varphi_k$ remains positive. ∂E_{φ_k} is a perturbed sphere.

Denote $\mathcal{S}'(\varphi)$ by $\tilde{\mathcal{L}}$. We derive a lemma for $\tilde{\mathcal{L}}$ similar to Lemma 5.3.

LEMMA 7.2. *Let Π be the same projection operator from $\mathcal{X}$ to $\mathcal{X}_*$.*

1. *There exists $C > 0$ such that for all $u \in \mathcal{X}_*$*

$$\|u\|_{W^{2,p}} \le C\rho^4 \|\Pi\tilde{\mathcal{L}}(u)\|_{L^p}.$$

2. *If* (2.8) *holds, then*

$$\|u\|_{W^{1,2}}^2 \le C\rho^4 \langle \Pi\tilde{\mathcal{L}}(u), u\rangle.$$

Proof. By Lemma 5.3, part 1, Lemma 6.1, and the fact $\|\varphi\|_{W^{2,p}} = O(\rho^5)$, we deduce that

$$\begin{aligned}\|\Pi\tilde{\mathcal{L}}(u)\|_{L^p} &\ge \|\Pi\mathcal{L}(u)\|_{L^p} - \|\Pi(\tilde{\mathcal{L}} - \mathcal{L})(u)\|_{L^p}\\ &\ge \frac{C}{\rho^4}\|u\|_{W^{2,p}} - \frac{C}{\rho^7}\|\varphi\|_{W^{2,p}}\|u\|_{W^{2,p}}\\ &\ge \frac{C}{\rho^4}\|u\|_{W^{2,p}} - \frac{C}{\rho^2}\|u\|_{W^{2,p}} \;\ge\; \frac{C}{\rho^4}\|u\|_{W^{2,p}}\end{aligned}$$

when ρ is small. This proves part 1 of Lemma 7.2.

Write $\tilde{\mathcal{L}} = \mathcal{H}'(\varphi) + \mathcal{A}'(\varphi) + \mathcal{B}'(\varphi) + \mathcal{C}'(\varphi) + \lambda'(\varphi)$. Then, according to (4.7),

$$\langle \mathcal{H}_k'(\varphi_k)(u_k), u_k\rangle = \int_{S^2}\left[\frac{\partial^2 L_k}{\partial\phi_k^2}u_k^2 + 2\sum_{i=1}^{2}\frac{\partial^2 L_k}{\partial\phi_k\partial\phi_{k,i}}u_k u_{k,i} + \sum_{i,j=1}^{2}\frac{\partial^2 L_k}{\partial\phi_{k,i}\partial\phi_{k,j}}u_{k,i}u_{k,j}\right]d\theta_k,$$

and a similar expression holds if we replace φ_k and $\varphi_{k,i}$ by 0 in the last formula.

With $\|\varphi\|_{W^{2,p}} = O(\rho^5)$, calculations show that

$$\begin{aligned}&|\langle(\mathcal{H}_k'(\varphi_k) - \mathcal{H}_k'(0))u_k, u_k\rangle|\\ &\quad\le \left|\int_{S^2}\left(\frac{\partial^2 L_k(\varphi_k)}{\partial\phi_k^2} - \frac{\partial^2 L_k(0)}{\partial\phi_k^2}\right)u_k^2\,d\theta_k\right|\\ &\qquad + 2\sum_{i=1}^{2}\left|\int_{S^2}\left(\frac{\partial^2 L_k(\varphi_k)}{\partial\phi_k\partial\phi_{k,i}} - \frac{\partial^2 L_k(0)}{\partial\phi_k\partial\phi_{k,i}}\right)u_k u_{k,i}\,d\theta_k\right|\\ &\qquad + \sum_{i,j=1}^{2}\left|\int_{S^2}\left(\frac{\partial^2 L_k(\varphi_k)}{\partial\phi_{k,i}\partial\phi_{k,j}} - \frac{\partial^2 L_k(0)}{\partial\phi_{k,i}\partial\phi_{k,j}}\right)u_{k,i}u_{k,j}\,d\theta_k\right|\\ &\quad\le \frac{C}{\rho^2}\|u\|_{L^2}^2 + \frac{C}{\rho^2}\|u\|_{L^2}\|Du\|_{L^2} + \frac{C}{\rho^2}\|Du\|_{L^2}^2 \;\le\; \frac{C}{\rho^2}\|u\|_{W^{1,2}}^2.\end{aligned} \tag{7.25}$$

Next we estimate $\|(\mathcal{A}_k'(\varphi_k) - \mathcal{A}_k'(0))u_k\|_{L^2}$ and revisit $\mathcal{A}_k''$. Arguing as in the proof of Lemma 6.1, part 2, we deduce that

$$\|\mathcal{A}_k''(\phi)(u_k, v_k)\|_{L^2} \le \frac{C}{\rho^7}\|u_k\|_{W^{1,2}}\|v_k\|_{W^{1,2}}.$$

This implies that in this lemma

$$\|(\mathcal{A}_k'(\varphi) - \mathcal{A}_k'(0))u_k\|_{L^2} \le \frac{C}{\rho^7}C\rho^5\|u_k\|_{W^{1,2}} \le \frac{C}{\rho^2}\|u_k\|_{W^{1,2}}.$$

Simpler arguments show that

$$\|(\mathcal{B}_k'(\varphi)-\mathcal{B}_k'(0))u_k\|_{L^2}\le\frac{C}{\rho^2}\|u_k\|_{W^{1,2}},\quad \|(\mathcal{C}'(\varphi)-\mathcal{C}'(0))u\|_{L^2}\le\frac{C}{\rho^2}\|u\|_{W^{1,2}}.$$

We obtain that

$$\|(\mathcal{A}'(\varphi)+\mathcal{B}'(\varphi)+\mathcal{C}'(\varphi)-\mathcal{A}'(0)-\mathcal{B}'(0)-\mathcal{C}'(0))u\|_{L^2}\le\frac{C}{\rho^2}\|u\|_{W^{1,2}}. \tag{7.26}$$

If (2.8) holds, we combine Lemma 5.3, part 3, (7.25), and (7.26) to deduce that

$$\langle\Pi\tilde{\mathcal{L}}(u),u\rangle=\langle\Pi\mathcal{L}(u),u\rangle+\langle\Pi(\tilde{\mathcal{L}}-\mathcal{L})u,u\rangle\ge\frac{C}{\rho^4}\|u\|^2_{W^{1,2}}-\frac{C}{\rho^2}\|u\|^2_{W^{1,2}}\ge\frac{C}{\rho^4}\|u\|^2_{W^{1,2}},$$

proving the second part. ▯

One consequence of Lemma 7.2, part 1, is an estimate of $\frac{\partial\varphi}{\partial\xi_{l,j}}$.

LEMMA 7.3. *The fixed point* φ *satisfies* $\left\|\frac{\partial\varphi}{\partial\xi_{l,j}}\right\|_{W^{2,p}}=O(\rho^4)$, $l=1,2,\dots,K$, $j=1,2,3$.

Proof. We prove this lemma by the implicit function theorem. Fix $l\in\{1,2,\dots,K\}$ and $j\in\{1,2,3\}$. Differentiating $\Pi\mathcal{S}(\varphi)$ with respect to $\xi_{l,j}$ we find that, for $k=1,2,\dots,K$, if $k=l$, then

$$\begin{aligned}\frac{\partial\Pi\mathcal{S}_l(\varphi)}{\partial\xi_{l,j}}&=\Pi\tilde{\mathcal{L}}_l\left(\frac{\partial\varphi}{\partial\xi_{l,j}}\right)+\Pi\frac{\gamma}{3}\\&\quad\times\int_{E_{\varphi_l}}\left[\frac{\partial R(\xi_l+(r_l^3+\varphi_l(\theta_l))^{1/3}\theta_l,y)}{\partial x_j}+\frac{\partial R(\xi_l+(r_l^3+\varphi_l(\theta_l))^{1/3}\theta_l,y)}{\partial y_j}\right]dy\\&\quad+\sum_{m\neq l}\Pi\frac{\gamma}{3}\int_{E_{\varphi_m}}\frac{\partial G(\xi_l+(r_l^3+\varphi_l(\theta_l))^{1/3}\theta_l,y)}{\partial x_j}\,dy,\end{aligned}$$

and if $k\neq l$,

$$\frac{\partial\Pi\mathcal{S}_k(\varphi)}{\partial\xi_{l,j}}=\Pi\tilde{\mathcal{L}}_k\left(\frac{\partial\varphi}{\partial\xi_{l,j}}\right)+\Pi\frac{\gamma}{3}\int_{E_{\varphi_l}}\frac{\partial G(\xi_k+(r_k^3+\varphi_k(\theta_k))^{1/3}\theta_k,y)}{\partial y_j}\,dy.$$

Here $R=R(x,y)$ and $G=G(x,y)$. It is clear that

$$\begin{aligned}\Bigg\|\frac{\gamma}{3}\int_{E_{\varphi_l}}\Bigg[&\frac{\partial R(\xi_l+(r_l^3+\varphi_l(\theta_l))^{1/3}\theta_l,y)}{\partial x_j}\\&+\frac{\partial R(\xi_l+(r_l^3+\varphi_l(\theta_l))^{1/3}\theta_l,y)}{\partial y_j}\Bigg]dy\Bigg\|_{L^p}=O(\gamma\rho^3),\end{aligned}$$

$$\left\|\frac{\gamma}{3}\int_{E_{\varphi_m}}\frac{\partial G(\xi_l+(r_l^3+\varphi_l(\theta_l))^{1/3}\theta_l,y)}{\partial x_j}\,dy\right\|_{L^p}=O(\gamma\rho^3),$$

$$\left\|\frac{\gamma}{3}\int_{E_{\varphi_l}}\frac{\partial G(\xi_k+(r_k^3+\varphi_k(\theta_k))^{1/3}\theta_k,y)}{\partial y_j}\,dy\right\|_{L^p}=O(\gamma\rho^3).$$

Therefore

$$\frac{\partial \Pi \mathcal{S}(\varphi)}{\partial \xi_{l,j}} = \Pi \tilde{\mathcal{L}} \left(\frac{\partial \varphi}{\partial \xi_{l,j}} \right) + W,$$

where $\|W\|_{L^p} = O(\gamma \rho^3) = O(1)$.

On the other hand

$$\frac{\partial \Pi \mathcal{S}(\varphi)}{\partial \xi_{l,j}} = 0,$$

since $\Pi \mathcal{S}(\varphi) = 0$.

By Lemma 7.2 we deduce that

$$\left\| \frac{\partial \varphi}{\partial \xi_{l,j}} \right\|_{W^{2,p}} \leq C\rho^4 O(1) \leq C\rho^4. \qquad \square$$

8. Solving the reduced problem. We now turn to solve $\mathcal{S}(\phi) = 0$.

LEMMA 8.1. *$J(E_\varphi) = J(B) + O(\rho^6)$. More explicitly*

$$J(E_\varphi) = \sum_{k=1}^{K} 4\pi r_k^2 + \frac{\gamma}{2} \Bigg\{ \sum_{k=1}^{K} \left[\frac{8\pi r_k^5}{15} + \left(\frac{4\pi}{3} \right)^2 r_k^6 R(\xi_k, \xi_k) \right] + \sum_{k=1}^{K} \sum_{l=1, l\neq k}^{K} \left(\frac{4\pi}{3} \right)^2 r_k^3 r_l^3 G(\xi_k, \xi_l) \Bigg\} + O(\rho^5).$$

Here $J(E_\varphi) = J(E_{\varphi(\cdot,\xi,r)})$ can be considered as a function of (ξ, r).

Proof. Expanding $J(E_\varphi)$ yields

$$J(E_\varphi) = J(B) + \sum_k \int_{S^2} \mathcal{S}_k(0)\varphi_k \, d\theta_k + \frac{1}{2} \sum_k \int_{S^2} \mathcal{L}_k(\varphi)\varphi_k \, d\theta_k + O(\rho^8). \tag{8.1}$$

The error term $O(\rho^8)$ in (8.1) is obtained in the same way that (7.18) is derived.

On the other hand $\Pi \mathcal{S}(\varphi) = 0$ implies that

$$\Pi(\mathcal{S}_k(0) + \mathcal{L}_k(\varphi) + \mathcal{N}_k(\varphi)) = 0,$$

where $\mathcal{N}$ is given in (7.7) and estimated in (7.18). We multiply the last equation by φ_k and integrate to derive

$$\int_{S^2} \mathcal{S}_k(0)\varphi_k \, d\theta_k + \int_{S^2} \mathcal{L}(\varphi_k)\varphi_k \, d\theta_k = O(\rho^8).$$

We can now rewrite (8.1) as

$$J(E_\varphi) = J(B) + \frac{1}{2} \sum_k \int_{S^2} \mathcal{S}_k(0)\varphi_k \, d\theta_k + O(\rho^8).$$

Note that $\mathcal{S}_k(0)$ is the sum of a number independent of θ_k and a quantity of order ρ by Lemma 3.1. Since φ_k satisfies (7.2), the inner product of the number and φ_k is zero, and hence

$$\int_{S^2} \mathcal{S}_k(0)\varphi_k \, d\theta = O(\rho^6).$$

Therefore

$$J(E_\varphi) = J(B) + O(\rho^6).$$

Lemma 3.2 implies that

$$\begin{aligned} J(E_\varphi) &= \sum_{k=1}^{K} 4\pi r_k^2 + \frac{\gamma}{2}\Bigg\{ \sum_{k=1}^{K} \left[\frac{8\pi r_k^5}{15} + \left(\frac{4\pi}{3}\right)^2 r_k^6 R(\xi_k,\xi_k) \right] \\ &\quad + \sum_{k=1}^{K} \sum_{l=1, l\neq k}^{K} \left(\frac{4\pi}{3}\right)^2 r_k^3 r_l^3 G(\xi_k,\xi_l) \\ &\quad + \sum_{k=1}^{K}\sum_{l=1}^{K} \left(\frac{4\pi}{3}\right)^2 \left(\frac{r_k^3 r_l^5}{10|D|} + \frac{r_k^5 r_l^3}{10|D|} \right) \Bigg\} + O(\rho^6) \\ &= \sum_{k=1}^{K} 4\pi r_k^2 + \frac{\gamma}{2}\Bigg\{ \sum_{k=1}^{K} \left[\frac{8\pi r_k^5}{15} + \left(\frac{4\pi}{3}\right)^2 r_k^6 R(\xi_k,\xi_k) \right] \\ &\quad + \sum_{k=1}^{K} \sum_{l=1, l\neq k}^{K} \left(\frac{4\pi}{3}\right)^2 r_k^3 r_l^3 G(\xi_k,\xi_l) \Bigg\} + O(\rho^5). \end{aligned}$$

This proves the lemma. □

LEMMA 8.2. *When* ρ *is sufficiently small,* $J(E_{\varphi(\cdot,\xi,r)})$ *is minimized at some* $(\xi,r) = (\zeta,s) \in U$. *As* $\rho \to 0$, $\frac{s}{\rho} \to (1,1,\dots,1)$, *and* $\zeta \to \zeta_0$ *along a subsequence where* $\zeta_0 \in U_1$ *is a global minimum of* F.

Proof. Let us rescale the problem with

$$R = \frac{r}{\rho}, \quad \tilde{J}(\xi,R) = \frac{2}{\gamma\rho^5} J(E_{\varphi(\cdot,\xi,r)}), \quad (\xi,R) \in U_1 \times \tilde{U}_2,$$

where

$$\tilde{U}_2 = \left\{ (R_1,R_2,\dots,R_K) : \ 1-\delta_2 < R_k < 1+\delta_2, \ \sum_{k=1}^{K} R_k^3 = K \right\}$$

is a scaled version of U_2. Note that by (2.5) and Lemma 8.1 that

$$\begin{aligned} \tilde{J}(\xi,R) &= \frac{8\pi}{\gamma\rho^3} \sum_{k=1}^{K} R_k^2 + \sum_{k=1}^{K} \frac{8\pi R_k^5}{15} \\ &\quad + \rho \left(\frac{4\pi}{3}\right)^2 \left[\sum_{k=1}^{K} (R_k^6 R(\xi_k,\xi_k)) + \sum_{k=1}^{K} \sum_{l\neq k} R_k^3 R_l^3 G(\xi_k,\xi_l) \right] + O(\rho^3). \end{aligned}$$

Again by (2.5) we may assume that along a subsequence

$$\frac{8\pi}{\gamma\rho^3} \to b_0 \le \frac{8\pi}{(3+\epsilon)\pi}, \text{ as } \rho \to 0. \tag{8.2}$$

Let (ζ,S) be the global minimum of $\tilde{J}$ on the closure of $U_1 \times \tilde{U}_2$. Here $S = \frac{s}{\rho}$. Let $(\zeta,S) \to (\zeta_0,S_0)$ along a subsequence as ρ tends to 0. First we claim that

$S_0 = (1, 1, \ldots, 1)$. Suppose this is false, i.e., $S_0 \neq (1, 1, \ldots, 1)$. Then as ρ tends to 0,

$$\begin{aligned} \tilde{J}(\zeta, (1, \ldots, 1)) - \tilde{J}(\zeta, S) &= \sum_k \frac{8\pi}{\gamma\rho^3} + \sum_k \frac{8\pi}{15} - \sum_k \frac{8\pi S_k^2}{\gamma\rho^3} - \sum_k \frac{8\pi S_k^5}{15} + O(\rho) \\ &\to \sum_k b_0 + \sum_k \frac{8\pi}{15} - \sum_k b_0 S_{0,k}^2 - \sum_k \frac{8\pi S_{0,k}^5}{15}. \end{aligned}$$

Because of (8.2) and the constraint $\sum_k S_{0,k}^3 = K$, it is easy to show that the last line is negative if δ_2 in (3.1) is small enough, depending on ϵ. For, under (8.2), the function

$$x \to b_0 x^{2/3} + \frac{8\pi}{15} x^{5/3}$$

is convex when x is near 1. The last assertion then follows from the Jensen's inequality, when x takes values $S_{0,k}^3$. This is a contradiction to that (ζ, S) is a minimum of $\tilde{J}$.

Next we claim that ζ_0 minimizes F in U_1. Suppose this is false. Let η be a minimum of F in U_1. Then $F(\eta) < F(\zeta_0)$. Consider

$$\begin{aligned} \frac{1}{\rho}\left(\frac{3}{4\pi}\right)^2 (\tilde{J}(\eta, S) - \tilde{J}(\zeta, S)) &= \sum_{k=1}^K S_k^6 R(\eta_k, \eta_k) + \sum_{k=1}^K \sum_{l \neq k} S_k^3 S_l^3 G(\eta_k, \eta_l) \\ &\quad - \sum_{k=1}^K S_k^6 R(\zeta_k, \zeta_k) - \sum_{k=1}^K \sum_{l \neq k} S_k^3 S_l^3 G(\zeta_k, \zeta_l) + O(\rho^2) \\ &\to F(\eta) - F(\zeta_0) \ < \ 0, \text{ as } \rho \to 0, \end{aligned}$$

another contradiction to that (ζ, S) minimizes $\tilde{J}$. Note that $(\zeta, S) \in U_1 \times \tilde{U_2}$ when ρ is small, since $(\zeta_0, S_0) \in U_1 \times \tilde{U_2}$. ◻

We show that $\varphi(\cdot, \zeta, s)$ is an exact solution of (1.1) in the next two lemmas. The first shows that $A_k = 0$ in (7.1) at $\xi = \zeta$ and $r = s$.

LEMMA 8.3. *At* $\xi = \zeta$ *and* $r = s$, $\mathcal{S}_k(\varphi(\cdot, \zeta, s))(\theta_k) = A_{k,1} \cos\theta_{k,1} \sin\theta_{k,2} + A_{k,2} \sin\theta_{k,1} \sin\theta_{k,2} + A_{k,3} \cos\theta_{k,2}$.

Proof. At each $(\xi, r) \in U$, let

$$p_k = r_k^3, \quad q_k = s_k^3. \tag{8.3}$$

Calculations show that

$$\begin{aligned} \frac{\partial J(E_\varphi)}{\partial p_k} &= \sum_{l=1}^K \int_{S^2} [\mathcal{S}_l(\varphi) - \lambda(\varphi)] \frac{\partial(p_l + \varphi_l)}{\partial p_k}\, d\theta_l \\ &= \int_{S^2} [\mathcal{S}_k(\varphi) - \lambda(\varphi)] \left(1 + \frac{\partial \varphi_k}{\partial p_k}\right) d\theta_k + \sum_{l \neq k} \int_{S^2} [\mathcal{S}_l(\varphi) - \lambda(\varphi)] \frac{\partial \varphi_l}{\partial p_k}\, d\theta_l \\ &= \int_{S^2} (A_{k,1} \cos\theta_{k,1} \sin\theta_{k,2} + A_{k,2} \sin\theta_{k,1} \sin\theta_{k,2} + A_{k,3} \cos\theta_{k,2} \\ &\qquad + A_k - \lambda(\varphi)) \left(1 + \frac{\partial \varphi_k}{\partial p_k}\right) d\theta_k \end{aligned}$$

$$
\begin{aligned}
&+\sum_{l\neq k}\int_{S^2}(A_{l,1}\cos\theta_{l,1}\sin\theta_{l,2}+A_{l,2}\sin\theta_{l,1}\sin\theta_{l,2}+A_{l,3}\cos\theta_{l,2}\\
&\qquad\qquad +A_l-\lambda(\varphi))\frac{\partial\varphi_l}{\partial p_k}\,d\theta_l\\
&=4\pi A_k-4\pi\lambda(\varphi).
\end{aligned}
$$

Here we have used the facts that

$$\frac{\partial\varphi_l}{\partial p_k}\perp\cos\theta_{l,1}\sin\theta_{l,2},\ \sin\theta_{l,1}\sin\theta_{l,2},\ \cos\theta_{l,2},\ 1$$

which follow from $\varphi\in\mathcal{X}_*$.

On the other hand at the minimum $p=q$ and $\xi=\zeta$ with respect to p, we must have

$$\frac{\partial J(E_\varphi)}{\partial p_k}|_{\xi=\zeta,p=q}=\mu$$

for all $k=1,2,\ldots,K$. Here μ is a Lagrange multiplier coming from the constraint

$$\sum_{k=1}^K p_k=\frac{3a|D|}{4\pi}.$$

Therefore we deduce that

$$A_k=\frac{\mu}{4\pi}+\lambda$$

which is independent of k. By (4.20) we derive that $\sum_{k=1}^K A_k=0$, and then we conclude that each A_k must be 0. ▯

Next we show that $A_{k,1}$, $A_{k,2}$, and $A_{k,3}$ in (7.1) are 0 at $\xi=\zeta$ and $r=s$. The proof uses a tricky reparametrization technique.

LEMMA 8.4. *At $\xi=\zeta$ and $r=s$, $\mathcal{S}(\varphi(\cdot,\zeta,s))=0$.*

Proof. To simplify notations in this proof, we do not explicitly indicate the dependence of φ on r, i.e., we write $\varphi(\cdot,\xi)$ instead of $\varphi(\cdot,\xi,r)$. For each $\xi_k=(\xi_{k,1},\xi_{k,2},\xi_{k,3})$ near ζ_k we reparametrize $\partial_D E_{\varphi_k(\cdot,\xi)}$. Let ζ_k be the center of new polar coordinates, $r_k^3+\psi_k$ the new radius cube, and η_k the new angle. A point on $\partial_D E_{\varphi_k(\cdot,\xi)}$ is described as $\zeta_k+(r_k^3+\psi_k)^{1/3}\eta_k$. It is related to the old polar coordinates via

$$\zeta_k+(r_k^3+\psi_k)^{1/3}\eta_k=\xi_k+(r_k^3+\varphi_k)^{1/3}\theta_k. \tag{8.4}$$

In the new coordinates E_{φ_k} becomes E_{ψ_k}. It is viewed as a perturbation of the ball centered at ζ_k with radius r_k. The perturbation is described by ψ_k which is a function of η_k and ξ.

The main effect of the new coordinates is to “freeze” the center. The center of the new polar system is ζ_k which is fixed while the center of the old polar system is ξ_k which varies in D.

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

$$\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial\xi_{k,j}}|_{\xi=\zeta}=\frac{\partial J(E_{\varphi(\cdot,\xi)})}{\partial\xi_{k,j}}|_{\xi=\zeta}=0,\quad j=1,2,3, \tag{8.5}$$

since ζ is a minimum.

On the other hand calculations show that

$$\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial \xi_{k,j}} = \sum_{l=1}^{K} \int_{S^2} \mathcal{S}_l(\psi(\cdot,\xi))(\eta_l) \frac{\partial \psi_l}{\partial \xi_{k,j}} \, d\eta_l. \tag{8.6}$$

We emphasize that (8.6) is obtained under the reparametrized coordinates, in which the dependence of $J(E_{\psi(\cdot,\xi)})$ on ξ is reflected only 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 $R(\xi_l + \cdots, \xi_l + \cdots)$ and $G(\xi_k + \cdots, \xi_l + \cdots)$. The result would have been very different from (8.6). See the proof of Lemma 7.3 which involves differentiation with respect to ξ in the original coordinates. In the derivation of (8.6) we have used the fact that $\sum_l \int_{S^2} \psi_l \, d\eta_l = 0$ which implies that $\sum_l \int_{S^2} \frac{\partial \psi_l}{\partial \xi_{k,j}} \, d\eta_l = 0$, so that $\sum_l \int_{S^2} \lambda(\psi) \frac{\partial \psi_l}{\partial \xi_{k,j}} \, d\eta_l = 0$, where $\lambda(\psi)$ is part of

$$\mathcal{S}_l(\psi) = \mathcal{H}_l(\psi) + \mathcal{A}_l(\psi) + \mathcal{B}_l(\psi) + \mathcal{C}_l(\psi) + \lambda(\psi),$$

and we can reach the right-hand side of (8.6).

The expression $\mathcal{S}(\phi)$ is invariant under reparametrization, i.e.,

$$\mathcal{S}_l(\varphi(\cdot,\xi))(\theta_l) = \mathcal{S}_l(\psi(\cdot,\xi))(\eta_l). \tag{8.7}$$

Now we return to the original coordinate system and integrate with respect to θ_l in (8.6). Then

$$\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial \xi_{k,j}} = \sum_{l=1}^{K} \int_{S^2} \mathcal{S}_l(\varphi(\cdot,\xi))(\theta_l) \frac{\partial \psi_l(\eta_l(\theta_l,\xi),\xi)}{\partial \xi_{k,j}} \left| \frac{\partial(\eta_{l,1},\eta_{l,2})}{\partial(\theta_{l,1},\theta_{l,2})} \right| \frac{\sin \eta_{l,2}}{\sin \theta_{l,2}} \, d\theta_l. \tag{8.8}$$

There are two cases: $l = k$ and $l \neq k$. We start with the first case. Recall that ψ_k and η_k are defined implicitly as functions of θ_k and ξ by (8.4). Let us agree that $\psi_k = \psi_k(\eta_k, \xi)$ is a function of η_k and ξ. Set $\Psi_k(\theta_k, \xi) = \psi_k(\eta_k(\theta_k, \xi), \xi)$. To simplify notations let us set

$$g = (r_k^3 + \Psi_k)^{1/3}, \quad \tilde{g} = (r_k^3 + \varphi_k)^{1/3}. \tag{8.9}$$

Implicit differentiation shows that, with the help of Lemmas 7.1 and 7.3,

$$\begin{bmatrix} \frac{\partial \eta_{k,1}}{\partial \theta_{k,1}} & \frac{\partial \eta_{k,1}}{\partial \theta_{k,2}} & \frac{\partial \eta_{k,1}}{\partial \xi_{k,1}} & \frac{\partial \eta_{k,1}}{\partial \xi_{k,2}} & \frac{\partial \eta_{k,1}}{\partial \xi_{k,3}} \\ \frac{\partial \eta_{k,2}}{\partial \theta_{k,1}} & \frac{\partial \eta_{k,2}}{\partial \theta_{k,2}} & \frac{\partial \eta_{k,2}}{\partial \xi_{k,1}} & \frac{\partial \eta_{k,2}}{\partial \xi_{k,2}} & \frac{\partial \eta_{k,2}}{\partial \xi_{k,3}} \\ \frac{\partial \Psi_k}{\partial \theta_{k,1}} & \frac{\partial \Psi_k}{\partial \theta_{k,2}} & \frac{\partial \Psi_k}{\partial \xi_{k,1}} & \frac{\partial \Psi_k}{\partial \xi_{k,2}} & \frac{\partial \Psi_k}{\partial \xi_{k,3}} \end{bmatrix} = -M^{-1}N, \tag{8.10}$$

where

$$M^{-1} = \begin{bmatrix} g\sin\eta_{k,1}\sin\eta_{k,2} & -g\cos\eta_{k,1}\cos\eta_{k,2} & -\frac{\cos\eta_{k,1}\sin\eta_{k,2}}{3g^2} \\ -g\cos\eta_{k,1}\sin\eta_{k,2} & -g\sin\eta_{k,1}\cos\eta_{k,2} & -\frac{\sin\eta_{k,1}\sin\eta_{k,2}}{3g^2} \\ 0 & g\sin\eta_{k,2} & -\frac{\cos\eta_{k,2}}{3g^2} \end{bmatrix}^{-1}$$

$$= \frac{1}{\sin\eta_{k,2}} \begin{bmatrix} \frac{\sin\eta_{k,1}}{g} & -\frac{\cos\eta_{k,1}}{g} & 0 \\ -\frac{\cos\eta_{k,1}\cos\eta_{k,2}\sin\eta_{k,2}}{g} & -\frac{\sin\eta_{k,1}\cos\eta_{k,2}\sin\eta_{k,2}}{g} & \frac{\sin^2\eta_{k,2}}{g} \\ -3g^2\cos\eta_{k,1}\sin^2\eta_{k,2} & -3g^2\sin\eta_{k,1}\sin^2\eta_{k,2} & -3g^2\cos\eta_{k,2}\sin\eta_{k,2} \end{bmatrix}$$

and $N = [N_{ij}]$ is a 3 by 5 matrix given by

$$N_{11} = \frac{\cos\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\theta_{k,1}} - \tilde{g}\sin\theta_{k,1}\sin\theta_{k,2},$$

$$N_{12} = \frac{\cos\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\theta_{k,2}} + \tilde{g}\cos\theta_{k,1}\cos\theta_{k,2}, \quad N_{13} = 1 + \frac{\cos\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,1}},$$

$$N_{14} = \frac{\cos\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,2}}, \quad N_{15} = \frac{\cos\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,3}}$$

$$N_{21} = \frac{\sin\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\theta_{k,1}} + \tilde{g}\cos\theta_{k,1}\sin\theta_{k,2},$$

$$N_{22} = \frac{\sin\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\theta_{k,2}} + \tilde{g}\sin\theta_{k,1}\cos\theta_{k,2},$$

$$N_{23} = \frac{\sin\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,1}}, \quad N_{24} = 1 + \frac{\sin\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,2}},$$

$$N_{25} = \frac{\sin\theta_{k,1}\sin\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,3}}, \quad N_{31} = \frac{\cos\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\theta_{k,1}},$$

$$N_{32} = \frac{\cos\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\theta_{k,2}} - \tilde{g}\sin\theta_{k,2}, \quad N_{33} = \frac{\cos\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,1}},$$

$$N_{34} = \frac{\cos\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,2}}, \quad N_{35} = 1 + \frac{\cos\theta_{k,2}}{3\tilde{g}^2}\frac{\partial\varphi_k}{\partial\xi_{k,3}}.$$

We write N as

$$\sin\theta_{k,2} \begin{bmatrix} -\tilde{g}\sin\theta_{k,1} + O(\rho^3) & \frac{\tilde{g}\cos\theta_{k,1}\cos\theta_{k,2}}{\sin\theta_{k,2}} + O(\rho^3) & \frac{1}{\sin\theta_{k,2}} + O(\rho^2) & O(\rho^2) & O(\rho^2) \\ \tilde{g}\cos\theta_{k,1} + O(\rho^3) & \frac{\tilde{g}\sin\theta_{k,1}\cos\theta_{k,2}}{\sin\theta_{k,2}} + O(\rho^3) & O(\rho^2) & \frac{1}{\sin\theta_{k,2}} + O(\rho^2) & O(\rho^2) \\ \frac{O(\rho^3)}{\sin\theta_{k,2}} & -\tilde{g} + \frac{O(\rho^3)}{\sin\theta_{k,2}} & \frac{O(\rho^2)}{\sin\theta_{k,2}} & \frac{O(\rho^2)}{\sin\theta_{k,2}} & \frac{1}{\sin\theta_{k,2}} + \frac{O(\rho^2)}{\sin\theta_{k,2}} \end{bmatrix}.$$

At $\xi = \zeta$, we have $\eta = \theta$ and $\Psi = \varphi$. Multiplying M^{-1} and N we deduce that (8.10) becomes

$$\begin{bmatrix} 1+O(\rho^2) & O(\rho^2) & -\frac{\sin\theta_{k,1}}{\sin\theta_{k,2}g}+O(\rho) & \frac{\cos\theta_{k,1}}{\sin\theta_{k,2}g}+O(\rho) & O(\rho) \\ O(\rho^2) & 1+O(\rho^2) & \frac{\cos\theta_{k,1}\cos\theta_{k,2}}{g}+O(\rho) & \frac{\sin\theta_{k,1}\cos\theta_{k,2}}{g}+O(\rho) & -\frac{\sin\theta_{k,2}}{g}+O(\rho) \\ O(\rho^5) & O(\rho^5) & 3g^2\cos\theta_{k,1}\sin\theta_{k,2}+O(\rho^4) & 3g^2\sin\theta_{k,1}\sin\theta_{k,2}+O(\rho^4) & 3g^2\cos\theta_{k,2}+O(\rho^4) \end{bmatrix} \tag{8.11}$$

when $\xi = \zeta$.

We have found from (8.11) that at $\xi = \zeta$,

$$\left(\frac{\partial\Psi_k}{\partial\xi_{k,1}}, \frac{\partial\Psi_k}{\partial\xi_{k,2}}, \frac{\partial\Psi_k}{\partial\xi_{k,3}}\right)|_{\xi=\zeta} = 3r_k^2\theta_k + O(\rho^4). \tag{8.12}$$

To compute $\frac{\partial\psi_k}{\partial\xi_{k,j}}$, we invert $\eta_k = \eta_k(\xi, \theta_k)$ to express $\theta_k = \Theta_k(\eta_k, \xi)$. Then

$$\frac{\partial\psi_k}{\partial\xi_{k,j}} = \frac{\partial\Psi_k}{\partial\xi_{k,j}} + \frac{\partial\Psi_k}{\partial\theta_{k,1}}\frac{\partial\Theta_{k,1}}{\partial\xi_{k,j}} + \frac{\partial\Psi_k}{\partial\theta_{k,2}}\frac{\partial\Theta_{k,2}}{\partial\xi_{k,j}}.$$

At $\xi = \zeta$, since, by (8.11),

$$\frac{\partial\Psi_k}{\partial\theta_{k,m}}|_{\xi=\zeta} = O(\rho^5) \tag{8.13}$$

and

$$\begin{aligned} \begin{bmatrix} \frac{\partial\Theta_{k,1}}{\partial\xi_{k,1}} & \frac{\partial\Theta_{k,1}}{\partial\xi_{k,2}} & \frac{\partial\Theta_{k,1}}{\partial\xi_{k,3}} \\ \frac{\partial\Theta_{k,2}}{\partial\xi_{k,1}} & \frac{\partial\Theta_{k,2}}{\partial\xi_{k,2}} & \frac{\partial\Theta_{k,2}}{\partial\xi_{k,3}} \end{bmatrix}_{\xi=\zeta} &= -\begin{bmatrix} \frac{\partial\eta_{k,1}}{\partial\theta_{k,1}} & \frac{\partial\eta_{k,1}}{\partial\theta_{k,2}} \\ \frac{\partial\eta_{k,2}}{\partial\theta_{k,1}} & \frac{\partial\eta_{k,2}}{\partial\theta_{k,2}} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial\eta_{k,1}}{\partial\xi_{k,1}} & \frac{\partial\eta_{k,1}}{\partial\xi_{k,2}} & \frac{\partial\eta_{k,1}}{\partial\xi_{k,3}} \\ \frac{\partial\eta_{k,2}}{\partial\xi_{k,1}} & \frac{\partial\eta_{k,2}}{\partial\xi_{k,2}} & \frac{\partial\eta_{k,2}}{\partial\xi_{k,3}} \end{bmatrix} \\ &= \frac{O\left(\frac{1}{\rho}\right)}{\sin\theta_{k,2}}, \end{aligned} \tag{8.14}$$

we deduce that

$$\left(\frac{\partial\psi_k}{\partial\xi_{k,1}}, \frac{\partial\psi_k}{\partial\xi_{k,2}}, \frac{\partial\psi_k}{\partial\xi_{k,3}}\right)|_{\xi=\zeta} = 3r_k^2\theta_k + \frac{O(\rho^4)}{\sin\theta_{k,2}}(1,1,1). \tag{8.15}$$

The second case $l \neq k$ is similar, for which we omit the details of our computation. At $\xi = \zeta$, we have

$$\left(\frac{\partial\psi_l}{\partial\xi_{k,1}}, \frac{\partial\psi_l}{\partial\xi_{k,2}}, \frac{\partial\psi_l}{\partial\xi_{k,3}}\right)|_{\xi=\zeta} = \frac{O(\rho^4)}{\sin\theta_{l,2}}(1,1,1). \tag{8.16}$$

Following (8.15), (8.16), and the fact that $|\frac{\partial(\eta_{l,1},\eta_{l,2})}{\partial(\theta_{l,1},\theta_{l,2})}|_{\xi=\zeta} = 1 + O(\rho^2)$, we find that (8.8) becomes

$$\begin{aligned}
\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial \xi_{k,1}}|_{\xi=\zeta} &= \int_{S^2} \mathcal{S}_k(\varphi) \Bigg(3r_k^2 \cos\theta_{k,1} \sin\theta_{k,2} \\
&\qquad + \frac{O(\rho^4)}{\sin\theta_{k,2}} \Bigg) \, d\theta_k + \sum_{l\neq k} \int_{S^2} \mathcal{S}_l(\varphi) \frac{O(\rho^4)}{\sin\theta_{l,2}} \, d\theta_l, \\
\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial \xi_{k,2}}|_{\xi=\zeta} &= \int_{S^2} \mathcal{S}_k(\varphi) \Bigg(3r_k^2 \sin\theta_{k,1} \sin\theta_{k,2} \\
&\qquad + \frac{O(\rho^4)}{\sin\theta_{k,2}} \Bigg) \, d\theta_k + \sum_{l\neq k} \int_{S^2} \mathcal{S}_l(\varphi) \frac{O(\rho^4)}{\sin\theta_{l,2}} \, d\theta_l, \\
\frac{\partial J(E_{\psi(\cdot,\xi)})}{\partial \xi_{k,3}}|_{\xi=\zeta} &= \int_{S^2} \mathcal{S}_k(\varphi) \left(3r_k^2 \cos\theta_{k,2} + \frac{O(\rho^4)}{\sin\theta_{k,2}} \right) d\theta_k \\
&\qquad + \sum_{l\neq k} \int_{S^2} \mathcal{S}_l(\varphi) \frac{O(\rho^4)}{\sin\theta_{l,2}} \, d\theta_l.
\end{aligned}$$

Now we combine (7.1), (8.5), and the above to derive that at $\xi = \zeta$ and $r = s$,

$$\begin{aligned}
&A_{k,1} \int_{S^2} \cos\theta_{k,1} \sin\theta_{k,2} \left(3r_k^2 \cos\theta_{k,1} \sin\theta_{k,2} + \frac{O(\rho^4)}{\sin\theta_{k,2}} \right) d\theta_k + A_{k,2} O(\rho^4) \\
&\quad + A_{k,3} O(\rho^4) + \sum_{l\neq k} A_{l,1} O(\rho^4) + \sum_{l\neq k} A_{l,2} O(\rho^4) + \sum_{l\neq k} A_{l,3} O(\rho^4) = 0, \\
&A_{k,1} O(\rho^4) + A_{k,2} \int_{S^2} \sin\theta_{k,1} \sin\theta_{k,2} \left(3r_k^2 \sin\theta_{k,1} \sin\theta_{k,2} + \frac{O(\rho^4)}{\sin\theta_{k,2}} \right) d\theta_k \\
&\quad + A_{k,3} O(\rho^4) + \sum_{l\neq k} A_{l,1} O(\rho^4) + \sum_{l\neq k} A_{l,2} O(\rho^4) + \sum_{l\neq k} A_{l,3} O(\rho^4) = 0, \\
&A_{k,1} O(\rho^4) + A_{k,2} O(\rho^4) + A_{k,3} \int_{S^2} \cos\theta_{k,2} \left(3r_k^2 \cos\theta_{k,2} + \frac{O(\rho^4)}{\sin\theta_{k,2}} \right) d\theta_k \\
&\quad + \sum_{l\neq k} A_{l,1} O(\rho^4) + \sum_{l\neq k} A_{l,2} O(\rho^4) + \sum_{l\neq k} A_{l,3} O(\rho^4) = 0.
\end{aligned}$$

Writing the system in matrix form

$$\left(\begin{bmatrix} 4\pi r_1^2 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 4\pi r_1^2 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 4\pi r_1^2 & 0 & \dots & 0 & 0 \\ .. & & & & & & \\ .. & & & & & & \\ 0 & 0 & 0 & 0 & \dots & 4\pi r_K^2 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 4\pi r_K^2 \end{bmatrix} + O(\rho^4) \right) \begin{bmatrix} A_{1,1} \\ A_{1,2} \\ A_{1,3} \\ \dots \\ \dots \\ A_{K,2} \\ A_{K,3} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \dots \\ \dots \\ 0 \\ 0 \end{bmatrix} \tag{8.17}$$

we deduce, since (8.17) is nonsingular when ρ is small, that $A_{k,1} = A_{k,2} = A_{k,3} = 0$. ◻

The existence part of Theorem 2.1 follows from Lemma 8.4. The centers ζ_k and radii s_k of the spheres are found in Lemma 8.2. In Lemma 7.1 we see that

$\|\varphi\|_{W^{2,p}} \leq c\rho^5$, which implies that the radius of a sphere is approximately

$$(s_k^3 + \varphi_k(\theta_k))^{1/3} = s_k + \frac{O(|\varphi_k(\theta_k)|)}{\rho^2} = s_k + O(\rho^3). \tag{8.18}$$

By Lemma 8.2, ζ is close to a minimum of F and s_k is close to ρ. The formula in Lemma 8.1 gives the free energy of our solution.

In Theorem 2.2, a solution is termed stable if it is a local minimizer of J in the space

$$U \times \Bigg\{ \phi = (\phi_1, \dots, \phi_K) : \ |\rho^3 + \phi_k| \geq \frac{\rho^3}{2}, \ \phi_k \in W^{1,2}(S^2), \\ \phi_k \perp 1, \ \phi_k \perp H_1, \ k = 1, 2, \dots, K \Bigg\}. \tag{8.19}$$

The condition $|\rho^3 + \phi_k| \geq \frac{\rho^3}{2}$ ensures that J is well defined in this space. Under the condition (2.8), Lemma 7.2, part 2, shows that each $\varphi(\cdot, \xi, r)$ we found in Lemma 7.1 locally minimizes J, with fixed $(\xi, r) \in U$, in $\{\phi : \ |\rho^3 + \phi_k| \geq \frac{\rho^3}{2}, \ \phi_k \in W^{1,2}(S^2), \ \phi_k \perp 1, \ \phi_k \perp H_1\}$. On the other hand $\varphi(\cdot, \zeta, s)$ minimizes $J(E_{\varphi(\cdot,\xi,r)})$ with respect to ξ and r. Hence $\varphi(\cdot, \zeta, s)$ is a local minimizer of J in (8.19).

If (2.9) holds, then we can find one eigenvalue $\lambda_{k,n}$ of $\mathcal{L}_1$, Lemma 5.1, for some $n \in \{2, 3, \dots\}$ such that

$$\lambda_{k,n} < -\frac{C}{\rho^4}, \quad \langle \mathcal{L}_1(e_{k,n}), e_{k,n} \rangle < -\frac{C}{\rho^4} \|e_{k,n}\|^2_{W^{1,2}},$$

where $e_{k,n}$ is an eigenvector corresponding to $\lambda_{k,n}$. By Lemma 5.2, the last inequality implies that

$$\langle \mathcal{L}(e_{k,n}), e_{k,n} \rangle < -\frac{C}{\rho^4} \|e_{k,n}\|^2_{W^{1,2}}.$$

Then by Lemma 6.1, parts 2, 3, and 4, and (7.25) in the proof of Lemma 7.2,

$$\langle \tilde{\mathcal{L}}(e_{k,n}), e_{k,n} \rangle < -\frac{C}{\rho^4} \|e_{k,n}\|^2_{W^{1,2}}.$$

Therefore the solution is unstable.

9. Discussion.

The functional (1.2) is derived as a Γ-limit of the free energy functional in the Ohta–Kawasaki theory of diblock copolymers in [20]. Ohta and Kawasaki use 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

$$I(u) = \int_D \left[\frac{\varepsilon^2}{2} |Du|^2 + W(u) + \frac{\sigma}{2} |(-\Delta)^{-1/2}(u - a)|^2 \right] dx, \tag{9.1}$$

where u is in

$$\{u \in H^1(D) : \overline{u} = a\}. \tag{9.2}$$

The ε in (9.1) is not to be confused with the ϵ that has appeared in this paper. 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 (9.1): ε, σ, and a, where ε is small and a is in $(0, 1)$.

These three-dimensionless parameters are related to several physical parameters of a diblock copolymer system. See [29] for the precise relationships between the dimensionless parameters here and the physical parameters.

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

$$\sigma = \varepsilon\gamma \tag{9.3}$$

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

$$J(E) = \tau|D\chi_E|(D) + \frac{\gamma}{2}\int_D |(-\Delta)^{-1/2}(\chi_E - a)|^2\,dx \tag{9.4}$$

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

$$\tau = \int_0^1 \sqrt{2W(q)}\,dq. \tag{9.5}$$

The functional (9.4) is defined on the same admissible set Σ, (1.3). In this paper we have taken $\tau = 1$ without loss of generality.

The theory of Γ-convergence was developed by De Giorgi [7], Modica and Mortola [14], Modica [13], and Kohn and Sternberg [11]. It was proved that $\varepsilon^{-1}I$ Γ-converges to J in the following sense.

Proposition 9.1 (see Ren and Wei [20]).

1. *For every family* $\{u_\varepsilon\}$ *of functions in* (9.2) *satisfying* $\lim_{\varepsilon\to0} u_\varepsilon = \chi_E$ *in* $L^2(D)$*,*
$$\liminf_{\varepsilon\to0} \varepsilon^{-1}I(u_\varepsilon) \ge J(E).$$
2. *For every* E *in* Σ*, there exists a family* $\{u_\varepsilon\}$ *of functions in* (9.2) *such that* $\lim_{\varepsilon\to0} u_\varepsilon = \chi_E$ *in* $L^2(D)$*, and*
$$\limsup_{\varepsilon\to0} \varepsilon^{-1}I(u_\varepsilon) \le J(E).$$

The relationship between I and J becomes more clear when a result of Kohn and Sternberg [11] was used to show the following.

Proposition 9.2 (see Ren and Wei [20]). *Let* $\delta > 0$ *and* $E \in \Sigma$ *be such 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* $\varepsilon_0 > 0$ *such that for all* $\varepsilon < \varepsilon_0$ *there exists* $u_\varepsilon \in B_{\delta/2}(\chi_E)$ *with* $I(u_\varepsilon) \le I(u)$ *for all* $u \in B_{\delta/2}(\chi_E)$*. In addition* $\lim_{\varepsilon\to0} \|u_\varepsilon - \chi_E\|_{L^2(D)} = 0$.

The existence of a stable solution $E_{\varphi(\cdot,\zeta,s)}$ to (1.1) in the sense of Theorem 2.1 does not quite imply the existence of a local minimizer, close to $\chi_{E_{\varphi(\cdot,\zeta,s)}}$ in $L^2(D)$, of I. One must show that $E_{\varphi(\cdot,\zeta,s)}$ is a strict local minimizer in the sense of Proposition 9.2. This issue requires more study.

Our work is the first mathematically rigorous confirmation of the spherical phase of diblock copolymer morphology. This phase, depicted in Figure 1.1, plot 1, has been observed in experiments for some time [1]. Our earlier work [31, 30] in two dimensions gave a mathematical proof of the existence of the cylindrical phase of diblock copolymer morphology; see Figure 1.1, plot 2. The results obtained here are analogous to the ones obtained in [30], but there are some notable differences.

In two dimensions we studied a cross section of the cylindrical phase and constructed a stable solution which is a union of many small, approximate discs under the condition that

$$\frac{1+\epsilon}{\rho^3 \log \frac{1}{\rho}} < \gamma < \frac{12-4\epsilon}{\rho^3}. \tag{9.6}$$

Here ρ is the average disc radius defined by $\rho = \sqrt{\frac{a|D|}{K\pi}}$. Note that the two bounds for γ in (9.6) are of different orders. Recall that in three dimensions we have (2.12), i.e.,

$$\frac{3+\epsilon}{\rho^3} < \gamma < \frac{30-4\epsilon}{\rho^3}, \tag{9.7}$$

where the two bounds are of the same order. In experiments it is more likely to see the cylindrical phase than the spherical phase (see [1]). The different bounds in (9.6) and (9.7) appear to offer an explanation.

In (8.18) we have proved that the perturbed "radius" is

$$(s_k^3 + \varphi_k(\theta_k))^{1/3} = s_k + O(\rho^3). \tag{9.8}$$

In other words the deviation of the "radius" of a perturbed ball from an exact ball is of the order $O(\rho^3)$. However, in two dimensions the corresponding quantity is

$$(s_k^2 + \varphi_k(\theta_k))^{1/2} = s_k + O(\rho^2), \tag{9.9}$$

a fact found after the proof of [30, Theorem 2.1]. The approximate balls in the spherical solution found here are more round than the approximate discs in the cylindrical solution found in [30].

Appendix A. We drop the subscript k in this appendix. The derivative of $\mathcal{A}$ at 0 has two terms according to (4.29). The first is

$$\frac{\gamma}{9r_k} \int_{S^2} \frac{u(\omega)}{4\pi|\theta-\omega|}\, d\omega.$$

The second is

$$-\frac{\gamma u(\theta)}{9r_k} \int_{B_1(0)} \frac{(\theta-y)\cdot\theta}{4\pi|\theta-y|^2}\, dy$$

for which we calculate the integral. Here $B_1(0)$ is the unit ball. This integral is independent of $\theta \in S^2$ so without loss of generality we assume that $\theta = (0,0,1)$. Write $y = (r\cos p, r\sin p, y_3)$ in the cylindrical coordinates. Then the integral becomes

$$\int_{B_1(0)} \frac{(\theta-y)\cdot\theta}{4\pi|\theta-y|^2}\, dy = \frac{1}{4\pi}\int_{-1}^{1}\int_0^{2\pi}\int_0^{\sqrt{1-y_3^2}} \frac{(1-y_3)r\, dr\, dp\, dy_3}{[(1-y_3)^2+r^2]^{3/2}} = \frac{1}{3}.$$

Appendix B. The integral operator

$$h(\theta) \to \int_{S^2} \frac{h(\omega)\, d\omega}{|\theta-\omega|} \tag{B.1}$$

acts on spherical harmonics $h \in H_n$ in a simple way. Here H_n is the space of spherical harmonics of degree n on S^2. In general one has

$$\int_{S^2} \Phi(\theta \cdot \omega) h(\omega)\, d\omega = \alpha_n(\Phi) h(\theta), \tag{B.2}$$

where

$$\alpha_n(\Phi) = 2\pi \int_{-1}^{1} \Phi(t) P_n(t)\, dt. \tag{B.3}$$

See, for instance, [10, Theorem 3.4.1]. Here P_n is the nth Legendre polynomial. In our case

$$\frac{1}{|\theta - \omega|} = \frac{1}{\sqrt{2 - 2\theta \cdot \omega}},$$

so we take

$$\Phi(t) = \frac{1}{\sqrt{2 - 2t}}. \tag{B.4}$$

The classical representation of Legendre polynomials in terms of generating functions [10, Formula 3.3.39]

$$\frac{1}{(1 + r^2 - 2rt)^{1/2}} = \sum_{n=0}^{\infty} P_n(t) r^n, \quad r, t \in (-1, 1) \tag{B.5}$$

shows that

$$\int_{-1}^{1} \frac{P_n(t)\, dt}{(1 + r^2 - 2rt)^{1/2}} = r^n \int_{-1}^{1} P_n^2(t)\, dt = \frac{2r^n}{2n+1},$$

where the orthogonality of the Legendre polynomials is used [10, Formula 3.3.16]:

$$\int_{-1}^{1} P_n(t) P_m(t)\, dt = \frac{2\delta_{nm}}{2n+1}.$$

By sending $r \to 1$ we find that

$$\alpha_n(\Phi) = \frac{4\pi}{2n+1}. \tag{B.6}$$

Appendix C. Here we calculate the improper integral

$$\int_{B_1(0)} \frac{|\theta - y|^2 - 3(1 - \theta \cdot y)^2}{|\theta - y|^5}\, dy, \tag{C.1}$$

where $B_1(0)$ is the unit ball centered at 0. This integral is independent of $\theta \in S^2$. We take $\theta = (0, 0, 1)$. Let $z = (0, 0, 1) - y$ and set $z = (r \cos p, r \sin p, z_3)$ in cylindrical coordinates. Then

$$\begin{aligned}
&\int_{B_1(0)} \frac{|\theta - y|^2 - 3(1 - \theta \cdot y)^2}{|\theta - y|^5}\, dy \\
&\quad = \int_{B_1(0,0,1)} \frac{|z|^2 - 3z_3^2}{|z|^5}\, dz \\
&\quad = \int_0^2 \int_0^{\sqrt{1-(1-z_3)^2}} \int_0^{2\pi} \frac{(r^2 + z_3^2) - 3z_3^2}{(r^2 + z_3^2)^{5/2}} r\, dp dr dz_3 \;=\; -\frac{8\pi}{3}.
\end{aligned}$$

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