The Diblock Copolymer Problem with Skewed Monomer Composition

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1 Introduction

A diblock copolymer molecule is a linear sub-chain of N_A A-monomers grafted covalently to another sub-chain of N_B B-monomers. Because of the repulsion between the unlike monomers, the different type sub-chains tend to segregate, but as they are chemically bonded in chain molecules, segregation of sub-chains cannot lead to a macroscopic phase separation. Only a local micro-phase separation occurs: micro-domains rich in A and B emerge. These micro-domains form morphology patterns/phases in a larger scale.

The Ohta-Kawasaki [13] free energy of an incompressible diblock copolymer melt is a functional of the A monomer density field. Let $u(x)$ be the relative A monomer number density at point x in the sample. When there is high A monomer concentration at x, $u(x)$ is close to 1; when there is high concentration of B monomers at x, $u(x)$ is close to 0. A value of $u(x)$ between 0 and 1 means that a mixture of A and B monomers occupies x. In one-dimension the re-scaled, dimensionless free energy of the system is

$$I(u) = \int_0^1 [\frac{\epsilon^2}{2}|u'|^2 + W(u) + \frac{\sigma}{2}|(-\Delta)^{-1/2}(u-a)|^2]\,dx \tag{1.1}$$

The functional I is defined in the admissible set

$$\mathcal{A} = \{u \in W^{1,2}(0,1) : \overline{u} = a\} \tag{1.2}$$

where $\overline{u} = \int_0^1 u\,dx$ is the average of u.

The term $W(u)$ is the internal energy field. We take it to be a smooth double well potential of equal depth. It has global minimum value 0 achieved at 0 and 1. We assume for simplicity that W is smooth, grows at least quadratically at $\pm\infty$, and symmetric about 1/2: $W(u) = W(1-u)$. 0 and 1 are non-degenerate: $W''(0) = W''(1) > 0$. An example of W is $W(u) = \frac{1}{4}(u^2-u)^2$.

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The other two terms in (1.1) give the entropy of the system. The peculiar nonlocal term is due to the fact that molecules in a diblock copolymer are connected long chains. It models a type of nonlocal interaction known as the Coulomb interaction. Mathematically we view $(-\Delta)^{-1}$ as a bounded positive operator from $\{\zeta \in L^2(0,1) : \overline{\zeta} = 0\}$ to $\{\xi \in W^{2,2}(0,1) : \overline{\xi} = 0,\ \xi'(0) = \xi'(1) = 0\}$: $\xi = (-\Delta)^{-1}\zeta$ if

$$-\xi'' = \zeta \text{ in } (0,1),\ \xi'(0) = \xi'(1) = 0,\ \ \overline{\xi} = 0.$$

Then $(-\Delta)^{-1/2}$ is the positive square root of $(-\Delta)^{-1}$.

Three positive parameters ϵ, σ and a appear in (1.1). ϵ is always a small parameter, and σ is proportional to the size of the sample. In earlier works a has been taken to be a fixed constant, independent of ϵ, in $(0,1)$. Then one may choose σ to be of order ϵ and apply the Γ-limit theory (De Giorgi [4], Modica [9], and Kohn and Sternberg [8]). This was the approach used in Ren and Wei [14]. In terms of N_A and N_B

$$a = \frac{N_A}{N_A + N_B}. \tag{1.3}$$

N_A and N_B are both large integers. The condition that $a \in (0,1)$ is independent of ϵ means that $N_A \sim N_B$.

In this paper we consider a case when N_A and N_B are large but not comparable. Namely we assume a skewed relationship

$$N_A \sim \sqrt{N_B}. \tag{1.4}$$

Hence N_A is a lot smaller than N_B. The condition (1.4) turns out to be equivalent (cf. Choksi and Ren [3]) to

$$a \sim \epsilon^{1/2},\ \sigma \sim 1 \tag{1.5}$$

Therefore we take the positive a to be

$$a = \epsilon^{1/2} a_0, \text{ where } \ a_0 > 0 \text{ is independent of } \epsilon. \tag{1.6}$$

In addition to its physical relevance, the condition (1.5) generates some interesting mathematical questions. Define a nonlinear operator

$$S(u) = -\epsilon^2 u'' + f(u) - \overline{f(u)} + \sigma(-\Delta)^{-1}(u - a) \tag{1.7}$$

where $f = W'$, from

$$\mathcal{X} = \{u \in W^{2,2}(0,0) : \overline{u} = a,\ u'(0) = u'(1) = 0,\} \tag{1.8}$$

to

$$\mathcal{Y} = \{z \in L^2(0,1) : \overline{z} = 0\} \tag{1.9}$$

The Euler-Lagrange equation of I is

$$S(u) = 0,\ u \in \mathcal{X}. \tag{1.10}$$

The standard Γ-limit approach used in [14] to solve (1.10) is to identify a limiting functional of I. The Γ-limit theory asserts that if one can find an isolated local minimizer of the limiting functional, then for small ϵ, I also has a local minimizer nearby. To identify the limiting functional in [14], the value a must be ϵ-independent. The parameter range (1.6) can not be dealt with by the straightforward Γ-limit argument. Instead we will use a Lyapunov-Schmidt reduction approach. The latter method is more complex because one must understand some properties of the linearization of S at some carefully constructed approximate solutions.

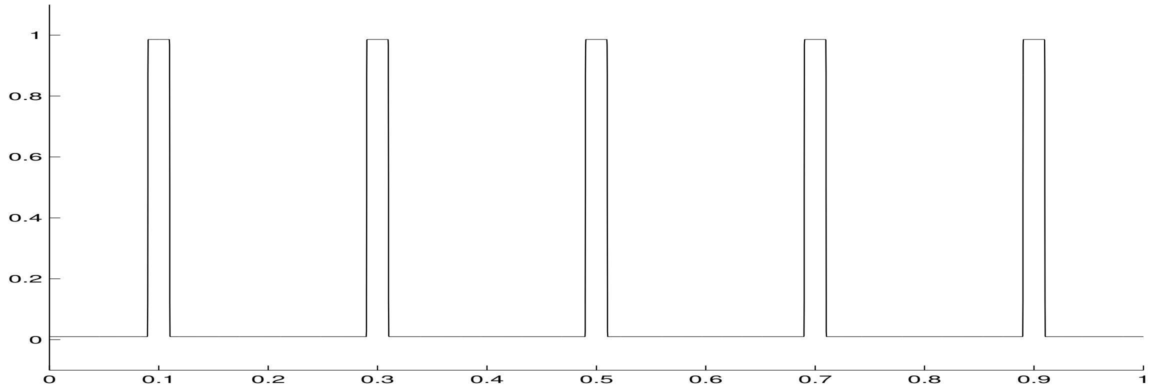

Figure 1: A solution with 5 droplets

The solutions of (1.10) we are interested will model the lamellar phase of a diblock copolymer. They must be non-constant local minimizers of I. Because of the skewed value (1.6), we want a solution to be close to 0 everywhere except near a finite points where the solution is close to 1 (Figure 1). We call the small regions where the solution is close to 1 droplets, and call the solution a droplet solution.

The parameter range (1.6) may also be an important threshold. The energy of a droplet solution will turn out to be of order ϵ. It is of the same order as the energy of the constant solution $u = a$. If we consider a parameter range where $a \ll \epsilon^{1/2}$, then the energy of the constant solution will be of lower order. Then it is doubtful that the Ohta-Kawasaki model will allow any non-constant morphology.

Finally we wish to gain some crucial ideas before we study the 2 and 3 dimensional versions of the skewed monomer composition cases. There one finds the more interesting cylindrical and spherical morphology phases (cf. Bates and Fredrickson [1]).

The main result of this paper is the following theorem.

Theorem 1.1 *For each positive integer N there exists a local minimizer of I with N small droplets when ϵ is sufficiently small. The free energy of the local minimizer is*

$$\epsilon(2N\tau + f'(0)a_0^2(\frac{1}{2} - \frac{\coth\beta - \operatorname{csch}\beta}{\beta})) + o(\epsilon)$$

where $\tau = \int_0^1 \sqrt{2W(z)}\,dz,\ \beta = \dfrac{\sqrt{\sigma}}{N\sqrt{f'(0)}}.$

In our Lyapunov-Schmidt reduction approach to prove Theorem 1.1, we construct a manifold $\mathcal{M}$ of approximate solutions w_ξ parameterized by a $2N$-vector ξ, together with a fiber $w_\xi + \mathcal{F}_\xi$ at each w_ξ (Section 2). The manifold $\mathcal{M}$ and its fibers $\xi + \mathcal{F}_\xi$ form a local decomposition of $\mathcal{X}$. In Section 3 we find ϕ_ξ so that $w_\xi + \phi_\xi$ solves (1.10) in the fiber direction. In Section 4 we prove that $w_\xi + \phi_\xi$ locally minimizes I in a similar fiber $w_\xi + \mathcal{P}_\xi$. Finally in Section 5 we find a particular ξ so that at this ξ, $w_\xi + \phi_\xi$ solves (1.10) in $\mathcal{X}$ and it is a local minimizer of I.

The mathematical literature on the diblock copolymer problem includes Nishiura and Ohnishi [11], Ohnishi *et al* [12], Ren and Wei [16, 15, 19, 17, 22, 21], Choksi [2], Fife and Hilhorst [5], Henry [7], and Teramoto and Nishiura [23]. More information on the model (1.1) and its extension to triblock copolymers may be found in Nakazawa and Ohta [10], and Ren and Wei [18].

In the notations of this paper, a quantity's dependence on ϵ is not emphasized. For example we write I instead of I_ϵ and S instead of S_ϵ. However whenever a quantity is independent of ϵ, we point out the fact. The L^∞ norm will simply be denoted by $\|\cdot\|$, and the $L^2(0,1)$ norm denoted by $\|\cdot\|_2$. The $L^2(0,1)$ inner product is denoted by $\langle\cdot,\cdot\rangle$. All projection operations used in the paper are derived from this inner product. Constants like C, C_1, C_2,..., are all independent of ϵ. They may vary from place to place.

2 The approximate manifold and its fibers

Let $\xi_1, \xi_2, ..., \xi_{2N}$ be $2N$ numbers in $(0,1)$, satisfying $\xi_1 < \xi_2 < ... < \xi_{2N}$. Given $\xi = (\xi_1, \xi_2, ..., \xi_{2N})$ we will build an approximate solution whose droplets interfaces are at ξ_j. The centers of the droplets are at ζ_k:

$$\zeta_k = \frac{\xi_{2k-1} + \xi_{2k}}{2}, \ k = 1, 2, ..., N \tag{2.1}$$

and the half widths, scaled by $\epsilon^{1/2}$, of the droplets are l_k:

$$l_k = \frac{\xi_{2k} - \xi_{2k-1}}{2\epsilon^{1/2}}, \ k = 1, 2, ..., N \tag{2.2}$$

We can express ξ in terms of $\zeta = (\zeta_1, \zeta_2, ..., \zeta_N)$ and $l = (l_1, l_2, ..., l_N)$:

$$\xi_{2k} = \zeta_k + \epsilon^{1/2} l_k, \ \xi_{2k-1} = \zeta_k - \epsilon^{1/2} l_k, \ k = 1, 2, ..., N. \tag{2.3}$$

The exact set $\Lambda \subset \mathbf{R}^{2N}$ in which ξ varies is

$$\Lambda = \{\xi \in \mathbf{R}^{2N} : \zeta_1 > \delta, \ \zeta_2 - \zeta_1 > \delta, \ \zeta_3 - \zeta_2 > \delta, \ ..., \ \zeta_N - \zeta_{N-1} > \delta, \ 1 - \zeta_N > \delta,$$
$$\frac{1}{\delta} > l_k > \delta, \ k = 1, 2, ..., N\} \tag{2.4}$$

where ξ is related to (ζ, l) via (2.3). In (2.4) δ is a positive constant independent of ϵ. It is small enough so that a particular (ζ^0, l^0) defined in Lemma 5.2, Section 5, satisfies the inequalities in (2.4).

We construct a manifold of approximate solutions parameterized by $\xi \in \Lambda$. First define

$$s_\xi(x) = 0 \text{ in } (0, \xi_1), \ 1 \text{ in } (\xi_1, \xi_2), \ 0 \text{ in } (\xi_2, \xi_3), \ \dots, 1 \text{ in } (\xi_{2N-1}, \xi_{2N}), \ 0 \text{ in } (\xi_{2N}, 1) \tag{2.5}$$

which gives a profile away from the interfaces. The interface profile is the solution H of the differential equation

$$-H'' + f(H) = 0, \ H(-\infty) = 0, \ H(\infty) = 1, \ H(0) = \frac{1}{2}. \tag{2.6}$$

Near ξ_j we use $H((x - \xi_j)/\epsilon)$ if j is odd, or $H(-(x - \xi_j)/\epsilon)$ if j is even. Then s_ξ and H must be connected by a smooth cut-off function χ

$$w_{\xi,1}(x) = \sum_{j=1}^{2N} \chi(x - \xi_j) H((-1)^{j+1} \frac{x - \xi_j}{\epsilon}) + (1 - \sum_{j=1}^{2N} \chi(x - \xi_j)) s_\xi(x). \tag{2.7}$$

where χ is defined to be

$$\chi(x)=\begin{cases} 1 & \text{in} \quad (-\epsilon^{\alpha},\epsilon^{\alpha}) \\ 0 & \text{in} \quad \mathbf{R}\backslash(-2\epsilon^{\alpha},2\epsilon^{\alpha}) \end{cases}. \tag{2.8}$$

The exponent α in (2.8) satisfies

$$\frac{1}{2}<\alpha<1. \tag{2.9}$$

χ satisfies

$$\chi=O(1),\ \chi'=O(\epsilon^{-\alpha}),\ \chi''=O(\epsilon^{-2\alpha}) \tag{2.10}$$

It turns out that $w_{\xi,1}$ is not accurate enough to be an approximate solution. A correction to $w_{\xi,1}$ is needed. Let $w_{\xi,2}$ be the solution of

$$f'(0)w_{\xi,2}+\sigma(-\Delta)^{-1}(w_{\xi,1}+w_{\xi,2}-a)=f'(0)\overline{w_{\xi,2}},\ \overline{w_{\xi,1}+w_{\xi,2}-a}=0 \tag{2.11}$$

which may be written as

$$-Dw''_{\xi,2}+w_{\xi,2}+w_{\xi,1}-a=0,\ w'_{\xi,2}(0)=w'_{\xi,2}(1)=0 \tag{2.12}$$

Here

$$D=\frac{f'(0)}{\sigma}. \tag{2.13}$$

$w_{\xi,2}$ is easily estimated. We denote the Green function of the last differential equation by G_D, i.e.

$$-D\frac{G^2(x,y)}{\partial x^2}+G(x,y)=\delta(x-y),\quad \frac{\partial G(0,y)}{\partial x}=\frac{\partial G(1,y)}{\partial x}=0. \tag{2.14}$$

Lemma 2.1

$$w_{\xi,2}(x)=\epsilon^{1/2}(a_0-\sum_{j=1}^{N}2l_jG_D(x,\zeta_j))+O(\epsilon).$$

In particular $w_{\xi,2}=O(\epsilon^{1/2})$.

Proof. Note that $\epsilon^{-1/2}w_{\xi,1}$ approaches $\sum_{j=1}^{K}2l_j\delta(\cdot-\zeta_j)$ in the sense of distributions, as $\epsilon\to 0$. The lemma then follows easily. □

Now we set an approximate solution

$$w_{\xi}=w_{\xi,1}+w_{\xi,2}\in\mathcal{X}. \tag{2.15}$$

As ξ varies in Λ w_ξ forms a $2N$-dimensional manifold which we denote by $\mathcal{M}$ embedded in $\mathcal{X}$:

$$\mathcal{M}=\{w_\xi\in\mathcal{X}:\xi\in\Lambda\} \tag{2.16}$$

The next lemma shows how accurate w_ξ is.

Lemma 2.2 $S(w_\xi)=(f'(w_{\xi,1})-f'(0))w_{\xi,2}+O(\epsilon)$.

Proof. First note that

$$\begin{aligned}
\overline{f(w_\xi)} &= \int_0^1 f(w_{\xi,1})\,dx + \int_0^1 f'(w_{\xi,1})w_{\xi,2}\,dx + O(\epsilon) \\
&= \int_0^1 f'(w_{\xi,1})w_{\xi,2}\,dx + O(\epsilon) \\
&= f'(0)\overline{w_{\xi,2}} + \int_0^1 [f'(w_{\xi,1}) - f'(0)]w_{\xi,2}\,dx + O(\epsilon) \\
&= f'(0)\overline{w_{\xi,2}} + O(\epsilon)
\end{aligned} \tag{2.17}$$

Then using (2.11) we find

$$\begin{aligned}
S(w_\xi) &= -\epsilon^2 w_\xi'' + f(w_\xi) + \sigma(-\Delta)^{-1}(w_\xi - a) - f'(0)\overline{w_{\xi,2}} + O(\epsilon) \\
&= -\epsilon^2 w_\xi'' + f(w_\xi) - f'(0)w_{\xi,2} + O(\epsilon) \\
&= -\epsilon^2 (w_{\xi,1})'' - \epsilon^2 (w_{\xi,2})'' + f(w_{\xi,1}) + f'(w_{\xi,1})w_{\xi,2} - f'(0)w_{\xi,2} + O(\epsilon) \\
&= (-\epsilon^2 (w_{\xi,1})'' + f(w_{\xi,1})) + (f'(w_{\xi,1}) - f'(0))w_{\xi,2} + O(\epsilon) \\
&= (f'(w_{\xi,1}) - f'(0))w_{\xi,2} + O(\epsilon)
\end{aligned}$$

This proves the lemma. □

Corollary 2.3 $S(w_\xi) = O(\epsilon^{1/2})$.

Proof. It follows from Lemmas 2.1 and 2.2. □

Note that Lemma 2.2 is a stronger statement than Corollary 2.3. Lemma 2.2 implies that $S(w_\xi)$ is $O(\epsilon^{1/2})$ in ϵ size neighborhoods of ξ_j. Elsewhere $S(w_\xi)$ is $O(\epsilon)$.

For each $j = 1, 2, ..., 2N$, let us define

$$h_j(x) = H'(\frac{x - x_j}{\epsilon})\kappa(\frac{x - x_j}{\sqrt{\epsilon}}) - \overline{H'(\frac{x - x_j}{\epsilon})\kappa(\frac{x - x_j}{\sqrt{\epsilon}})} = H'(\frac{x - x_j}{\epsilon}) - \epsilon + O(e^{-C/\epsilon}). \tag{2.18}$$

where κ is a smooth, even cut-off function

$$\kappa(s) = \left\{ \begin{array}{ll} 1 & \text{if } |s| \le 1 \\ 0 & \text{if } |s| \ge 2 \end{array} \right. .$$

Here $O(e^{-C/\epsilon})$ is an exponentially small quantity with respect to ϵ because of the exponentially fast decay rate of H': $H'(t) \le C_1 e^{-C_2|t|}$. Therefore $h_j'(0) = h_j'(1) = 0$, $\|h_j' - \epsilon^{-1}H''(\frac{\cdot - x_j}{\epsilon})\|_\infty = O(\epsilon^{-C/\epsilon})$, and $\|h_j'' - \epsilon^{-2}H'''(\frac{\cdot - x_j}{\epsilon})\|_\infty = O(\epsilon^{-C/\epsilon})$.

At each w_ξ of the manifold we define the space

$$\mathcal{F}_\xi = \{\phi \in W^{2,2}(0,1) : \ \overline{\phi} = 0, \ \phi'(0) = \phi'(1) = 0, \ \ \phi \perp h_j, \ j = 1, 2, ..., 2N\} \tag{2.19}$$

where $\perp$ is defined from the $L^2(0,1)$ inner product. Then $w_\xi + \mathcal{E}_\xi$ is a subset of $\mathcal{X}$, which we call the ξ-fiber of $\mathcal{M}$ in $\mathcal{X}$. Define $\mathcal{E}_\xi$ to be the subspace

$$\mathcal{E}_\xi = \{q \in L^2(0,1) : \overline{q} = 0, \ q \perp h_j, \ j = 1, 2, ..., 2N\} \tag{2.20}$$

of $\mathcal{Y}$. Let the projection to $\mathcal{E}_\xi$ be π_ξ

$$\pi_\xi : \mathcal{Y} \to \mathcal{E}_\xi \tag{2.21}$$

3 Solvability in fibers

At each w_ξ we look for a $\phi_\xi \in \mathcal{F}_\xi$ so that

$$\pi_\xi \circ S(w_\xi + \phi_\xi) = 0 \tag{3.1}$$

For each $\phi \in \mathcal{F}_\xi$ we expand

$$S(w_\xi + \phi) = S(w_\xi) + L_\xi(\phi) + R_\xi(\phi) \tag{3.2}$$

where

$$L_\xi(\phi) = -\epsilon^2 \phi'' + f'(w_\xi)\phi - \overline{f'(w_\xi)\phi} + \sigma(-\Delta)^{-1}\phi \tag{3.3}$$

is the linearization of S at w_ξ, and

$$R_\xi(\phi) = f(w_\xi + \phi) - f(w_\xi) - f'(w_\xi)\phi - \overline{f(w_\xi + \phi) - f(w_\xi) - f'(w_\xi)\phi} \tag{3.4}$$

Then (3.1) is written as

$$\pi_\xi \circ S(w_\xi) + \pi_\xi \circ L_\xi(\phi_\xi) + \pi_\xi \circ R_\xi(\phi_\xi) = 0 \tag{3.5}$$

Regarding the the linear operator $\pi_\xi \circ L_\xi$:

$$\pi_\xi \circ L_\xi : \mathcal{F}_\xi \to \mathcal{E}_\xi$$

we have the following lemma.

Lemma 3.1 *1. There exists $C_1 > 0$ independent of ϵ such that $\|\phi\| \le C_1 \|\pi_\xi \circ L_\xi(\phi)\|$ for all $\phi \in \mathcal{F}_\xi$. In particular $\pi_\xi \circ L_\xi$ is one-to-one from $\mathcal{F}_\xi$ to $\mathcal{E}_\xi$.*

2. $\pi_\xi \circ L_\xi$ is onto from $\mathcal{F}_\xi$ to $\mathcal{E}_\xi$.

Proof. To prove part 1 we argument by contradiction. Suppose the conclusion is false. Then there exists $\psi \in \mathcal{F}_\xi$ for each ϵ such that $\|\psi\| = 1$ and along a subsequence of $\epsilon \to 0$,

$$\|\pi_\xi \circ L_\xi(\psi)\| \to 0. \tag{3.6}$$

Write (3.6) as

$$-\epsilon^2 \psi'' + f'(w_\xi)\psi - \overline{f'(w_\xi)\psi} + \sigma(-\Delta)^{-1}\psi - \sum_{j=1}^{2N} \beta_j h_j = o(1) \tag{3.7}$$

for some $\beta_j \in \mathbf{R}$. We multiply the last equation by ψ and integrate. Denoting $\varphi = (-\Delta)^{-1}\psi$, we deduce

$$\int_0^1 [\epsilon^2 |\psi'|^2 + f'(w_\xi)\psi^2 + \sigma|\varphi'|^2]\, dx = o(1).$$

Since $f'(w_\xi)$ may only be negative in ϵ-size neighborhoods of ξ_j, the last equation implies

$$\int_0^1 |\varphi'|^2\, dx = o(1).$$

The Sobolev imbedding theory yields

$$\|\varphi\| = o(1) \tag{3.8}$$

We must estimate the size of β_j. To this end we multiply (3.7) by h_k and integrate. Then

$$\int_0^1 [(-\epsilon^2\psi'' + f'(w_\xi)\psi + \sigma\varphi)h_k]\,dx + \sum_{j=1}^{2N} \beta_j \langle h_j, h_k\rangle = o(\epsilon)$$

Simple calculations simplify the second part on the left side, so

$$\int_0^1 (-\epsilon^2\psi'' + f'(w_\xi) + \sigma\varphi)h_k\,dx + \sum_{j=1}^{2N} \beta_j(\epsilon\tau\delta_{jk} + O(\epsilon^2)) = o(\epsilon) \tag{3.9}$$

where we have used another way to describe τ:

$$\tau = \int_{\mathbf{R}} (H')^2\,dt. \tag{3.10}$$

The first part of the left side is estimated as follows:

$$\begin{aligned}
&\int_0^1 [(-\epsilon^2\psi'' + f'(w_\xi)\psi + \sigma\varphi)(H'(\frac{x-\xi_k}{\epsilon}) - \overline{H'(\frac{x-\xi_k}{\epsilon})})]\,dx \\
= &\int_0^1 [-\psi f'(w_\xi)\overline{H'(\frac{x-\xi_k}{\epsilon})} + \sigma\varphi(H'(\frac{x-\xi_k}{\epsilon}) - \overline{H'(\frac{x-\xi_k}{\epsilon})})]\,dx \;=\; O(\epsilon)
\end{aligned}$$

This simplifies (3.9) to

$$\sum_{j=1}^{2N} \beta_j(\epsilon\tau\delta_{jk} + O(\epsilon^2)) = O(\epsilon).$$

Hence

$$\beta_j = O(1). \tag{3.11}$$

Let $y \in [0,1]$ such that, without the loss of generality, $\psi(y) = \|\psi\| = 1$. We claim that $y - \xi_j = O(\epsilon)$ for some j. Otherwise, at y, because of (3.8),

$$\begin{aligned}
L_\xi(\psi)(y) &= -\epsilon^2\psi''(y) + f'(w_\xi(y))\psi(y) - \overline{f'(w_\xi)\psi} + \sigma((-\Delta)^{-1}\psi)(y) \\
&\geq 0 + f'(w_\xi(y)) - \overline{(f'(w_\xi) - f'(0))\psi} + \sigma((-\Delta)^{-1}\psi)(y) \\
&= f'(w_\xi(y)) + \sigma\varphi(y) + O(\epsilon) \;=\; f'(w_\xi(y)) + o(1) \\
&= f'(0) + o(1)
\end{aligned} \tag{3.12}$$

Combining (3.11) and (3.12), we obtain

$$\pi_\xi \circ L_\xi(\psi)(y) \geq f'(0) - \sum_{j=1}^{2N} \beta_j h_j(y) + o(1) \geq f'(0) + o(1)$$

which contradicts (3.6).

We have thus proved that $y - \xi_j = O(\epsilon)$ for some j, along a subsequence of $\epsilon \to 0$. Define $\Psi(t) = \psi(\xi_j + \epsilon t)$. Then (3.7), (3.8), and (3.11) imply

$$-\Psi'' + f'(w_\xi(\xi_j + \epsilon t))\Psi - \beta_j H' \to 0$$

uniformly on any compact subset of $\mathbf{R}$. From here we may pass the limit and find Ψ_∞ and β_j^0 so that $\Psi \to \Psi_\infty$ in $C^2_{loc}(\mathbf{R})$ and $\beta_j \to \beta_j^0$. Moreover $\Psi_\infty \neq 0$ since $\Psi((y - \xi_j)/\epsilon) = 1$, and

$$-\Psi''_\infty + f'(H)\Psi_\infty - \beta_j^0 H' = 0.$$

If we multiply the last equation by H' and integrate over $\mathbf{R}$, we find $\beta_j^0 = 0$. Then Ψ_∞ satisfies

$$-\Psi''_\infty + f'(H)\Psi_\infty = 0.$$

The bounded solutions of this equation are scalar multiples of H'. Hence $\Psi_\infty = cH'$ for some $c \neq 0$.
On the other hand, sine $\psi \in \mathcal{F}_\xi$ means that $\psi \perp h_j$ and $\overline{\psi} = 0$, so we deduce that

$$0 = \langle \psi, h_j \rangle = \epsilon \int_{-\xi_j/\epsilon}^{(1-\xi_j)/\epsilon} \Psi(t)(H'(t) - O(e^{-C/\epsilon}))\, dt = \epsilon(c \int_{\mathbf{R}} (H'(t))^2\, dt + o(1))$$

which is impossible. We have thus proved part 1 of the lemma.
To prove part 2 of the lemma we need to solve

$$\pi_\xi \circ L_\xi(\phi) = p \tag{3.13}$$

in $\mathcal{F}_\xi$ for any given $p \in \mathcal{E}_\xi$. By applying $\pi_\xi \circ (-\Delta)^{-1}$ to both sides of (3.13) we consider the equation

$$\pi_\xi \circ (-\Delta)^{-1} \circ \pi_\xi \circ L_\xi(\phi) = \pi_\xi \circ (-\Delta)^{-1} p \tag{3.14}$$

The linear operator $\pi_\xi \circ (-\Delta)^{-1} \circ \pi_\xi \circ L_\xi$ on the left side maps from $\mathcal{F}_\xi$ to itself and has the form

$$\epsilon^2(\text{Identity Operator}) + \text{Compact Operator}. \tag{3.15}$$

According to the Fredholm Alternative, (3.14) is solvable if

$$\pi_\xi \circ (-\Delta)^{-1} \circ \pi_\xi \circ L_\xi(\phi) = 0 \tag{3.16}$$

only has the trivial solution. To see this we write (3.16) as

$$(-\Delta)^{-1} \circ \pi_\xi \circ L_\xi(\phi) = \sum_{j=1}^{2N} \alpha_j h_j$$

for some $\alpha_j \in \mathbf{R}$. Apply $-\Delta$ to the last equation to find

$$\pi_\xi \circ L_\xi(\phi) = \sum_{j=1}^{2N} \alpha_j(-h''_j). \tag{3.17}$$

We multiply it by h_k and integrate to deduce

$$0=\sum_{j=1}^{2N}\alpha_j\int_0^1 h_j'h_k'\,dx=\sum_{j=1}^{2N}\alpha_j\epsilon(\tau\delta_{jk}+O(\epsilon)),\ \ k=1,2,...,2N,$$

which implies that $\alpha_j=0$, $j=1,2,...,2N$. Then (3.17) becomes

$$\pi_\xi\circ L_\xi(\phi)=0.$$

The first part of the lemma implies that $\phi=0$.

Hence (3.14) is solvable, i.e. for any $p\in\mathcal{E}_\xi$ there exist $\phi\in\mathcal{F}_\xi$ and $\beta_j\in\mathbf{R}$ such that

$$(-\Delta)^{-1}\circ\pi_\xi\circ L_\xi(\phi)=(-\Delta)^{-1}p+\sum_{j=1}^{2N}\beta_j h_j.$$

Apply $-\Delta$ to the last equation to deduce

$$\pi_\xi\circ L_\xi(\phi)=p+\sum_{j=1}^{2N}\beta_j(-h_j''). \tag{3.18}$$

We multiply by h_k and integrate to obtain

$$0=\sum_{j=1}^{2N}\beta_j\int_0^1 h_j'h_k'\,dx=\sum_{j=1}^{2N}\beta_j\epsilon(\tau\delta_{jk}+O(\epsilon)),\ \ k=1,2,...,2N,$$

which implies that $\beta_j=0$, for all $j=1,2,...,2N$. Then (3.18) becomes (3.13). $\square$

We are now ready to solve (3.1).

Lemma 3.2 *There exists $\phi_\xi\in\mathcal{F}_\xi$ with $\|\phi_\xi\|=O(\epsilon^{1/2})$ so that $\pi_\xi\circ S(w_\xi+\phi_\xi)=0$.*

Proof. We write (3.5) in a fixed point form:

$$\phi_\xi=(\pi_\xi\circ L_\xi)^{-1}(-\pi_\xi\circ S(w_\xi)-\pi_\xi\circ R_\xi(\phi_\xi)) \tag{3.19}$$

We define the operator T_ξ from $\mathcal{D}(T_\xi)$ to itself

$$T_\xi(\phi)=(\pi_\xi\circ L_\xi)^{-1}(-\pi_\xi\circ S(w_\xi)-\pi_\xi\circ R_\xi(\phi)) \tag{3.20}$$

where the domain $\mathcal{D}(T_\xi)$ of T_ξ is

$$\mathcal{D}(T_\xi)=\{\phi\in L^\infty(0,1):\overline{\phi}=0,\ \phi\perp h_j,\ j=1,2,...,2N\} \tag{3.21}$$

Let $\mathcal{B}_\xi$ be a closed ball in $\mathcal{D}(T_\xi)$ defined by

$$\mathcal{B}_\xi=\{\phi\in\mathcal{D}(T_\xi):\|\phi\|\le C_2\epsilon^{1/2}\} \tag{3.22}$$

where C_2 is a constant independent of ϵ to be determined soon. For every $\phi \in \mathcal{B}_\xi$, by Corollary 2.3

$$\begin{aligned}\|T_\xi(\phi)\| &\leq C_1\|\pi_\xi \circ S(w_\xi)\| + C_1\|\pi_\xi \circ R_\xi(\phi)\| \\ &\leq C_3\epsilon^{1/2} + C_5(1 + O(\|\phi\|))\|\phi\|^2 \\ &\leq C_3\epsilon^{1/2} + C_6C_2^2(1 + C_2\epsilon^{1/2})\epsilon \end{aligned} \tag{3.23}$$

where we have estimated $R_\xi(\phi)$ as follows:

$$\|R_\xi(\phi)\| \leq 2\|f(w_\xi + \phi) - f(w_\xi) - f'(w_\xi)\phi\| \leq C_4(1 + O(\|\phi\|))\|\phi\|^2$$

for some C_4 depending on f only. In (3.23) the constants C_3 and C_6 are again independent of ϵ. If we choose C_2 to be sufficiently large, then when ϵ is small enough (3.23) is bounded by $C_2\epsilon^{1/2}$. Therefore by choosing such C_2 we see that $\mathcal{D}(T_\xi)$ maps $\mathcal{B}_\xi$ to itself.

Next we prove that T_ξ is a contraction mapping in $\mathcal{D}(T_\xi)$. Take ϕ_1 and ϕ_2 in $\mathcal{D}(T_\xi)$. Then

$$\begin{aligned}\|T_\xi(\phi_1) - T_\xi(\phi_2)\| &\leq C_1\|\pi_\xi \circ (R_\xi(\phi_1) - R_\xi(\phi_2))\| \;\leq\; C_7\|R_\xi(\phi_1) - R_\xi(\phi_2)\| \\ &\leq C_8\|f(w_\xi + \phi_1) - f(w_\xi + \phi_2) - f'(w_\xi)(\phi_1 - \phi_2)\| \\ &\leq C_8\|f'(w_\xi + \phi_2 + \theta(\phi_1 - \phi_2))(\phi_1 - \phi_2) - f'(w_\xi)(\phi_1 - \phi_2)\| \\ &\leq C_8\|f'(w_\xi + \phi_2 + \theta(\phi_1 - \phi_2)) - f'(w_\xi)\|\;\|\phi_1 - \phi_2\| \\ &\leq O(\|\phi_1\| + \|\phi_2\|)\;\|\phi_1 - \phi_2\| \\ &\leq C_9\epsilon^{1/2}\|\phi_1 - \phi_2\|\end{aligned}$$

which implies that T_ξ is a contraction mapping if ϵ is sufficiently small. In these estimates $\theta = \theta(x) \in (0,1)$ comes from the mean value theorem. $\square$

4 Stability in fibers

The manifold $\mathcal{M}$ is also embedded in $\mathcal{A}$. At each w_ξ we define

$$\mathcal{P}_\xi = \{\psi \in W^{1,2}(0,1) : \overline{\psi} = 0,\ \psi \perp h_j,\ j = 1, 2, ..., 2N\} \tag{4.1}$$

Then $w_\xi + \mathcal{P}_\xi$ is a subset of $\mathcal{A}$, which we call the ξ-fiber of $\mathcal{M}$ in $\mathcal{A}$. Note that $\mathcal{F}_\xi \subset \mathcal{P}_\xi$.

In this section we show that $w_\xi + \phi_\xi$ found in the last section locally minimizer I in $w_\xi + \mathcal{P}_\xi$. We first study the linearization of S at $w_\xi + \phi_\xi$. Set

$$\lambda = \inf\{\frac{1}{2}\int_0^1 [\epsilon^2(\psi')^2 + f'(w_\xi + \phi_\xi)\psi^2 + \sigma|(-\Delta)^{-1/2}\psi|^2]\,dx : \psi \in \mathcal{P}_\xi,\ \int_0^1 \psi^2\,dx = 1\} \tag{4.2}$$

Lemma 4.1 $\liminf_{\epsilon \to 0} \lambda > 0$.

Proof. In this proof we denote $w_\xi + \phi_\xi$ by g_ξ. We argue by contradiction. Assume $\liminf_{\epsilon\to 0} \lambda \leq 0$. Clearly λ is achieved by a ψ in $\mathcal{P}_\xi$. Scaling ψ by a constant multiple, we may assume that $\|\psi\| = 1$ and ψ satisfies

$$-\epsilon^2\psi'' + f'(g_\xi)\psi - \overline{f'(g_\xi)\psi} + \sigma(-\Delta)^{-1}\psi = \lambda\psi + \sum_{j=1}^{2N}\beta_j h_j \tag{4.3}$$

for some $\beta_j \in \mathbf{R}$. Note that $\overline{\psi} = 0$, $\psi \perp h_j$, and $\|\psi\| = 1$, but $\int_0^1 \psi^2 \, dx$ is no longer equal to 1.

First multiply (4.3) by ψ, denote $\varphi = (-\Delta)^{-1}\psi$, and integrate to obtain

$$\int_0^1 [\epsilon^2(\psi')^2 + f'(g_\xi)\psi^2 + \sigma(\varphi')^2] \, dx = \lambda \int_0^1 \psi^2 \, dx \tag{4.4}$$

Since $f'(g_\xi)$ may only be negative in ϵ-size neighborhoods of ξ_j, we deduce from (4.4) that

$$O(\epsilon) + \sigma \int_0^1 (\varphi')^2 \, dx \leq \lambda_+ \tag{4.5}$$

where

$$\lambda_+ = \begin{cases} 0 & \text{if} \quad \lambda \leq 0 \\ \lambda & \text{if} \quad \lambda > 0 \end{cases} \tag{4.6}$$

The assumption $\liminf_{\epsilon \to 0} \lambda \leq 0$ implies that

$$\lambda_+ = o(1). \tag{4.7}$$

By the Sobolev embedding theory, (4.5) and (4.7) imply that

$$\|\varphi\| = O(\sqrt{\lambda_+ + \epsilon}) = o(1). \tag{4.8}$$

Next multiply (4.3) by h_k and integrate to deduce

$$\int_0^1 [-\epsilon^2\psi'' h_k + f'(g_\xi)\psi h_k + \sigma\varphi h_k] \, dx = \sum_{j=1}^{2N} \beta_j \epsilon(\tau\delta_{jk} + O(\epsilon)) \tag{4.9}$$

As in the argument leading to (3.11) we find that

$$\beta_j = O(1), \ j = 1, 2, ..., 2N. \tag{4.10}$$

Thirdly we let $y \in [0, 1]$ so that $\psi(y) = \|\psi\| = 1$. We show that y must be in an ϵ-size neighborhood of some ξ_k. Otherwise (4.3) is not valid at y, for as in (3.12)

$$f'(0) + o(1) \leq -\epsilon^2\psi''(y) + f'(g_\xi(y))\psi(y) - \overline{f'(g_\xi)\psi} + \sigma\varphi(y) = \lambda\psi(y) + \sum_{j=1}^{2N} \beta_j h_j(y) = \lambda + o(1)$$

with the help of (4.10). But this is impossible since we have assumed that $\liminf_{\epsilon \to 0} \lambda \leq 0$.

Finally we assume that $y - \xi_k = O(\epsilon)$ for some k and look for a contradiction. Let $\Psi(t) = \psi(\xi_j + \epsilon t)$. Then

$$-\Psi''(t) + f'(g_\xi(\xi_j + \epsilon t)) + o(1) = \lambda\Psi(t) + \sum_{j=1}^{2N} \beta_j h_j(\xi_k + \epsilon t), \ t \in (-\frac{\xi_k}{\epsilon}, \frac{1 - \xi_k}{\epsilon}).$$

As in the proof of Lemma 3.1 Ψ converges in Ψ_∞ in $C^2_{loc}(\mathbf{R})$. $\Psi_\infty \neq 0$ since $\Psi((y - \xi_k)/\epsilon) = 1$, and Ψ_∞ satisfies

$$-\Psi''_\infty + f'(H)\Psi_\infty = (\liminf_{\epsilon \to 0} \lambda)\Psi_\infty + \beta_k^0 H' \tag{4.11}$$

where $\beta_k^0 = \lim \beta_k$. Since $\psi \perp h_k$ and $\overline{\psi} = 0$,

$$0 = \int_0^1 \psi h_k \, dx = \int_0^1 \psi(H'(\frac{x - \xi_\epsilon}{\epsilon}) + O(e^{-C/\epsilon})) \, dx = \epsilon \int_{\mathbf{R}} \Psi_\infty(t) H'(t) \, dt + o(\epsilon).$$

Therefore

$$\int_{\mathbf{R}} \Psi_\infty H' \, dt = 0. \tag{4.12}$$

We multiply (4.11) by H' and integrate. Because of (4.12) we obtain from (4.11) that

$$0 = \beta_k^0 \int_{\mathbf{R}} (H')^2 \, dt, \text{ i.e. } \beta_k^0 = 0.$$

Then (4.11) becomes

$$-\Psi_\infty'' + f'(H)\Psi_\infty = (\liminf_{\epsilon \to 0} \lambda)\Psi_\infty \tag{4.13}$$

The equation (4.13) has no bounded solution if $\liminf \lambda < 0$. Hence $\liminf \lambda = 0$. Then the only bounded solutions are scalar multiples of H'. Hence $\Psi_\infty = cH'$ for some $c \neq 0$. But this contradicts (4.12). □

We are now ready to show that $w_\xi + \phi_\xi$ locally minimizes I in the ξ-fiber.

Lemma 4.2 *There exists an non-empty open $\mathcal{N}_\xi \subset \mathcal{P}_\xi$ containing 0 such that for every $\psi \in \mathcal{N}_\xi$, $\psi \neq 0$, $I(w_\xi + \phi_\xi) < I(w_\xi + \phi_\xi + \psi)$.*

Proof. We again denote $w_\xi + \phi_\xi$ by g_ξ. Let $\psi \in \mathcal{P}_\xi$ and expand

$$I(g_\xi + \psi) = I(g_\xi) + \int_0^1 S(g_\xi)\psi + \frac{1}{2}\int_0^1 [\epsilon^2(\psi')^2 + f'(g_\xi)\psi^2 + \sigma|(-\Delta)^{-1/2}\psi|^2] \, dx + \frac{1}{6}\int_0^1 f''(..)\psi^3 \, dx$$

Because $\pi_\xi \circ S(g_\xi) = 0$ and $\psi \perp h_j$, we deduce

$$I(g_\xi + \psi) = I(g_\xi) + \frac{1}{2}\int_0^1 [\epsilon^2(\psi')^2 + f'(g_\xi)\psi^2 + \sigma|(-\Delta)^{-1/2}\psi|^2] \, dx + O(\|\psi\|) \, \|\psi\|_2^2 \tag{4.14}$$

which by (4.2) implies

$$I(g_\xi + \psi) \geq I(g_\xi) + (\lambda - O(\|\psi\|)) \, \|\psi\|_2^2 \tag{4.15}$$

where C is independent of ϵ. We define a non-empty open subset

$$\mathcal{N}_\xi = \{\psi \in \mathcal{P}_\xi : \|\psi\| < C_1\} \tag{4.16}$$

of $\mathcal{P}_\xi$ for some $C_1 > 0$. If we take C_1 to be sufficiently small (but independent of ϵ), then (4.15) and Lemma 4.1 imply that there exists $C_2 > 0$, independent of ϵ, so that

$$I(g_\xi + \psi) \geq I(g_\xi) + C_2 \, \|\psi\|_2^2, \text{ for all } \psi \in \mathcal{N}_\xi \tag{4.17}$$

Lemma 4.2 follows from (4.17). □

5 The reduced problem

In this section we find a particular $\tilde{\xi}$ so that $\tilde{\xi}$ locally minimizes $I(w_\xi + \phi_\xi)$ with respect to ξ and $S(w_{\tilde{\xi}} + \phi_{\tilde{\xi}}) = 0$. Let

$$J(\zeta, l) = I(w_\xi + \phi_\xi) \tag{5.1}$$

where ζ and l are related to ξ via (2.3).

Lemma 5.1 *For $\xi \in \Lambda$ we have*

$$J(\zeta, l) = \epsilon[2N\tau + 4f'(0)Q(\zeta, l)] + O(\epsilon^{3/2})$$

uniformly with respect to (ζ, l). Here Q is an ϵ-independent function

$$Q(\zeta, l) = \frac{1}{2}\sum_{k,j=1}^{N} l_k l_j G_D(\zeta_k, \zeta_j) - \frac{a_0}{2}\sum_{j=1}^{N} l_j + \frac{a_0^2}{8}$$

for (ζ, l) that satisfy

$$0 < \zeta_1 < \zeta_2 < ... < \zeta_N < 1,\ l_j > 0,\ j = 1, 2, ..., 2N.$$

Proof. Clearly

$$\begin{aligned}
J(\zeta, l) &= I(w_\xi) + I'(\xi)(\phi_\xi) + \frac{1}{2}I''(\xi)(\phi_\xi, \phi_\xi) + O(\epsilon^{3/2}) \\
&= I(w_\xi) + \int_0^1 S(w_\xi)\phi_\xi + \frac{1}{2}\int_0^1 [\epsilon^2|\phi_\xi'|^2 + f'(w_\xi)\phi_\xi^2 + \sigma|(-\Delta)^{-1/2}\phi_\xi|^2]\,dx + O(\epsilon^{3/2})
\end{aligned}$$

The equation $\pi_\xi \circ S(w_\xi + \phi_\xi) = 0$ implies that

$$-\epsilon^2\phi_\xi'' + f'(w_\xi)\phi_\xi - \overline{f'(w_\xi)\phi_\xi} + \sigma(-\Delta)^{-1}\phi_\xi + S(w_\xi) + O(\|\phi_\xi\|^2) = \sum_{j=1}^{2N}\beta_j h_j \tag{5.2}$$

for some $\beta_j \in \mathbf{R}$. Multiply (5.2) by ϕ_ξ and integrate to find

$$\int_0^1 [\epsilon^2|\phi_\xi'|^2 + f'(w_\xi)\phi_\xi^2 + \sigma|(-\Delta)^{-1/2}\phi_\xi|^2]\,dx + \int_0^1 S(w_\xi)\phi_\xi\,dx + O(\epsilon^{3/2}) = 0 \tag{5.3}$$

Substituting (5.3) to the earlier estimate of $M(\zeta, l)$ we deduce

$$J(\zeta, l) = I(w_\xi) + \frac{1}{2}\int_0^1 S(w_\xi)\phi_\xi\,dx + O(\epsilon^{3/2}) \tag{5.4}$$

By Lemma 2.2 we obtain

$$\int_0^1 S(w_\xi)\phi_\xi\,dx = \int_0^1 (f'(w_{\xi,1}) - f'(0))w_{\xi,2}\,dx + O(\epsilon^{3/2}) = O(\epsilon^{3/2}) \tag{5.5}$$

To see the last equation note that only on intervals of size ϵ near ξ_j, $f'(w_{\xi,1}) - f'(0)$ is of order 1. Elsewhere $f'(w_{\xi,1}) - f'(0) = O(\epsilon)$. Now (5.4) becomes

$$J(\zeta, l) = I(w_\xi) + O(\epsilon^{3/2}) \tag{5.6}$$

We turn our attention to $I(w_\xi)$. Note that

$$\begin{aligned}
I(w_\xi) &= \frac{\epsilon^2}{2}\int_0^1 |w'_{\xi,1}|^2\,dx + \epsilon^2\int_0^1 w'_{\xi,1}w'_{\xi,2}\,dx \\
&\quad + \int_0^1 W(w_{\xi,1})\,dx + \int_0^1 f(w_{\xi,1})w_{\xi,2}\,dx + \frac{1}{2}\int_0^1 f'(w_{\xi,1})w_{\xi,2}^2\,dx \\
&\quad + \frac{\sigma}{2}\int_0^1 |(-\Delta)^{-1/2}(w_{\xi,1}+w_{\xi,2}-a)|^2\,dx + O(\epsilon^{3/2}) \\
&= \frac{\epsilon^2}{2}\int_0^1 |w'_{\xi,1}|^2\,dx + \int_0^1 W(w_{\xi,1})\,dx \\
&\quad + \epsilon^2\int_0^1 w'_{\xi,1}w'_{\xi,2}\,dx + \int_0^1 f(w_{\xi,1})w_{\xi,2}\,dx \\
&\quad + \frac{1}{2}\int_0^1 f'(w_{\xi,1})w_{\xi,2}^2\,dx + \frac{\sigma}{2}\int_0^1 |(-\Delta)^{-1/2}(w_{\xi,1}+w_{\xi,2}-a)|^2\,dx + O(\epsilon^{3/2}) \\
&= 2N\tau\epsilon + \frac{1}{2}\int_0^1 f'(w_{\xi,1})w_{\xi,2}^2 + \frac{\sigma}{2}\int_0^1 (w_{\xi,1}+w_{\xi,2}-a)(-\Delta)^{-1}(w_{\xi,1}+w_{\xi,2}-a) + O(\epsilon^{3/2}) \\
&= 2N\tau\epsilon + \frac{1}{2}\int_0^1 f'(w_{\xi,1})w_{\xi,2}^2\,dx - \frac{f'(0)}{2}\int_0^1 (w_{\xi,1}+w_{\xi,2}-a)w_{\xi,2}\,dx + O(\epsilon^{3/2}) \\
&= 2N\tau\epsilon + \frac{1}{2}\int_0^1 (f'(w_{\xi,1})-f'(0))w_{\xi,2}^2\,dx - \frac{f'(0)}{2}\int_0^1 (w_{\xi,1}-a)w_{\xi,2}\,dx + O(\epsilon^{3/2}) \\
&= 2N\tau\epsilon - \frac{f'(0)}{2}\int_0^1 (w_{\xi,1}-a)w_{\xi,2}\,dx + O(\epsilon^{3/2}) \\
&= 2N\tau\epsilon - \frac{f'(0)\epsilon}{2}\int_0^1 (\frac{w_{\xi,1}}{\epsilon^{1/2}} - a_0)(a_0 - \sum_{j=1}^N 2l_j G_D(x,\zeta_j))\,dx + O(\epsilon^{3/2}) \\
&= 2N\tau\epsilon - \frac{f'(0)\epsilon}{2}[\int_0^1 \frac{w_{\xi,1}}{\epsilon^{1/2}}a_0\,dx - 2\int_0^1 \frac{w_{\xi,1}}{\epsilon^{1/2}}(\sum_{j=1}^N l_j G_D(x,\zeta_j))\,dx \\
&\quad - a_0^2 + 2a_0\int_0^1 (\sum_{j=1}^N l_j G_D(x,\zeta_j))\,dx] + O(\epsilon^{3/2}) \\
&= 2N\tau\epsilon - \frac{f'(0)\epsilon}{2}[2a_0\sum_{j=1}^N l_j - 4\sum_{k=1}^N\sum_{j=1}^N l_k l_j G_D(\zeta_k,\zeta_j) - a_0^2 + 2a_0\sum_{j=1}^N l_j] + O(\epsilon^{3/2}) \\
&= 2N\tau\epsilon + 2f'(0)\epsilon[\sum_{k,j=1}^N l_k l_j G_D(\zeta_k,\zeta_j) - a_0\sum_{j=1}^N l_j + \frac{a_0^2}{4}] + O(\epsilon^{3/2}). \quad \square
\end{aligned} \tag{5.7}$$

Lemma 5.2 *Q has a unique critical point* (ζ^0, l^0) *where*

$$\zeta_1^0 = \frac{1}{2N},\ \zeta_2^0 = \frac{3}{2N},\ \zeta_3^0 = \frac{5}{2N},\ ...,\ \zeta_j^0 = \frac{2j-1}{2N},\ ...,\ \zeta_N^0 = \frac{2N-1}{2N}$$

and

$$l_j^0 = a_0\sqrt{D}(\coth\frac{1}{N\sqrt{D}} - \operatorname{csch}\frac{1}{N\sqrt{D}}),\ j = 1, 2, ..., N.$$

Proof. For any (ζ, l) we define a $C^{0,1}[0,1]$ function p by

$$p(x) = \sum_{k=1}^{N} G_D(x, \zeta_k) l_k. \tag{5.8}$$

Calculations show that

$$\frac{\partial Q}{\partial \zeta_j} = l_j(p'(\zeta_j-) + p'(\zeta_j+)), \tag{5.9}$$

$$\frac{\partial Q}{\partial l_j} = \sum_{k=1}^{N} G_D(\zeta_j, \zeta_k) l_k - \frac{a_0}{2} = p(\zeta_j) - \frac{a_0}{2}. \tag{5.10}$$

Now we assume that (ζ, l) is a critical point of Q. Then (5.9) and (5.10) imply that

$$p'(\zeta_j-) + p'(\zeta_j+) = 0, \tag{5.11}$$

$$p(\zeta_j) = \frac{a_0}{2}. \tag{5.12}$$

Since p satisfies the linear differential equation

$$-Dp'' + p = 0,\ \text{in } (0,1)\backslash\{\zeta_1, \zeta_2, ..., \zeta_N\},\ \text{and } p'(0) = p'(1) = 0,$$

(5.11) and (5.12) imply that

$$\zeta_1 = \frac{1}{2N},\ \zeta_2 = \frac{3}{2N}, \zeta_3 = \frac{5}{2N},\ ...,\ \zeta_j = \frac{2i-1}{2N},\ ...,\ \zeta_N = \frac{2N-1}{2N}. \tag{5.13}$$

At a critical point (ζ, l), (5.10) implies that l satisfy the linear system

$$\begin{bmatrix} G_D(\zeta_1,\zeta_1) & G_D(\zeta_1,\zeta_2) & ... & G_D(\zeta_1,\zeta_N) \\ G_D(\zeta_2,\zeta_1) & G_D(\zeta_2,\zeta_2) & ... & G_D(\zeta_2,\zeta_N) \\ & ... & & \\ G_D(\zeta_N,\zeta_1) & G_D(\zeta_N,\zeta_2) & ... & G_D(\zeta_N,\zeta_N) \end{bmatrix} \begin{bmatrix} l_1 \\ l_2 \\ ... \\ l_N \end{bmatrix} = \frac{1}{2} \begin{bmatrix} a_0 \\ a_0 \\ ... \\ a_0 \end{bmatrix} \tag{5.14}$$

It is shown in the appendix that at (5.13) the symmetric $N \times N$ matrix $[G_D(\zeta_j, \zeta_k)]$ is non-singular and

$$\sum_{k=1}^{N} G_D(\zeta_j, \zeta_k) = \frac{1}{2\sqrt{D}} \frac{1}{\coth(1/(N\sqrt{D})) - \operatorname{csch}(1/(N\sqrt{D}))}. \tag{5.15}$$

Note that the right side of (5.15) is independent of j. Therefore the unique solution to (5.14) is

$$l_j = a_0\sqrt{D}(\coth\frac{1}{N\sqrt{D}} - \operatorname{csch}\frac{1}{N\sqrt{D}}). \ \square \tag{5.16}$$

Lemma 5.3 *The second derivative matrix of Q at (ζ^0, l^0) is positive definite.*

Proof. We calculate the second derivative of Q at (ζ^0, l^0). First

$$\frac{\partial^2 Q}{\partial l_j \partial l_k}(\zeta^0, l^0) = G_D(\zeta_j^0, \zeta_k^0). \tag{5.17}$$

We define a matrix $\mathbf{A}$ whose ik-entry a_{jk} is given by (5.17).

Next we write G_D as

$$G_D(x, y) = \Gamma(|x - y|) + R(x, y) \tag{5.18}$$

where Γ is the fundamental solution and R is the smooth regular part:

$$\Gamma(z) = \frac{1}{2\sqrt{D}} \exp(-\frac{z}{\sqrt{D}}), \quad R(x, y) = \frac{\cosh \frac{x+y-1}{\sqrt{D}} + \exp(-\frac{1}{\sqrt{D}}) \cosh \frac{x-y}{\sqrt{D}}}{2\sqrt{D} \sinh \frac{1}{\sqrt{D}}}. \tag{5.19}$$

Then we calculate

$$\begin{aligned} \frac{\partial Q}{\partial \zeta_j} &= \frac{1}{2} \frac{\partial}{\partial \zeta_j}[G_D(\zeta_j, \zeta_j) l_j^2] + \frac{\partial}{\partial \zeta_j}[\sum_{k \neq j} G_D(\zeta_j, \zeta_k) l_j l_k] \\ &= R_1(\zeta_j, \zeta_j) l_j^2 + l_j \sum_{k \neq j} [\Gamma'(|\zeta_j - \zeta_k|)(\pm 1) + R_1(\zeta_j, \zeta_k)] l_k \end{aligned}$$

where $\pm 1 = 1$ if $\zeta_j - j_k > 0$ and $\pm = -1$ if $\zeta_j - \zeta_k < 0$. Let

$$\iota = l_1^0 = l_2^0 = ... = l_N^0 = a_0 \sqrt{D} (\coth \frac{1}{N\sqrt{D}} - \operatorname{csch} \frac{1}{N\sqrt{D}}). \tag{5.20}$$

Then if $k \neq j$

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j \partial l_k} = \iota(\Gamma'(|\zeta_j^0 - \zeta_k^0|)(\pm 1) + R_1(\zeta_j^0, \zeta_k^0)), \ j \neq k. \tag{5.21}$$

If $k = j$,

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j \partial l_j} = 2\iota R_1(\zeta_j^0, \zeta_j^0) + \iota \sum_{k \neq j} (\Gamma'(|\zeta_j^0 - \zeta_k^0|)(\pm 1) + R_1(\zeta_j^0, \zeta_k^0)). \tag{5.22}$$

We define a matrix $\mathbf{B}$ whose jk-entry b_{jk} is given by (5.21) and (5.22).

If $k \neq j$,

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j \partial \zeta_k} = \iota^2(-\Gamma''(|\zeta_j^0 - \zeta_k^0|) + R_{12}(\zeta_j^0, \zeta_k^0)) \tag{5.23}$$

If $k = j$,

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j^2} = \iota^2(R_{11}(\zeta_j^0, \zeta_j^0) + R_{12}(\zeta_j^0, \zeta_j^0)) + \iota^2 \sum_{k \neq j} [\Gamma''(|\zeta_j^0 - \zeta_k^0|) + R_{11}(\zeta_j^0, \zeta_k^0)].$$

Using the the equation that G_D solves we may simply the second part on the right side and obtain

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j^2} = \iota^2(-\Gamma''(0) + R_{12}(\zeta_j^0, \zeta_j^0)) + \frac{\iota^2}{D} \sum_{k=1}^{N} G_D(\zeta_j^0, \zeta_k^0). \tag{5.24}$$

We define a matrix $\mathbf{C}$ whose jk-entry c_{jk} is given by (5.23) and (5.24).

The second derivative of Q at (ζ^0, l^0) is the symmetric matrix

$$\mathbf{H} = \left[\begin{array}{cc} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{C} \end{array} \right]. \tag{5.25}$$

The matrix $\mathbf{H}$ turns out to be the same matrix studied in Wei and Winter ??. There it was proved that the matrix is positive definite. We include it in the appendix. $\square$

Proof of Theorem 1.1. Let us denote w_ξ and ϕ_ξ by $w_{\zeta,l}$ and $\phi_{\zeta,l}$ respectively where ξ is related to ζ and l via (2.3). In Λ, according to Lemma 5.1, $\epsilon^{-1}J$ uniformly converges to $2N\tau + 4f'(0)Q$ as $\epsilon \to 0$. Lemmas 5.2 and 5.3 imply that (ζ^0, l^0) is a strict local minimizer of $2N\tau + 4f'(0)Q$. Our choice of δ in the definition (2.4) of Λ ensures that $(\zeta^0, l^0) \in \Lambda$. Near (ζ^0, l^0) there exists a local minimizer $(\tilde{\zeta}, \tilde{l})$ of J when ϵ is sufficiently small. Moreover $(\tilde{\zeta}, \tilde{l}) \to (\zeta^0, l^0)$ as $\epsilon \to 0$. It is standard to prove that $S(w_{\tilde{\zeta},\tilde{l}} + \phi_{\tilde{\zeta},\tilde{l}}) = 0$. The detailed argument may be found in papers like [6, 20]. Lemma 4.2 states that for each (ζ, l), $w_{\zeta,l} + \phi_{\zeta,l}$ locally minimizes I in the fiber $w_{\zeta,l} + \mathcal{P}_{\zeta,l}$. Then $w_{\tilde{\zeta},\tilde{l}} + \phi_{\tilde{\zeta},\tilde{l}}$ locally minimizes I in $\mathcal{A}$. $\square$

6 Discussion

If in Theorem 1.1 we expand

$$\frac{\coth\beta - \operatorname{csch}\beta}{\beta} = \frac{1}{2} - \frac{\beta^2}{24} + ... \tag{6.1}$$

for small β, i.e. large N, we find that the free energy of the N droplet solution is approximately

$$\epsilon(2N\tau + \frac{a_0^2\sigma}{24N^2}). \tag{6.2}$$

The last expression is minimized at

$$N_{opt} = (\frac{a_0^2\sigma}{24\tau})^{1/3} \tag{6.3}$$

with respect to N. This N_{opt} gives the optimal number of droplets.

Another interesting consequence of our work concerns the distribution of A-monomers. The area under each droplet of an N-droplet local minimizer, by (5.16), is

$$\frac{2a_0}{N\beta}(\coth\beta - \operatorname{csch}\beta)\epsilon^{1/2} + o(\epsilon^{1/2}). \tag{6.4}$$

Taking all the droplets into consideration, the area under all the droplets is

$$\frac{2a_0}{\beta}(\coth\beta - \operatorname{csch}\beta)\epsilon^{1/2} + o(\epsilon^{1/2}). \tag{6.5}$$

On the other hand the total area under the graph of local minimizer is $a = a_0\epsilon^{1/2}$. Since (6.1) implies that

$$\frac{2a_0}{\beta}(\coth\beta - \operatorname{csch}\beta) < a_0, \tag{6.6}$$

we discover that a significant portion of the area $a_0\epsilon^{1/2}$ is under the part where the graph is close to 0. In other words the A-monomers form droplets and at the same time spread through the entire sample with the B-monomers.

Appendix

Here we show that $G_D(\zeta_j^0,\zeta_k^0)$ is non-singular, verify (5.15), and prove that all the eigenvalues of $\mathbf{H}$ are positive.

Arguing as in [17, Section 7] we find that the inverse matrix of $\mathbf{A}$ has the tridiagonal form

$$\mathbf{A}^{-1}=\sqrt{D}\begin{bmatrix} 2\coth\beta-\operatorname{csch}\beta & -\operatorname{csch}\beta & 0 & 0 & \dots & 0 \\ -\operatorname{csch}\beta & 2\coth\beta & -\operatorname{csch}\beta & 0 & \dots & 0 \\ 0 & -\operatorname{csch}\beta & 2\coth\beta & -\operatorname{csch}\beta & \dots & 0 \\ \dots \\ 0 & 0 & 0 & 0 & \dots & 2\coth\beta-\operatorname{csch}\beta \end{bmatrix} \tag{A.1}$$

where

$$\beta=\frac{1}{N\sqrt{D}}. \tag{A.2}$$

One rewrites (A.1) as

$$\mathbf{A}^{-1}=-\sqrt{D}\operatorname{csch}\beta\begin{bmatrix} 1 & 1 & 0 & 0 & \dots & 0 \\ 1 & 0 & 1 & 0 & \dots & 0 \\ 0 & 1 & 0 & 1 & \dots & 0 \\ \dots \\ 0 & 0 & 0 & 0 & \dots & 1 \end{bmatrix}+2\sqrt{D}\coth\beta\,\mathbf{I} \tag{A.3}$$

where $\mathbf{I}$ is the $N\times N$ identity matrix. One just needs to diagonalized the first matrix on the right side of (A.3). It turns out that $\mathbf{A}^{-1}$ is diagonalized by the orthogonal matrix of eigenvectors

$$\mathbf{P}=\sqrt{\frac{2}{N}}\begin{bmatrix} \frac{1}{\sqrt{2}} & \cos(\frac{\pi}{N}(2-1)(1-\frac{1}{2})) & \dots & \cos(\frac{\pi}{N}(N-1)(1-\frac{1}{2})) \\ \frac{1}{\sqrt{2}} & \cos(\frac{\pi}{N}(2-1)(2-\frac{1}{2})) & \dots & \cos(\frac{\pi}{N}(N-1)(2-\frac{1}{2})) \\ \dots \\ \frac{1}{\sqrt{2}} & \cos(\frac{\pi}{N}(2-1)(N-\frac{1}{2})) & \dots & \cos(\frac{\pi}{N}(N-1)(N-\frac{1}{2})) \end{bmatrix} \tag{A.4}$$

and that

$$\mathbf{P}^T\mathbf{A}^{-1}\mathbf{P}=-\sqrt{D}\operatorname{csch}\beta\begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \dots \\ 0 & 0 & \dots & \lambda_N \end{bmatrix}+2\sqrt{D}\coth\beta\,\mathbf{I} \tag{A.5}$$

where

$$\lambda_j=2\cos\frac{\pi(j-1)}{N},\ j=1,2,...,N. \tag{A.6}$$

Therefore

$$\mathbf{P}^T\mathbf{A}\mathbf{P}=\begin{bmatrix} a_1 & 0 & \dots & 0 \\ 0 & a_2 & \dots & 0 \\ \dots \\ 0 & 0 & \dots & a_N \end{bmatrix} \tag{A.7}$$

where the eigenvalues of $\mathbf{A}$ are

$$a_j = \frac{1}{\sqrt{D}} \frac{1}{\coth\beta - \operatorname{csch}\beta \cos\frac{\pi(j-1)}{N}} > 0, \; j = 1, 2, ..., N. \tag{A.8}$$

Hence all the eigenvalues of $G_D(\zeta_j^0, \zeta_k^0)$ are positive and

$$\sum_{k=1}^{N} G_D(\zeta_j^0, \zeta_k^0) = a_1 = \frac{1}{2\sqrt{D}} \frac{1}{\coth\beta - \operatorname{csch}\beta} \tag{A.9}$$

is independent of j, proving (5.15).

The formula (A.9) also allows us to simplify $\mathbf{C}$ to

$$\mathbf{C} = -\iota^2\mathbf{D} + \frac{\iota^2}{2D^{3/2}(\coth\beta - \operatorname{csch}\beta)}\,\mathbf{I} \tag{A.10}$$

where the jk entry of $\mathbf{D}$ is

$$d_{jk} = \Gamma''(|\zeta_j^0 - \zeta_k^0|) - R_{12}(\zeta_j^0, \zeta_k^0). \tag{A.11}$$

However from (5.19) we find that

$$\Gamma''(|x-y|) - R_{12}(x, y) \tag{A.12}$$

is the Green function of

$$-Dz'' + z = \delta(\cdot - y), \; z(0) = z(1) = 1 \tag{A.13}$$

divided by D. Argument similar to [17, Section 7] shows that

$$\mathbf{D}^{-1} = D^{3/2} \begin{bmatrix} 2\coth\beta + \operatorname{csch}\beta & -\operatorname{csch}\beta & 0 & 0 & ... & 0 \\ -\operatorname{csch}\beta & 2\coth\beta & -\operatorname{csch}\beta & 0 & ... & 0 \\ 0 & -\operatorname{csch}\beta & 2\coth\beta & -\operatorname{csch}\beta & ... & 0 \\ ... & & & & & \\ 0 & 0 & 0 & 0 & ... & 2\coth\beta + \operatorname{csch}\beta \end{bmatrix} \tag{A.14}$$

$\mathbf{D}^{-1}$ is diagonalized by

$$\mathbf{Q} = \sqrt{\frac{2}{N}} \begin{bmatrix} \frac{-1}{\sqrt{2}} & \sin(\frac{\pi}{N}(2-1)(1-\frac{1}{2})) & ... & \sin(\frac{\pi}{N}(N-1)(1-\frac{1}{2})) \\ \frac{1}{\sqrt{2}} & \sin(\frac{\pi}{N}(2-1)(2-\frac{1}{2})) & ... & \sin(\frac{\pi}{N}(N-1)(2-\frac{1}{2})) \\ ... & & & \\ \frac{(-1)^N}{\sqrt{2}} & \sin(\frac{\pi}{N}(2-1)(N-\frac{1}{2})) & ... & \sin(\frac{\pi}{N}(N-1)(N-\frac{1}{2})) \end{bmatrix} \tag{A.15}$$

Then

$$\mathbf{Q}^T\mathbf{D}^{-1}\mathbf{Q} = -\,D^{3/2}\operatorname{csch}\beta \begin{bmatrix} \mu_1 & 0 & ... & 0 \\ 0 & \mu_2 & ... & 0 \\ ... & & & \\ 0 & 0 & ... & \mu_N \end{bmatrix} + 2D^{3/2}\coth\beta\,\mathbf{I} \tag{A.16}$$

where the μ_j's are

$$\mu_1 = -2, \; \mu_j = 2\cos\frac{\pi(j-1)}{N}, \; j = 2, 3, ..., N. \tag{A.17}$$

Hence

$$\mathbf{Q}^T\mathbf{C}\mathbf{Q} = \begin{bmatrix} c_1 & 0 & ... & 0 \\ 0 & c_2 & ... & 0 \\ ... & & & \\ 0 & 0 & ... & c_N \end{bmatrix} \tag{A.18}$$

where

$$c_1 \;=\; \frac{\iota^2}{2D^{3/2}}\left(\frac{1}{\coth\beta - \operatorname{csch}\beta} - \frac{1}{\coth\beta + \operatorname{csch}\beta}\right) \;>\; 0, \tag{A.19}$$

$$c_j \;=\; \frac{\iota^2}{2D^{3/2}}\left(\frac{1}{\coth\beta - \operatorname{csch}\beta} - \frac{1}{\coth\beta - \operatorname{csch}\beta\cos\frac{\pi(j-1)}{N}}\right) \;>\; 0,\; j = 2, 3, ..., N. \tag{A.20}$$

We will use

$$\begin{bmatrix} \mathbf{P} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q} \end{bmatrix} \tag{A.21}$$

to diagonalize $\mathbf{H}$ to 2×2 blocks. We must compute $\mathbf{Q}^T\mathbf{B}\mathbf{P}$. Let

$$\mathbf{B} = \iota(\mathbf{E} + \mathbf{F}) \tag{A.22}$$

where the jk entry e_{jk} of $\mathbf{E}$ is

$$e_{jk} = \begin{cases} \Gamma'(|\zeta_j^0 - \zeta_k^0|)(\pm 1) + R_1(\zeta_j^0, \zeta_k^0) & \text{if} \quad j \neq k \\ R_1(\zeta_j^0, \zeta_j^0) & \text{if} \quad j = k \end{cases} \tag{A.23}$$

and $\mathbf{F}$ is diagonal whose jj entry is

$$f_{jj} = R_1(\zeta_j^0, \zeta_j^0) + \sum_{k\neq j}(\Gamma'(|\zeta_j^0 - \zeta_k^0|)(\pm 1) + R_1(\zeta_j^0, \zeta_k^0)). \tag{A.24}$$

To study $\mathbf{Q}^T\mathbf{E}\mathbf{P}$, we write $\mathbf{E}$ as $\mathbf{M}\mathbf{A}$ where, after some calculations we find that

$$\mathbf{M} = \mathbf{E}\mathbf{A}^{-1} = \frac{\operatorname{csch}\beta}{2\sqrt{D}}\begin{bmatrix} -1 & 1 & 0 & 0 & ... & 0 \\ -1 & 0 & 1 & 0 & ... & 0 \\ 0 & -1 & 0 & 1 & ... & 0 \\ ... & & & & & \\ 0 & 0 & 0 & 0 & ... & -1 \end{bmatrix}. \tag{A.25}$$

Then

$$\mathbf{Q}^T\mathbf{E}\mathbf{P} = (\mathbf{M}^T\mathbf{Q})^T(\mathbf{A}\mathbf{P}). \tag{A.26}$$

If we denote the columns of $\mathbf{P}$ by $\mathbf{p}_1$, $\mathbf{p}_2$, ..., $\mathbf{p}_N$, then

$$\mathbf{A}\mathbf{P} = [a_1\mathbf{p}_1, a_2\mathbf{p}_2, ..., a_N\mathbf{p}_N], \tag{A.27}$$

and

$$\mathbf{M}^T\mathbf{Q} = -\frac{\operatorname{csch}\beta}{\sqrt{D}}[0\mathbf{p}_1, \sin\frac{\pi}{N}\mathbf{p}_2, ..., \sin\frac{(N-1)\pi}{N}\mathbf{p}_N]. \tag{A.28}$$

Therefore

$$\mathbf{Q}^T\mathbf{E}\mathbf{P} = -\frac{\operatorname{csch}\beta}{\sqrt{D}}\begin{bmatrix} 0 & 0 & 0 & ... & 0 \\ 0 & a_2\sin\frac{\pi}{N} & 0 & ... & 0 \\ 0 & 0 & a_3\sin\frac{2\pi}{N} & ... & 0 \\ ... & & & & \\ 0 & 0 & 0 & ... & a_N\sin\frac{(N-1)\pi}{N} \end{bmatrix}. \tag{A.29}$$

If we write $\mathbf{F} = \mathbf{Q}^T\mathbf{E}\mathbf{P}$ and observe the first columns of the equation $\mathbf{E}\mathbf{P} = \mathbf{Q}\mathbf{F}$, then we find that

$$\sum_{k=1}^{N} e_{jk} = 0,\ j = 1, 2, ..., N. \tag{A.30}$$

Thus f_{jj} defined in (A.24) are all 0 and

$$\mathbf{B} = \iota\mathbf{E}. \tag{A.31}$$

So we find that

$$\mathbf{P}^T\mathbf{B}\mathbf{Q} = \begin{bmatrix} b_1 & 0 & ... & 0 \\ 0 & b_2 & ... & 0 \\ ... & & & \\ 0 & 0 & ... & b_N \end{bmatrix} \tag{A.32}$$

where

$$b_j = -\frac{\iota\operatorname{csch}\beta\sin\frac{\pi(j-1)}{N}}{2D(\coth\beta - \operatorname{csch}\beta\cos(\frac{\pi(j-1)}{N}))},\ j = 1, 2, ..., N. \tag{A.33}$$

Hence

$$\begin{bmatrix} \mathbf{P} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q} \end{bmatrix}^T \mathbf{H} \begin{bmatrix} \mathbf{P} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q} \end{bmatrix} = \begin{bmatrix} a_1 & 0 & ... & 0 & b_1 & 0 & ... & 0 \\ 0 & a_2 & ... & 0 & 0 & b_2 & ... & 0 \\ ... & & & & & & & \\ 0 & 0 & ... & a_N & 0 & 0 & ... & b_N \\ b_1 & 0 & ... & 0 & c_1 & 0 & ... & 0 \\ 0 & b_2 & ... & 0 & 0 & c_2 & ... & 0 \\ ... & & & & & & & \\ 0 & 0 & ... & b_N & 0 & 0 & ... & c_N \end{bmatrix} \tag{A.34}$$

which is indeed a matrix of diagonal 2×2 blocks

$$\begin{bmatrix} a_j & b_j \\ b_j & c_j \end{bmatrix} \tag{A.35}$$

after we re-label the rows and the columns in (A.34). For (A.35) we already know that a_j and c_j are positive (A.8, A.19, A.20), a bit more calculations show that the determinants of the 2×2 blocks are again positive. Hence all the eigenvalues of $\mathbf{H}$ are all positive.

References

[1] F.S. Bates and G.H. Fredrickson. Block copolymers - designer soft materials. *Physics Today*, 52(2):32–38, 1999.

[2] R. Choksi. Scaling laws in microphase separation of diblock copolymers. *J. Nonlinear Sci.*, 11(3):223–236, 2001.

[3] R. Choksi and X. Ren. On the derivation of a density functional theory for microphase separation of diblock copolymers. *J. Statist. Phys.*, 113(1-2):151–176, 2003.

[4] E. De Giorgi. Sulla convergenza di alcune successioni di integrali del tipo della'area. *Rendiconti di Matematica*, 8:277–294, 1975.

[5] P.C. Fife and D. Hilhorst. The Nishiura-Ohnishi free boundary problem in the 1D case. *SIAM J. Math. Anal.*, 33(3):589–606, 2001.

[6] C. Gui and J. Wei. Multiple interior peak solutions for some singular perturbation problems. *J. Diff. Eqns.*, 158:1–27, 1999.

[7] M. Henry. Singular limit of a fourth order problem arising in the micro-phase separation of diblock copolymers. *Adv. Differential Equations*, 6(9):1049–1114, 2001.

[8] R. Kohn and P. Sternberg. Local minimisers and singular perturbations. *Proc. Roy. Soc. Edinburgh Sect. A*, 111(1-2):69–84, 1989.

[9] L. Modica. The gradient theory of phase transitions and the minimal interface criterion. *Arch. Rat. Mech. Anal.*, 98(2):123–142, 1987.

[10] H. Nakazawa and T. Ohta. Microphase separation of ABC-type triblock copolymers. *Macromolecules*, 26(20):5503–5511, 1993.

[11] Y. Nishiura and I. Ohnishi. Some mathematical aspects of the microphase separation in diblock copolymers. *Physica D*, 84:31–39, 1995.

[12] I. Ohnishi, Y. Nishiura, M. Imai, and Y. Matsushita. Analytical solutions describing the phase separation driven by a free energy functional containing a long-range interaction term. *Chaos*, 9(2):329–341, 1999.

[13] T. Ohta and K. Kawasaki. Equilibrium morphology of block copolymer melts. *Macromolecules*, 19(10):2621–2632, 1986.

[14] X. Ren and J. Wei. On the multiplicity of solutions of two nonlocal variational problems. *SIAM J. Math. Anal.*, 31(4):909–924, 2000.

[15] X. Ren and J. Wei. Concentrically layered energy equilibria of the di-block copolymer problem. *European J. Appl. Math.*, 13(5):479–496, 2002.

[16] X. Ren and J. Wei. On energy minimizers of the di-block copolymer problem. *Interfaces Free Bound.*, 5(2):193–238, 2003.

[17] X. Ren and J. Wei. On the spectra of 3-D lamellar solutions of the diblock copolymer problem. *SIAM J. Math. Anal.*, 35(1):1–32, 2003.

[18] X. Ren and J. Wei. Triblock copolymer theory: Free energy, disordered phase and weak segregation. *Physica D*, 178(1-2):103–117, 2003.

[19] X. Ren and J. Wei. Triblock copolymer theory: Ordered ABC lamellar phase. *J. Nonlinear Sci.*, 13(2):175–208, 2003.

[20] X. Ren and J. Wei. Nucleation in the FitzHugh-Nagumo system: interface-spike solutions. preprint.

[21] X. Ren and J. Wei. Stability of spot and ring solutions of the diblock copolymer equation. preprint.

[22] X. Ren and J. Wei. Wriggled lamellar solutions and their stability in the diblock copolymer problem. preprint.

[23] T. Teramoto and Y. Nishiura. Double gyroid morphology in a gradient system with nonlocal effects. *Journal of the Physical Society of Japan*, 71(7):161 1–1614, 2002.