Droplet Solutions in the Diblock Copolymer Problem with Skewed Monomer Composition

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

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

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Abstract

A droplet solution characterizes the lamellar phase of a diblock copolymer when the two composing monomers maintain a skewed ratio. We study the threshold case where the free energy of a droplet solution is comparable to the free energy of the constant solution. Using a Lyapunov-Schmidt reduction approach, adapted to calculus of variations, we prove the existence of a free energy local minimizer with a given number of droplets. Also determined are the free energy, the droplet location, and the droplet size.

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 [15] 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

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

*Corresponding author. Phone: 1 435 797-0755, Fax 1 435 797-1822, E-mail: ren@math.usu.edu
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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 $W(u) = \frac{1}{4}(u^2 - u)^2$.

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

$$-\xi'' = \zeta \text{ in } (0,1),\ \xi'(0) = \xi'(1) = 0,\ \ \overline{\xi} = 0. \tag{1.3}$$

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 and Mortola [11], Modica [10], and Kohn and Sternberg [9]). This was the approach used in Ren and Wei [16]. In terms of the number of A-monomers and B-monomers, N_A and N_B, in each chain molecule

$$a = \frac{N_A}{N_A + N_B}. \tag{1.4}$$

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

$$N_A \sim N_B. \tag{1.5}$$

In [16] we found local minimizers that characterize the lamellar phase of a diblock copolymer. A typical local minimizer is shown in Figure 1. It is close to 0 in some intervals and close to 1 in other intervals. The two types of intervals are comparable in length, and they are separated by sharp interfaces.

In this paper we consider a case where N_A and N_B are large but *not comparable*. Namely we assume a skewed relationship that N_A and $\sqrt{N_B}$ are comparable:

$$N_A \sim \sqrt{N_B}. \tag{1.6}$$

Hence N_A is a lot smaller than N_B. The condition (1.6) turns out to be equivalent to (cf. Choksi and Ren [3])

$$a \sim \epsilon^{1/2},\ \sigma \sim 1. \tag{1.7}$$

Therefore throughout this paper we take the positive a to be

$$a = \epsilon^{1/2} a_0,\ \text{where}\ \ a_0 > 0 \text{ is independent of } \epsilon, \tag{1.8}$$

and assume that σ is independent of ϵ.

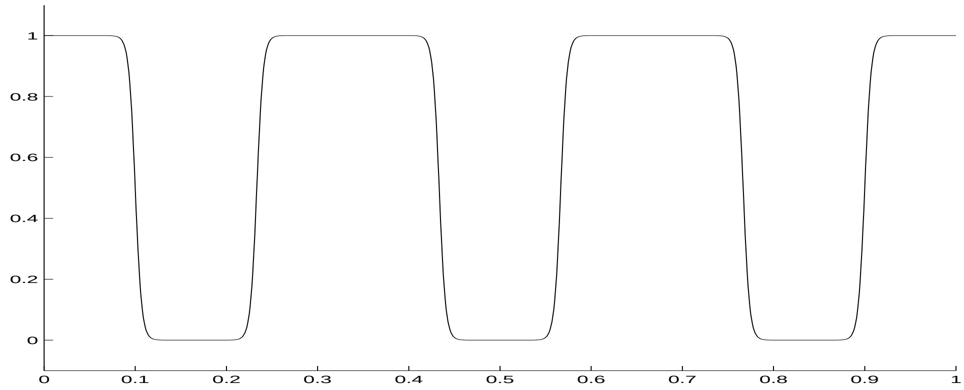

Figure 1: A local minimizer with 6 interfaces in the case (1.5).

In addition to its physical relevance, the condition (1.7) generates some interesting mathematical questions. Define a nonlinear operator

$$S(u) = -\epsilon^2 u'' + f(u) - \overline{f(u)} + \sigma(-\Delta)^{-1}(u - a) \tag{1.9}$$

where $f = W'$. If W is the particular $W(u) = \frac{1}{4}(u^2 - u)^2$, then f is $f(u) = u(u - \frac{1}{2})(u - 1)$. S is defined from the space

$$\mathcal{X} = \{u \in W^{2,2}(0,0) : \overline{u} = a,\ u'(0) = u'(1) = 0,\} \tag{1.10}$$

to the space

$$\mathcal{Y} = \{z \in L^2(0,1) : \overline{z} = 0\} \tag{1.11}$$

The Euler-Lagrange equation of I is

$$S(u) = 0,\ u \in \mathcal{X}. \tag{1.12}$$

The standard Γ-limit approach used in [16] to solve (1.12) is to identify a limiting functional of $\epsilon^{-1}I$. 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 [16], the value a must be ϵ *independent*. The parameter range (1.8) can not be dealt with by straightforward Γ-limit argument. Instead we will use a Lyapunov-Schmidt reduction approach, adapted specifically for calculus of variations. The latter method is more complex because one must understand the linearization of S at some carefully constructed approximate solutions. One may roughly regard the Γ-limit theory as a C^0 singular limit theory and the Lyapunov-Schmidt theory as a C^2 theory.

The solutions of (1.12) that we are interested in will model the lamellar phase of a diblock copolymer. They must be non-constant local minimizers of I. Because of the skewed value (1.8), we want a solution to be close to 0 everywhere except in some small intervals where the solution is close to 1 (Figure 2). We call these small intervals droplets, and call the solution a droplet solution. The condition (1.7) ensures that (1.6) is met, and the sample is of the proper size so a finite number of droplets are observed. We will show that the size of the droplets is of order $\epsilon^{1/2}$.

The parameter range (1.7) 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 $u = a$.

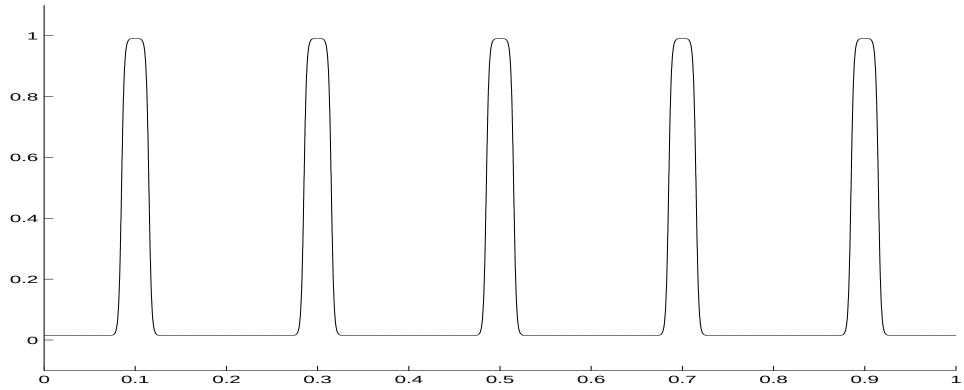

Figure 2: A local minimizer with 5 droplets in the case (1.6).

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*

$$\epsilon[2N\tau + f'(0)a_0^2(\frac{1}{2} - \frac{\coth\beta - \operatorname{csch}\beta}{\beta})] + o(\epsilon) \tag{1.13}$$

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

More information about the N-droplet local minimizer will be available as we prove the theorem. In particular we will know the location and the size of the droplets.

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 $w_\xi + \mathcal{F}_\xi$ form a local decomposition of $\mathcal{X}$. In Section 3 we find ϕ_ξ so that $w_\xi + \phi_\xi$ solves (1.12) in the fiber direction. In Section 4 we prove that $w_\xi + \phi_\xi$ locally minimizes I in a similar fiber $w_\xi + \mathcal{P}_\xi$. To our knowledge this is the first time in the literature of Lyapunov-Schmidt reduction when the fiber solution is connected to the variational structure. Finally in Section 5 we find a particular ξ so that at this ξ, $w_\xi + \phi_\xi$ solves (1.12) in $\mathcal{X}$ and it is a local minimizer of I. A few remarks are included in Section 6 and some technical proofs are in the appendix.

The mathematical literature on the diblock copolymer problem includes Nishiura and Ohnishi [13], Ohnishi *et al* [14], Ren and Wei [18, 17, 21, 19, 24, 22, 25], Choksi [2], Fife and Hilhorst [5], Henry [7], and Teramoto and Nishiura [26]. More information on the model (1.1) and its extension to triblock copolymers may be found in Nakazawa and Ohta [12], and Ren and Wei [20].

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 interfaces are at the ξ_j's. An interface is a point where the approximate solution changes between 0 and 1. Mathematically we require that the approximate solution is equal to $1/2$ at an interface 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:

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

Hence the first droplet is bounded by the interfaces ξ_1 and ξ_2, and the second droplet is bounded by the interfaces ξ_3 and ξ_4, etc. 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

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

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). Because l_k is of order 1, the size of each droplet is of order $\epsilon^{1/2}$.

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

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

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

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

$H(t)$ approaches 0 (or 1 respectively) exponentially fast as t tends to $-\infty$ (or ∞ respectively) in the sense that there exist positive C_1, C_2 so that

$$0 < H(t) < C_1 e^{C_2 t} \text{ if } t < 0, \text{ and } 0 < 1 - H(t) < C_1 e^{-C_2 t} \text{ if } t > 0. \tag{2.7}$$

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 to make

$$w_{\xi,1}(x)=\sum_{j=1}^{2N}\chi(x-\xi_j)H((-1)^{j+1}\frac{x-\xi_j}{\epsilon})+(1-\sum_{j=1}^{2N}\chi(x-\xi_j))s_\xi(x). \tag{2.8}$$

where χ is defined to be

$$\chi(x)=\begin{cases}1 & \text{in} \quad (-\epsilon^\alpha,\epsilon^\alpha)\\ 0 & \text{in} \quad \mathbf{R}\backslash(-2\epsilon^\alpha,2\epsilon^\alpha)\end{cases}. \tag{2.9}$$

The exponent α in (2.9) satisfies

$$\frac{1}{2}<\alpha<1. \tag{2.10}$$

χ satisfies

$$\chi=O(1),\ \chi'=O(\epsilon^{-\alpha}),\ \chi''=O(\epsilon^{-2\alpha}). \tag{2.11}$$

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

$$f'(0)w_{\xi,2}+\sigma(-\Delta)^{-1}(w_{\xi,1}+w_{\xi,2}-a)=f'(0)\overline{w_{\xi,2}},\ \overline{w_{\xi,1}+w_{\xi,2}-a}=0 \tag{2.12}$$

which may be written as

$$-Dw''_{\xi,2}+w_{\xi,2}+w_{\xi,1}-a=0,\ w'_{\xi,2}(0)=w'_{\xi,2}(1)=0. \tag{2.13}$$

Here

$$D=\frac{f'(0)}{\sigma}. \tag{2.14}$$

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

$$-D\frac{G^2(x,y)}{\partial x^2}+G(x,y)=\delta(x-y),\quad \frac{\partial G(0,y)}{\partial x}=\frac{\partial G(1,y)}{\partial x}=0 \tag{2.15}$$

where $\delta(\cdot)$ is the delta measure.

Lemma 2.1

$$w_{\xi,2}(x)=\epsilon^{1/2}(a_0-\sum_{j=1}^{N}2l_jG_D(x,\zeta_j))+O(\epsilon). \tag{2.16}$$

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

$$w_\xi=w_{\xi,1}+w_{\xi,2}\in\mathcal{X}. \tag{2.17}$$

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

$$\mathcal{M}=\{w_\xi\in\mathcal{X}:\xi\in\Lambda\}. \tag{2.18}$$

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

$$\begin{aligned}
\overline{f(w_\xi)} &= \int_0^1 f(w_{\xi,1})\,dx + \int_0^1 f'(w_{\xi,1})w_{\xi,2}\,dx + O(\epsilon) && (2.19)\\
&= \int_0^1 f'(w_{\xi,1})w_{\xi,2}\,dx + O(\epsilon) && (2.20)\\
&= f'(0)\overline{w_{\xi,2}} + \int_0^1 [f'(w_{\xi,1}) - f'(0)]w_{\xi,2}\,dx + O(\epsilon) && (2.21)\\
&= f'(0)\overline{w_{\xi,2}} + O(\epsilon). && (2.22)
\end{aligned}$$

To reach (2.22) we have used the fact that $f'(w_{\xi,1}) - f'(0) = O(1)$ only on ϵ-size neighborhoods of ξ_j. Elsewhere $w_{\xi,1}$ is exponentially close to 0 or 1, and hence $f'(w_{\xi,1}) - f'(0)$ is exponentially close to 0. Then using (2.12) we find that

$$\begin{aligned}
S(w_\xi) &= -\epsilon^2 w_\xi'' + f(w_\xi) + \sigma(-\Delta)^{-1}(w_\xi - a) - f'(0)\overline{w_{\xi,2}} + O(\epsilon) && (2.23)\\
&= -\epsilon^2 w_\xi'' + f(w_\xi) - f'(0)w_{\xi,2} + O(\epsilon) && (2.24)\\
&= -\epsilon^2 w_{\xi,1}'' - \epsilon^2 w_{\xi,2}'' + f(w_{\xi,1}) + f'(w_{\xi,1})w_{\xi,2} - f'(0)w_{\xi,2} + O(\epsilon) && (2.25)\\
&= (-\epsilon^2 w_{\xi,1}'' + f(w_{\xi,1})) + (f'(w_{\xi,1}) - f'(0))w_{\xi,2} + O(\epsilon) && (2.26)\\
&= (f'(w_{\xi,1}) - f'(0))w_{\xi,2} + O(\epsilon). && (2.27)
\end{aligned}$$

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

$$h_j(x) = H'(\frac{x - x_j}{\epsilon})\kappa(\frac{x - x_j}{\sqrt{\epsilon}}) - \overline{H'(\frac{x - x_j}{\epsilon})\kappa(\frac{x - x_j}{\sqrt{\epsilon}})} = H'(\frac{x - x_j}{\epsilon}) - \epsilon + O(e^{-C/\epsilon}). \tag{2.28}$$

where κ is a smooth, even cut-off function

$$\kappa(s) = \begin{cases} 1 & \text{if } |s| \le 1 \\ 0 & \text{if } |s| \ge 2 \end{cases}. \tag{2.29}$$

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 $\|h_j'' - \epsilon^{-2}H'''(\frac{\cdot - x_j}{\epsilon})\|_\infty = O(\epsilon^{-C/\epsilon})$. Not emphasized in the notation, the h_j's defined in (2.28) depend on ξ.

At each w_ξ of the manifold we define the space

$$\mathcal{F}_\xi = \{\phi \in W^{2,2}(0,1) :\ \overline{\phi} = 0,\ \phi'(0) = \phi'(1) = 0,\ \ \phi \perp h_j,\ j = 1, 2, ..., 2N\} \tag{2.30}$$

where $\perp$ is defined from the $L^2(0,1)$ inner product. Then $w_\xi + \mathcal{F}_\xi$ 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

$$\mathcal{E}_\xi = \{q \in L^2(0,1) : \overline{q} = 0,\ q \perp h_j,\ j = 1, 2, ..., 2N\} \tag{2.31}$$

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

$$\pi_\xi : \mathcal{Y} \to \mathcal{E}_\xi. \tag{2.32}$$

3 Solvability in fibers

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

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

This means that we solve $S(u) = 0$ in the fiber direction. 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 $\pi_\xi \circ L_\xi$:

$$\pi_\xi \circ L_\xi : \mathcal{F}_\xi \to \mathcal{E}_\xi \tag{3.6}$$

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 $\epsilon \to 0$,

$$\|\pi_\xi \circ L_\xi(\psi)\| \to 0. \tag{3.7}$$

Write (3.7) as

$$-\epsilon^2\psi'' + f'(w_\xi)\psi - \overline{f'(w_\xi)\psi} + \sigma(-\Delta)^{-1}\psi - \sum_{j=1}^{2N} \beta_j h_j = o(1) \tag{3.8}$$

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

$$\int_0^1 [\epsilon^2|\psi'|^2 + f'(w_\xi)\psi^2 + \sigma|\varphi'|^2]\,dx = o(1). \tag{3.9}$$

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

$$\int_0^1 |\varphi'|^2\,dx = o(1). \tag{3.10}$$

The Sobolev embedding theory yields

$$\|\varphi\| = o(1). \tag{3.11}$$

We must estimate the size of β_j. To this end we multiply (3.8) by h_k and integrate. Then

$$\int_0^1 [(-\epsilon^2\psi'' + f'(w_\xi)\psi + \sigma\varphi)h_k]\,dx + \sum_{j=1}^{2N} \beta_j\langle h_j, h_k\rangle = o(\epsilon). \tag{3.12}$$

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

$$\int_0^1 (-\epsilon^2\psi'' + f'(w_\xi) + \sigma\varphi)h_k\,dx + \sum_{j=1}^{2N} \beta_j(\epsilon\tau\delta_{jk} + O(\epsilon^2)) = o(\epsilon) \tag{3.13}$$

where $\delta_{jk} = 1$ if $j \neq k$ and 0 if $j = k$. Also we have used the fact that

$$\tau = \int_{\mathbf{R}} (H')^2\,dt. \tag{3.14}$$

The first part of the left side of (3.13) is estimated as follows:

$$\int_0^1 [(-\epsilon^2\psi'' + f'(w_\xi)\psi + \sigma\varphi)h_k]\,dx \tag{3.15}$$

$$= \int_0^1 (-\epsilon^2 h_k''\psi + f'(w_\xi)\psi h_k)\,dx + \int_0^1 \sigma\varphi h_k\,dx \tag{3.16}$$

$$= \int_0^1 [(-H'''(\frac{x-\xi_k}{\epsilon}) + f'(w_\xi)H(\frac{x-\xi_k}{\epsilon}))\psi - f'(w_\xi)\psi\epsilon]\,dx + \int_0^1 \sigma\varphi h_k\,dx \tag{3.17}$$

$$= O(\epsilon). \tag{3.18}$$

This simplifies (3.13) to

$$\sum_{j=1}^{2N} \beta_j(\epsilon\tau\delta_{jk} + O(\epsilon^2)) = O(\epsilon). \tag{3.19}$$

Hence

$$\beta_j = O(1). \tag{3.20}$$

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 (3.11),

$$\begin{aligned} L_\xi(\psi)(y) &= -\epsilon^2\psi''(y) + f'(w_\xi(y))\psi(y) - \overline{f'(w_\xi)\psi} + \sigma((-\Delta)^{-1}\psi)(y) && (3.21)\\ &\geq 0 + f'(w_\xi(y)) - \overline{(f'(w_\xi) - f'(0))\psi} + \sigma((-\Delta)^{-1}\psi)(y) && (3.22)\\ &= f'(w_\xi(y)) + \sigma\varphi(y) + O(\epsilon) \;=\; f'(w_\xi(y)) + o(1) && (3.23)\\ &= f'(0) + o(1). && (3.24) \end{aligned}$$

Combining (3.20) and (3.24), we obtain

$$\pi_\xi \circ L_\xi(\psi)(y) \geq f'(0) - \sum_{j=1}^{2N} \beta_j h_j(y) + o(1) \geq f'(0) + o(1) \tag{3.25}$$

which contradicts (3.7).

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 (3.8), (3.11), and (3.20) imply

$$-\Psi'' + f'(w_\xi(\xi_j + \epsilon t))\Psi - \beta_j H' \to 0 \tag{3.26}$$

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

$$-\Psi''_\infty + f'(H)\Psi_\infty - \beta_j^0 H' = 0. \tag{3.27}$$

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

$$-\Psi''_\infty + f'(H)\Psi_\infty = 0. \tag{3.28}$$

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 $\overline{\psi} = 0$, we deduce that

$$0 = \langle \psi, h_j \rangle = \epsilon \int_{-\xi_j/\epsilon}^{(1-\xi_j)/\epsilon} \Psi(t)(H'(t) - O(e^{-C/\epsilon}))\, dt = \epsilon(c \int_{\mathbf{R}} (H'(t))^2\, dt + o(1)) \tag{3.29}$$

which is impossible. We have thus proved part 1 of the lemma.

To prove part 2 of the lemma we need to solve

$$\pi_\xi \circ L_\xi(\phi) = p \tag{3.30}$$

in $\mathcal{F}_\xi$ for any given $p \in \mathcal{E}_\xi$. By applying $\pi_\xi \circ (-\Delta)^{-1}$ to both sides of (3.30) we consider the equation

$$\pi_\xi \circ (-\Delta)^{-1} \circ \pi_\xi \circ L_\xi(\phi) = \pi_\xi \circ (-\Delta)^{-1} p. \tag{3.31}$$

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. For this operator F_ξ is viewed as a Banach space whose norm is inherited from the $W^{2,2}(0,1)$ norm. The operator has the form

$$\epsilon^2(\text{Identity Operator}) + \text{Compact Operator}. \tag{3.32}$$

According to the Fredholm Alternative, (3.31) is solvable if

$$\pi_\xi \circ (-\Delta)^{-1} \circ \pi_\xi \circ L_\xi(\phi) = 0 \tag{3.33}$$

only has the trivial solution. To see this we write (3.33) as

$$(-\Delta)^{-1} \circ \pi_\xi \circ L_\xi(\phi) = \sum_{j=1}^{2N} \alpha_j h_j \tag{3.34}$$

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

$$\pi_\xi \circ L_\xi(\phi) = \sum_{j=1}^{2N} \alpha_j(-h_j''). \tag{3.35}$$

We multiply it by h_k and integrate to deduce

$$0 = \sum_{j=1}^{2N} \alpha_j \int_0^1 h_j' h_k' \, dx = \alpha_k \int_0^1 |h_k'|^2 \, dx, \ \ k = 1, 2, ..., 2N, \tag{3.36}$$

which implies that $\alpha_j = 0$, $j = 1, 2, ..., 2N$. Then (3.35) becomes

$$\pi_\xi \circ L_\xi(\phi) = 0. \tag{3.37}$$

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

Hence (3.31) 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

$$(-\Delta)^{-1} \circ \pi_\xi \circ L_\xi(\phi) = (-\Delta)^{-1} p + \sum_{j=1}^{2N} \beta_j h_j. \tag{3.38}$$

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

$$\pi_\xi \circ L_\xi(\phi) = p + \sum_{j=1}^{2N} \beta_j(-h_j''). \tag{3.39}$$

We multiply by h_k and integrate to obtain

$$0 = \sum_{j=1}^{2N} \beta_j \int_0^1 h_j' h_k' \, dx = \beta_k \int_0^1 |h_k'|^2 \, dx, \ \ k = 1, 2, ..., 2N, \tag{3.40}$$

which implies that $\beta_j = 0$, for all $j = 1, 2, ..., 2N$. Then (3.39) becomes (3.30). $\square$

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:

$$\phi_\xi = (\pi_\xi \circ L_\xi)^{-1}(-\pi_\xi \circ S(w_\xi) - \pi_\xi \circ R_\xi(\phi_\xi)) \tag{3.41}$$

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

$$T_\xi(\phi) = (\pi_\xi \circ L_\xi)^{-1}(-\pi_\xi \circ S(w_\xi) - \pi_\xi \circ R_\xi(\phi)) \tag{3.42}$$

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

$$\mathcal{D}(T_\xi) = \{\phi \in L^\infty(0,1) : \overline{\phi} = 0,\ \phi \perp h_j,\ j = 1, 2, ..., 2N\} \tag{3.43}$$

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

$$\mathcal{B}_\xi = \{\phi \in \mathcal{D}(T_\xi) : \|\phi\| \leq C_2\epsilon^{1/2}\} \tag{3.44}$$

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

$$\begin{aligned} \|T_\xi(\phi)\| &\leq C_1\|\pi_\xi \circ S(w_\xi)\| + C_1\|\pi_\xi \circ R_\xi(\phi)\| && (3.45)\\ &\leq C_3\epsilon^{1/2} + C_5(1 + O(\|\phi\|))\|\phi\|^2 && (3.46)\\ &\leq C_3\epsilon^{1/2} + C_6C_2^2(1 + C_2\epsilon^{1/2})\epsilon && (3.47) \end{aligned}$$

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

$$\|R_\xi(\phi)\| \leq 2\|f(w_\xi + \phi) - f(w_\xi) - f'(w_\xi)\phi\| \leq C_4(1 + O(\|\phi\|))\|\phi\|^2 \tag{3.48}$$

for some C_4 depending on f only. In (3.47) 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 (3.47) 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

$$\begin{aligned} \|T_\xi(\phi_1) - T_\xi(\phi_2)\| &\leq C_1\|\pi_\xi \circ (R_\xi(\phi_1) - R_\xi(\phi_2))\| \ \leq\ C_7\|R_\xi(\phi_1) - R_\xi(\phi_2)\| && (3.49)\\ &\leq C_8\|f(w_\xi + \phi_1) - f(w_\xi + \phi_2) - f'(w_\xi)(\phi_1 - \phi_2)\| && (3.50)\\ &\leq C_8\|f'(w_\xi + \phi_2 + \theta(\phi_1 - \phi_2))(\phi_1 - \phi_2) - f'(w_\xi)(\phi_1 - \phi_2)\| && (3.51)\\ &\leq C_8\|f'(w_\xi + \phi_2 + \theta(\phi_1 - \phi_2)) - f'(w_\xi)\|\ \|\phi_1 - \phi_2\| && (3.52)\\ &\leq O(\|\phi_1\| + \|\phi_2\|)\ \|\phi_1 - \phi_2\| && (3.53)\\ &\leq C_9\epsilon^{1/2}\|\phi_1 - \phi_2\| && (3.54) \end{aligned}$$

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. □

4 Stability in fibers

In this section we connect the fiber solution $w_\xi + \phi_\xi$ to the variational structure I. The manifold $\mathcal{M}$ is also embedded in the admissible set $\mathcal{A}$ defined in (1.2). At each w_ξ we let

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

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 minimizes I in $w_\xi + \mathcal{P}_\xi$. We first study the linearization of S at $w_\xi + \phi_\xi$. Set

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

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 $\liminf_{\epsilon\to 0} \lambda \le 0$. 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

$$-\epsilon^2\psi'' + f'(g_\xi)\psi - \overline{f'(g_\xi)\psi} + \sigma(-\Delta)^{-1}\psi = \lambda\psi + \sum_{j=1}^{2N}\beta_j h_j,\ \psi'(0) = \psi'(1) = 0, \tag{4.3}$$

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

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

where

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

The assumption $\liminf_{\epsilon\to 0} \lambda \le 0$ 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 (3.20) 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 (3.24)

$$f'(0)+o(1) \leq -\epsilon^2\psi''(y)+f'(g_\xi(y))\psi(y)-\overline{f'(g_\xi)\psi}+\sigma\varphi(y) = \lambda\psi(y)+\sum_{j=1}^{2N}\beta_j h_j(y) = \lambda+o(1) \quad (4.11)$$

with the help of (4.8) and (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

$$-\Psi''(t) + f'(g_\xi(\xi_j + \epsilon t))\Psi + o(1) = \lambda\Psi(t) + \sum_{j=1}^{2N}\beta_j h_j(\xi_k + \epsilon t), \; t \in (-\frac{\xi_k}{\epsilon}, \frac{1-\xi_k}{\epsilon}). \quad (4.12)$$

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

$$-\Psi''_\infty + f'(H)\Psi_\infty = (\liminf_{\epsilon\to 0} \lambda)\Psi_\infty + \beta^0_k H' \quad (4.13)$$

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

$$0 = \int_0^1 \psi h_k \, dx = \int_0^1 \psi(H'(\frac{x-\xi_\epsilon}{\epsilon}) + O(e^{-C/\epsilon}))\, dx = \epsilon \int_{\mathbf{R}} \Psi_\infty(t)H'(t)\, dt + o(\epsilon). \quad (4.14)$$

Therefore

$$\int_{\mathbf{R}} \Psi_\infty H' \, dt = 0. \quad (4.15)$$

We multiply (4.13) by H' and integrate. Because of (4.15) we obtain from (4.13) that

$$0 = \beta^0_k \int_{\mathbf{R}} (H')^2 \, dt, \text{ i.e. } \beta^0_k = 0. \quad (4.16)$$

Then (4.13) becomes

$$-\Psi''_\infty + f'(H)\Psi_\infty = (\liminf_{\epsilon\to 0} \lambda)\Psi_\infty. \quad (4.17)$$

The equation (4.17) 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 (4.15). □

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

$$I(g_\xi+\psi) = I(g_\xi)+\int_0^1 S(g_\xi)\psi+\frac{1}{2}\int_0^1 [\epsilon^2(\psi')^2+f'(g_\xi)\psi^2+\sigma|(-\Delta)^{-1/2}\psi|^2]+\frac{1}{6}\int_0^1 f''(..)\psi^3. \quad (4.18)$$

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

$$I(g_\xi + \psi) = I(g_\xi) + \frac{1}{2}\int_0^1 [\epsilon^2(\psi')^2 + f'(g_\xi)\psi^2 + \sigma|(-\Delta)^{-1/2}\psi|^2]\, dx + O(\|\psi\|)\ \|\psi\|_2^2 \tag{4.19}$$

which by (4.2) implies

$$I(g_\xi + \psi) \geq I(g_\xi) + (\frac{\lambda}{2} - O(\|\psi\|))\ \|\psi\|_2^2 \tag{4.20}$$

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

$$\mathcal{N}_\xi = \{\psi \in \mathcal{P}_\xi : \|\psi\| < C_1\} \tag{4.21}$$

of $\mathcal{P}_\xi$ for some $C_1 > 0$. If we take C_1 to be sufficiently small (but independent of ϵ), then (4.20) and Lemma 4.1 imply that there exists $C_2 > 0$, independent of ϵ, so that

$$I(g_\xi + \psi) \geq I(g_\xi) + C_2\ \|\psi\|_2^2,\ \text{for all } \psi \in \mathcal{N}_\xi. \tag{4.22}$$

Lemma 4.2 follows from (4.22). □

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*

$$J(\zeta, l) = \epsilon[2N\tau + 4f'(0)Q(\zeta, l)] + O(\epsilon^{3/2}) \tag{5.2}$$

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

$$Q(\zeta, l) = \frac{1}{2}\sum_{k,j=1}^{N} l_k l_j G_D(\zeta_k, \zeta_j) - \frac{a_0}{2}\sum_{j=1}^{N} l_j + \frac{a_0^2}{8} \tag{5.3}$$

for (ζ, l) that satisfies $0 < \zeta_1 < \zeta_2 < ... < \zeta_N < 1$, $l_j > 0$, for $j = 1, 2, ..., 2N$.

Proof. We expand the energy of $w_\xi + \phi_\xi$ to find

$$J(\zeta, l) = I(w_\xi) + \int_0^1 S(w_\xi)\phi_\xi + \frac{1}{2}\int_0^1 [\epsilon^2|\phi_\xi'|^2 + f'(w_\xi)\phi_\xi^2 + \sigma|(-\Delta)^{-1/2}\phi_\xi|^2]\, dx + O(\epsilon^{3/2}). \tag{5.4}$$

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

$$-\epsilon^2\phi_\xi'' + f'(w_\xi)\phi_\xi - \overline{f'(w_\xi)\phi_\xi} + \sigma(-\Delta)^{-1}\phi_\xi + S(w_\xi) + O(\|\phi_\xi\|^2) = \sum_{j=1}^{2N}\beta_j h_j \tag{5.5}$$

for some $\beta_j \in \mathbf{R}$. Multiply (5.5) by ϕ_ξ and integrate to find

$$\int_0^1 [\epsilon^2|\phi_\xi'|^2 + f'(w_\xi)\phi_\xi^2 + \sigma|(-\Delta)^{-1/2}\phi_\xi|^2]\,dx + \int_0^1 S(w_\xi)\phi_\xi\,dx + O(\epsilon^{3/2}) = 0. \tag{5.6}$$

Substituting (5.6) to (5.4) we deduce

$$J(\zeta, l) = I(w_\xi) + \frac{1}{2}\int_0^1 S(w_\xi)\phi_\xi\,dx + O(\epsilon^{3/2}) \tag{5.7}$$

By Lemma 2.2 we obtain

$$\int_0^1 S(w_\xi)\phi_\xi\,dx = \int_0^1 (f'(w_{\xi,1}) - f'(0))w_{\xi,2}\phi_\xi\,dx + O(\epsilon^{3/2}) = O(\epsilon^{3/2}). \tag{5.8}$$

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 (5.7) becomes

$$J(\zeta, l) = I(w_\xi) + O(\epsilon^{3/2}). \tag{5.9}$$

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

$$\begin{aligned}
I(w_\xi) &= \frac{\epsilon^2}{2}\int_0^1 |w_{\xi,1}'|^2\,dx + \epsilon^2\int_0^1 w_{\xi,1}'w_{\xi,2}'\,dx && (5.10)\\
&+ \int_0^1 W(w_{\xi,1})\,dx + \int_0^1 f(w_{\xi,1})w_{\xi,2}\,dx + \frac{1}{2}\int_0^1 f'(w_{\xi,1})w_{\xi,2}^2\,dx && (5.11)\\
&+ \frac{\sigma}{2}\int_0^1 |(-\Delta)^{-1/2}(w_{\xi,1} + w_{\xi,2} - a)|^2\,dx + O(\epsilon^{3/2}) && (5.12)\\
&= \frac{\epsilon^2}{2}\int_0^1 |w_{\xi,1}'|^2\,dx + \int_0^1 W(w_{\xi,1})\,dx && (5.13)\\
&+ \epsilon^2\int_0^1 w_{\xi,1}'w_{\xi,2}'\,dx + \int_0^1 f(w_{\xi,1})w_{\xi,2}\,dx && (5.14)\\
&+ \frac{1}{2}\int_0^1 f'(w_{\xi,1})w_{\xi,2}^2\,dx + \frac{\sigma}{2}\int_0^1 |(-\Delta)^{-1/2}(w_{\xi,1} + w_{\xi,2} - a)|^2\,dx + O(\epsilon^{3/2}) && (5.15)\\
&= 2N\tau\epsilon + \frac{1}{2}\int_0^1 f'(w_{\xi,1})w_{\xi,2}^2 && (5.16)\\
&+ \frac{\sigma}{2}\int_0^1 (w_{\xi,1} + w_{\xi,2} - a)(-\Delta)^{-1}(w_{\xi,1} + w_{\xi,2} - a) + O(\epsilon^{3/2}) && (5.17)\\
&= 2N\tau\epsilon + \frac{1}{2}\int_0^1 f'(w_{\xi,1})w_{\xi,2}^2 - \frac{f'(0)}{2}\int_0^1 (w_{\xi,1} + w_{\xi,2} - a)w_{\xi,2} + O(\epsilon^{3/2}) && (5.18)\\
&= 2N\tau\epsilon + \frac{1}{2}\int_0^1 (f'(w_{\xi,1}) - f'(0))w_{\xi,2}^2 - \frac{f'(0)}{2}\int_0^1 (w_{\xi,1} - a)w_{\xi,2} + O(\epsilon^{3/2}) && (5.19)\\
&= 2N\tau\epsilon - \frac{f'(0)}{2}\int_0^1 (w_{\xi,1} - a)w_{\xi,2}\,dx + O(\epsilon^{3/2}) && (5.20)
\end{aligned}$$

$$= \quad 2N\tau\epsilon - \frac{f'(0)\epsilon}{2}\int_0^1 (\frac{w_{\xi,1}}{\epsilon^{1/2}} - a_0)(a_0 - \sum_{j=1}^N 2l_j G_D(x,\zeta_j))\,dx + O(\epsilon^{3/2}) \tag{5.21}$$

$$= \quad 2N\tau\epsilon - \frac{f'(0)\epsilon}{2}[\int_0^1 \frac{w_{\xi,1}}{\epsilon^{1/2}} a_0\,dx - 2\int_0^1 \frac{w_{\xi,1}}{\epsilon^{1/2}}(\sum_{j=1}^N l_j G_D(x,\zeta_j))\,dx \tag{5.22}$$

$$-a_0^2 + 2a_0\int_0^1 (\sum_{j=1}^N l_j G_D(x,\zeta_j))\,dx] + O(\epsilon^{3/2})$$

$$= \quad 2N\tau\epsilon - \frac{f'(0)\epsilon}{2}[2a_0\sum_{j=1}^N l_j - 4\sum_{k,j=1}^N l_k l_j G_D(\zeta_k,\zeta_j) - a_0^2 + 2a_0\sum_{j=1}^N l_j] + O(\epsilon^{3/2}) \tag{5.23}$$

$$= \quad 2N\tau\epsilon + 4f'(0)\epsilon[\frac{1}{2}\sum_{k,j=1}^N l_k l_j G_D(\zeta_k,\zeta_j) - \frac{a_0}{2}\sum_{j=1}^N l_j + \frac{a_0^2}{8}] + O(\epsilon^{3/2}). \tag{5.24}$$

This proves the lemma. □

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

$$\zeta_1^0 = \frac{1}{2N},\ \zeta_2^0 = \frac{3}{2N},\ \zeta_3^0 = \frac{5}{2N},\ \ldots,\ \zeta_j^0 = \frac{2j-1}{2N},\ \ldots,\ \zeta_N^0 = \frac{2N-1}{2N} \tag{5.25}$$

and

$$l_j^0 = a_0\sqrt{D}(\coth\frac{1}{N\sqrt{D}} - \operatorname{csch}\frac{1}{N\sqrt{D}}),\ j = 1, 2, \ldots, N. \tag{5.26}$$

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

$$p(x) = \sum_{k=1}^N G_D(x,\zeta_k) l_k. \tag{5.27}$$

Calculations show that

$$\frac{\partial Q}{\partial \zeta_j} \quad = \quad \frac{l_j}{2}(p'(\zeta_j-) + p'(\zeta_j+)), \tag{5.28}$$

$$\frac{\partial Q}{\partial l_j} \quad = \quad \sum_{k=1}^N G_D(\zeta_j,\zeta_k) l_k - \frac{a_0}{2} \ = \ p(\zeta_j) - \frac{a_0}{2}. \tag{5.29}$$

Now we assume that (ζ, l) is a critical point of Q. Then (5.28) and (5.29) imply that

$$p'(\zeta_j-) + p'(\zeta_j+) \quad = \quad 0, \tag{5.30}$$

$$p(\zeta_j) \quad = \quad \frac{a_0}{2}. \tag{5.31}$$

Since p satisfies the linear differential equation

$$-Dp'' + p = 0,\ \text{in } (0,1)\backslash\{\zeta_1, \zeta_2, \ldots, \zeta_N\},\ \text{and } p'(0) = p'(1) = 0, \tag{5.32}$$

(5.30) and (5.31) imply that

$$\zeta_1 = \frac{1}{2N},\ \zeta_2 = \frac{3}{2N},\ \zeta_3 = \frac{5}{2N},\ ...,\ \zeta_j = \frac{2j-1}{2N},\ ...,\ \zeta_N = \frac{2N-1}{2N}. \tag{5.33}$$

At a critical point (ζ, l), (5.29) implies that l satisfies the linear system

$$\begin{bmatrix} G_D(\zeta_1,\zeta_1) & G_D(\zeta_1,\zeta_2) & ... & G_D(\zeta_1,\zeta_N) \\ G_D(\zeta_2,\zeta_1) & G_D(\zeta_2,\zeta_2) & ... & G_D(\zeta_2,\zeta_N) \\ & ... & & \\ G_D(\zeta_N,\zeta_1) & G_D(\zeta_N,\zeta_2) & ... & G_D(\zeta_N,\zeta_N) \end{bmatrix} \begin{bmatrix} l_1 \\ l_2 \\ ... \\ l_N \end{bmatrix} = \frac{1}{2} \begin{bmatrix} a_0 \\ a_0 \\ ... \\ a_0 \end{bmatrix}. \tag{5.34}$$

It is shown in the appendix that at (5.33) the symmetric $N \times N$ matrix $[G_D(\zeta_j, \zeta_k)]$ is non-singular and

$$\sum_{k=1}^{N} G_D(\zeta_j, \zeta_k) = \frac{1}{2\sqrt{D}} \ \frac{1}{\coth(1/(N\sqrt{D})) - \operatorname{csch}(1/(N\sqrt{D}))}. \tag{5.35}$$

Note that the right side of (5.35) is independent of j. Therefore the unique solution to (5.34) is

$$l_j = a_0\sqrt{D}(\coth\frac{1}{N\sqrt{D}} - \operatorname{csch}\frac{1}{N\sqrt{D}}). \tag{5.36}$$

This proves the lemma. □

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

$$\frac{\partial^2 Q}{\partial l_j \partial l_k}(\zeta^0, l^0) = G_D(\zeta_j^0, \zeta_k^0). \tag{5.37}$$

We define a matrix $\mathbf{A}$ whose ik-entry a_{jk} is given by (5.37).

Next we write G_D as

$$G_D(x, y) = \Gamma(|x - y|) + R(x, y) \tag{5.38}$$

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

$$\Gamma(z) = \frac{1}{2\sqrt{D}}\exp(-\frac{z}{\sqrt{D}}),\quad R(x, y) = \frac{\cosh\frac{x+y-1}{\sqrt{D}} + \exp(-\frac{1}{\sqrt{D}})\cosh\frac{x-y}{\sqrt{D}}}{2\sqrt{D}\sinh\frac{1}{\sqrt{D}}}. \tag{5.39}$$

Then we calculate

$$\frac{\partial Q}{\partial \zeta_j} = \frac{1}{2}\frac{\partial}{\partial \zeta_j}[G_D(\zeta_j, \zeta_j) l_j^2] + \frac{\partial}{\partial \zeta_j}[\sum_{k\neq j} G_D(\zeta_j, \zeta_k) l_j l_k] \tag{5.40}$$

$$= R_1(\zeta_j, \zeta_j) l_j^2 + l_j \sum_{k \neq j} [\Gamma'(|\zeta_j - \zeta_k|)(\pm 1) + R_1(\zeta_j, \zeta_k)] l_k \tag{5.41}$$

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

$$\iota = l_1^0 = l_2^0 = ... = l_N^0 = a_0\sqrt{D}(\coth\frac{1}{N\sqrt{D}} - \operatorname{csch}\frac{1}{N\sqrt{D}}). \tag{5.42}$$

Then if $k \neq j$

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j \partial l_k} = \iota(\Gamma'(|\zeta_j^0 - \zeta_k^0|)(\pm 1) + R_1(\zeta_j^0, \zeta_k^0)), \ j \neq k. \tag{5.43}$$

If $k = j$,

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j \partial l_j} = 2\iota R_1(\zeta_j^0, \zeta_j^0) + \iota \sum_{k \neq j} (\Gamma'(|\zeta_j^0 - \zeta_k^0|)(\pm 1) + R_1(\zeta_j^0, \zeta_k^0)). \tag{5.44}$$

We define a matrix $\mathbf{B}$ whose jk-entry b_{jk} is given by (5.43) and (5.44).

If $k \neq j$,

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j \partial \zeta_k} = \iota^2(-\Gamma''(|\zeta_j^0 - \zeta_k^0|) + R_{12}(\zeta_j^0, \zeta_k^0)). \tag{5.45}$$

If $k = j$,

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j^2} = \iota^2(R_{11}(\zeta_j^0, \zeta_j^0) + R_{12}(\zeta_j^0, \zeta_j^0)) + \iota^2 \sum_{k \neq j} [\Gamma''(|\zeta_j^0 - \zeta_k^0|) + R_{11}(\zeta_j^0, \zeta_k^0)]. \tag{5.46}$$

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

$$\frac{\partial^2 Q(\zeta^0, l^0)}{\partial \zeta_j^2} = \iota^2(-\Gamma''(0) + R_{12}(\zeta_j^0, \zeta_j^0)) + \frac{\iota^2}{D} \sum_{k=1}^{N} G_D(\zeta_j^0, \zeta_k^0). \tag{5.47}$$

We define a matrix $\mathbf{C}$ whose jk-entry c_{jk} is given by (5.45) and (5.47).

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

$$\mathbf{H} = \left[\begin{array}{cc} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{C} \end{array} \right]. \tag{5.48}$$

It turns out that the matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ also appear in the stability analysis of multiple spike solutions to the Gierer-Meinhardt system. See Iron, Ward and Wei [8], and Wei and Winter [27]. By using the spectral information of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ we can show that the matrix $\mathbf{H}$ is positive definite. The argument is a bit long. We leave the complete proof to the appendix. □

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, 23]. 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 $\mathcal{A}$.

The energy estimate of the local minimizer is derived from Lemma 5.1, and the values of ζ^0 and l^0 are given in Lemma 5.2, and (5.35). □

6 Discussion

The size of each droplet of the local minimizer constructed in Theorem 1.1 is of order $\epsilon^{1/2}$ and the free energy of the local minimizer is of order ϵ. Interestingly the free energy of the constant a, which is also a local minimizer, is

$$\frac{f'(0)a_0^2}{2}\epsilon + O(\epsilon^{3/2}), \tag{6.1}$$

again of order ϵ. This suggests that if $a \ll \epsilon^{1/2}$, any droplet solution, if it exists, will have free energy much larger than the free energy of the constant a. So our parameter range (1.7) may well be an important threshold.

If in Theorem 1.1 we expand

$$\frac{\coth\beta - \operatorname{csch}\beta}{\beta} = \frac{1}{2} - \frac{\beta^2}{24} + ... \tag{6.2}$$

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

$$\epsilon(2N\tau + \frac{a_0^2\sigma}{24N^2}). \tag{6.3}$$

The last expression is minimized at

$$N_{opt} = (\frac{a_0^2\sigma}{24\tau})^{1/3} \tag{6.4}$$

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

Another interesting consequence of our work concerns the distribution of the A-monomers. The area under each droplet of an N-droplet local minimizer, by (5.36), is

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

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

$$\frac{2a_0}{\beta}(\coth\beta - \operatorname{csch}\beta)\epsilon^{1/2} + o(\epsilon^{1/2}). \tag{6.6}$$

On the other hand the total area under the graph of the local minimizer is $a = a_0\epsilon^{1/2}$. Since (6.2) implies that

$$\frac{2a_0}{\beta}(\coth\beta - \operatorname{csch}\beta) < a_0, \tag{6.7}$$

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 (5.35), and prove that all the eigenvalues of $\mathbf{H}$ are positive.

Arguing as in [19, Section 7] we find that the inverse matrix of $\mathbf{A}$ has the tridiagonal form

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

where

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

One rewrites (A.1) as

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

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

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

and that

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

where

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

Therefore

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

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

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

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 (5.35).

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 (5.39) 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 [19, Section 7] shows that

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

which 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 $\mathbf{Q}^T\mathbf{BP}$. 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

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

Recall that $\pm 1 = -1$ if $\zeta_j^0 < \zeta_k^0$ and $\pm 1 = 1$ if $\zeta_j^0 > \zeta_k^0$.

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

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

Then

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

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

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

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 by (A.26, A.27, A.28) we obtain

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

If we write $\mathbf{F} = \mathbf{Q}^T\mathbf{EP}$ and observe the first columns of the two sides of the equation $\mathbf{EP} = \mathbf{QF}$, 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 (A.22) simplifies to

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

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 using (A.8, A.19, A.20, A.33) show that the determinants of the 2×2 blocks (A.35) are again positive. Hence all the eigenvalues of $\mathbf{H}$ are positive.

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