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Droplet solutions in the diblock copolymer problem with skewed monomer composition

Accepted: 19 October 2005 / Published online: 24 October 2005
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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

Supported in part by a Direct Grant from CUHK and an earmarked Grant of RGC of Hong Kong.

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that a mixture of A - and B -monomers occupies x . In one-dimension the re-scaled, dimensionless free energy of the system is

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

The functional I is defined in the admissible set

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

where $\bar{u} = \int_0^1 u \, dx$ 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 non-local 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 $\{\zeta \in L^2(0, 1) : \bar{\zeta} = 0\}$ to $\{\xi \in W^{2,2}(0, 1) : \bar{\xi} = 0, \xi'(0) = \xi'(1) = 0\}$: $\xi = (-\Delta)^{-1}\zeta$ if

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

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

$$a = \frac{N_A}{N_A + N_B}. \quad (1.4)$$

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

$$N_A \sim N_B. \quad (1.5)$$

In [16] we found local minimizers that characterize the lamellar phase of a diblock copolymer. A typical local minimizer is shown in Fig. 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:

$$N_A \sim \sqrt{N_B}. \quad (1.6)$$

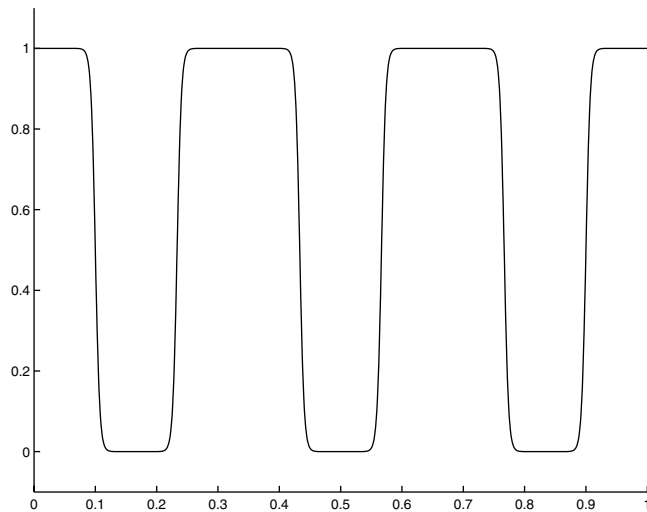


Fig. 1 A local minimizer with 6 interfaces in the case (1.5).

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 .

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

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

to the space

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

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 (Fig. 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 $u = a$. 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*

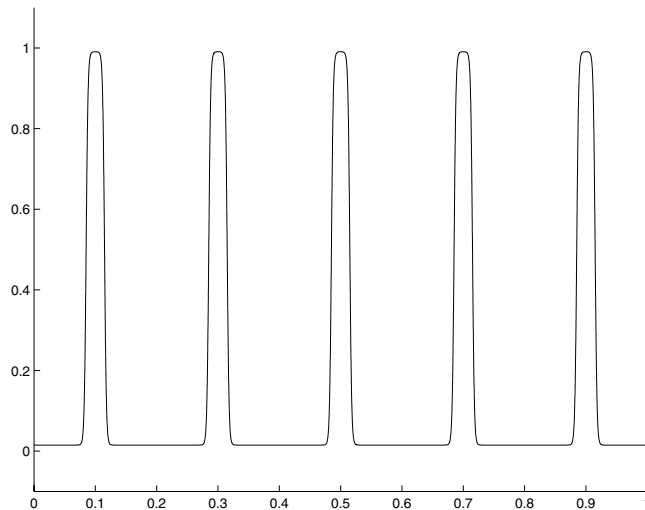


Fig. 2 A local minimizer with 5 droplets in the case (1.6).

minimizer is

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

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

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 (Sect. 2). The manifold \mathcal{M} and its fibers $w_\xi + \mathcal{F}_\xi$ form a local decomposition of \mathcal{X} . In Sect. 3 we find ϕ_ξ so that $w_\xi + \phi_\xi$ solves (1.12) in the fiber direction. In Sect. 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 Sect. 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 Sect. 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 [17, 18, 19, 21, 22, 24, 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, \dots , are all independent of ϵ . They may vary from place to place.

2 The approximate manifold and its fibers

Let $\xi_1, \xi_2, \dots, \xi_{2N}$ be $2N$ numbers in $(0, 1)$, satisfying $\xi_1 < \xi_2 < \dots < \xi_{2N}$. Given $\xi = (\xi_1, \xi_2, \dots, \xi_{2N})$ 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 :

$$\zeta_k = \frac{\xi_{2k-1} + \xi_{2k}}{2}, \quad k = 1, 2, \dots, N \quad (2.1)$$

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

$$l_k = \frac{\xi_{2k} - \xi_{2k-1}}{2\epsilon^{1/2}}, \quad k = 1, 2, \dots, N. \quad (2.2)$$

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 $\zeta = (\zeta_1, \zeta_2, \dots, \zeta_N)$ and $l = (l_1, l_2, \dots, l_N)$:

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

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

$$\begin{aligned} \Lambda = \{ \xi \in \mathbf{R}^{2N} : \zeta_1 > \delta, \zeta_2 - \zeta_1 > \delta, \dots, \zeta_N - \zeta_{N-1} > \delta, 1 - \zeta_N \\ > \delta, \frac{1}{\delta} > l_k > \delta, k = 1, \dots, N \} \end{aligned} \quad (2.4)$$

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, Sect. 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

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

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

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

$H(t)$ 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

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

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

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

where χ is defined to be

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

The exponent α in (2.9) satisfies

$$\frac{1}{2} < \alpha < 1. \quad (2.10)$$

χ satisfies

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

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

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

which may be written as

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

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

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

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 $\epsilon \rightarrow 0$. 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

$$\overline{f(w_\xi)} = \int_0^1 f(w_{\xi,1}) dx + \int_0^1 f'(w_{\xi,1})w_{\xi,2} dx + O(\epsilon) \tag{2.19}$$

$$= \int_0^1 f'(w_{\xi,1})w_{\xi,2} dx + O(\epsilon) \tag{2.20}$$

$$= f'(0)\overline{w_{\xi,2}} + \int_0^1 [f'(w_{\xi,1}) - f'(0)]w_{\xi,2} dx + O(\epsilon) \tag{2.21}$$

$$= f'(0)\overline{w_{\xi,2}} + O(\epsilon). \tag{2.22}$$

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

$$S(w_\xi) = -\epsilon^2 w_\xi'' + f(w_\xi) + \sigma(-\Delta)^{-1}(w_\xi - a) - f'(0)\overline{w_{\xi,2}} + O(\epsilon) \quad (2.23)$$

$$= -\epsilon^2 w_\xi'' + f(w_\xi) - f'(0)w_{\xi,2} + O(\epsilon) \quad (2.24)$$

$$= -\epsilon^2 w_{\xi,1}'' - \epsilon^2 w_{\xi,2}'' + f(w_{\xi,1}) + f'(w_{\xi,1})w_{\xi,2} - f'(0)w_{\xi,2} + O(\epsilon) \quad (2.25)$$

$$= (-\epsilon^2 w_{\xi,1}'' + f(w_{\xi,1})) + (f'(w_{\xi,1}) - f'(0))w_{\xi,2} + O(\epsilon) \quad (2.26)$$

$$= (f'(w_{\xi,1}) - f'(0))w_{\xi,2} + O(\epsilon). \quad (2.27)$$

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 $j = 1, 2, \dots, 2N$, let us define

$$\begin{aligned} h_j(x) &= H'\left(\frac{x-x_j}{\epsilon}\right)\kappa\left(\frac{x-x_j}{\sqrt{\epsilon}}\right) - \overline{H'\left(\frac{x-x_j}{\epsilon}\right)\kappa\left(\frac{x-x_j}{\sqrt{\epsilon}}\right)} \\ &= H'\left(\frac{x-x_j}{\epsilon}\right) - \epsilon + O(e^{-C/\epsilon}). \end{aligned} \quad (2.28)$$

where κ is a smooth, even cut-off function

$$\kappa(s) = \begin{cases} 1 & \text{if } |s| \leq 1 \\ 0 & \text{if } |s| \geq 2 \end{cases}. \quad (2.29)$$

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

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

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}_ξ to be the subspace

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

of \mathcal{Y} . Let the projection to \mathcal{E}_ξ be π_ξ

$$\pi_\xi : \mathcal{Y} \rightarrow \mathcal{E}_\xi. \quad (2.32)$$

3 Solvability in fibers

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

$$\pi_\xi \circ S(w_\xi + \phi_\xi) = 0. \quad (3.1)$$

This means that we solve $S(u) = 0$ in the fiber direction. For each $\phi \in \mathcal{F}_\xi$ we expand

$$S(w_\xi + \phi) = S(w_\xi) + L_\xi(\phi) + R_\xi(\phi) \quad (3.2)$$

where

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

is the linearization of S at w_ξ , and

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

Then (3.1) is written as

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

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

$$\pi_\xi \circ L_\xi : \mathcal{F}_\xi \rightarrow \mathcal{E}_\xi \quad (3.6)$$

we have the following lemma.

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

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 $\epsilon \rightarrow 0$,

$$\|\pi_\xi \circ L_\xi(\psi)\| \rightarrow 0. \quad (3.7)$$

Write (3.7) as

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

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

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

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

$$\int_0^1 |\varphi'|^2 dx = o(1). \quad (3.10)$$

The Sobolev embedding theory yields

$$\|\varphi\| = o(1). \quad (3.11)$$

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

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

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

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

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

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

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

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

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

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

$$= O(\epsilon). \quad (3.18)$$

This simplifies (3.13) to

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

Hence

$$\beta_j = O(1). \quad (3.20)$$

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),

$$L_\xi(\psi)(y) = -\epsilon^2 \psi''(y) + f'(w_\xi(y)) \psi(y) - \overline{f'(w_\xi) \psi} + \sigma ((-\Delta)^{-1} \psi)(y) \quad (3.21)$$

$$\geq 0 + f'(w_\xi(y)) - \overline{(f'(w_\xi) - f'(0)) \psi} + \sigma ((-\Delta)^{-1} \psi)(y) \quad (3.22)$$

$$= f'(w_\xi(y)) + \sigma \varphi(y) + O(\epsilon) = f'(w_\xi(y)) + o(1) \quad (3.23)$$

$$= f'(0) + o(1). \quad (3.24)$$

Combining (3.20) and (3.24), we obtain

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

which contradicts (3.7).

We have thus proved that $y - \xi_j = O(\epsilon)$ for some j , along a subsequence of $\epsilon \rightarrow 0$. Define $\Psi(t) = \psi(\xi_j + \epsilon t)$. Then (3.8), (3.11), and (3.20) imply

$$-\Psi'' + f'(w_\xi(\xi_j + \epsilon t))\Psi - \beta_j H' \rightarrow 0 \quad (3.26)$$

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

$$-\Psi_\infty'' + f'(H)\Psi_\infty - \beta_j^0 H' = 0. \quad (3.27)$$

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

$$-\Psi_\infty'' + f'(H)\Psi_\infty = 0. \quad (3.28)$$

The bounded solutions of this equation are scalar multiples of H' . Hence $\Psi_\infty = cH'$ for some $c \neq 0$.

On the other hand, since $\psi \in \mathcal{F}_\xi$ means that $\psi \perp h_j$ and $\bar{\psi} = 0$, we deduce that

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

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

To prove part 2 of the lemma we need to solve

$$\pi_\xi \circ L_\xi(\phi) = p \quad (3.30)$$

in \mathcal{F}_ξ 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

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

The linear operator $\pi_\xi \circ (-\Delta)^{-1} \circ \pi_\xi \circ L_\xi$ on the left side maps from \mathcal{F}_ξ to itself. For this operator \mathcal{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

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

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

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

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

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

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

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

We multiply it by h_k and integrate to deduce

$$0 = \sum_{j=1}^{2N} \alpha_j \int_0^1 h_j' h_k' dx = \sum_{j=1}^{2N} \alpha_j \epsilon (\tau \delta_{jk} + O(\epsilon)), \quad k = 1, 2, \dots, 2N, \quad (3.36)$$

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

$$\pi_\xi \circ L_\xi(\phi) = 0. \quad (3.37)$$

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

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

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

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

We multiply by h_k and integrate to obtain

$$0 = \sum_{j=1}^{2N} \beta_j \int_0^1 h_j' h_k' dx = \sum_{j=1}^{2N} \beta_j \epsilon (\tau \delta_{jk} + O(\epsilon)), \quad k = 1, 2, \dots, 2N, \quad (3.40)$$

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

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:

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

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

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

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

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

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

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

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

$$\|T_\xi(\phi)\| \leq C_1\|\pi_\xi \circ S(w_\xi)\| + C_1\|\pi_\xi \circ R_\xi(\phi)\| \quad (3.45)$$

$$\leq C_3\epsilon^{1/2} + C_5(1 + O(\|\phi\|))\|\phi\|^2 \quad (3.46)$$

$$\leq C_3\epsilon^{1/2} + C_6C_2^2(1 + C_2\epsilon^{1/2})\epsilon \quad (3.47)$$

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

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

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 T_ξ maps \mathcal{B}_ξ to itself.

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

$$\|T_\xi(\phi_1) - T_\xi(\phi_2)\| \leq C_1\|\pi_\xi \circ (R_\xi(\phi_1) - R_\xi(\phi_2))\| \leq C_7\|R_\xi(\phi_1) - R_\xi(\phi_2)\| \quad (3.49)$$

$$\leq C_8\|f(w_\xi + \phi_1) - f(w_\xi + \phi_2) - f'(w_\xi)(\phi_1 - \phi_2)\| \quad (3.50)$$

$$\leq C_8\|f'(w_\xi + \phi_2 + \theta(\phi_1 - \phi_2))(\phi_1 - \phi_2) - f'(w_\xi)(\phi_1 - \phi_2)\| \quad (3.51)$$

$$\leq C_8\|f'(w_\xi + \phi_2 + \theta(\phi_1 - \phi_2)) - f'(w_\xi)\|\|\phi_1 - \phi_2\| \quad (3.52)$$

$$\leq O(\|\phi_1\| + \|\phi_2\|)\|\phi_1 - \phi_2\| \quad (3.53)$$

$$\leq C_9\epsilon^{1/2}\|\phi_1 - \phi_2\| \quad (3.54)$$

which implies that T_ξ is a contraction map 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

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

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

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

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

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

Proof In this proof we denote $w_\xi + \phi_\xi$ by g_ξ . We argue by contradiction. Assume $\liminf_{\epsilon \rightarrow 0} \lambda \leq 0$. Clearly λ is achieved by a ψ in \mathcal{P}_ξ . 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 $\bar{\psi} = 0, \psi \perp h_j$, 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

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

The assumption $\liminf_{\epsilon \rightarrow 0} \lambda \leq 0$ 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 (3.20) we find that

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

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)

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

with the help of (4.8) and (4.10). But this is impossible since we have assumed that $\liminf_{\epsilon \rightarrow 0} \lambda \leq 0$.

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

$$\begin{aligned} -\Psi''(t) + f'(g_\xi(\xi_j + \epsilon t)) \Psi + o(1) &= \lambda \Psi(t) + \sum_{j=1}^{2N} \beta_j h_j(\xi_k + \epsilon t), \\ &\times t \in \left(-\frac{\xi_k}{\epsilon}, \frac{1 - \xi_k}{\epsilon} \right). \end{aligned} \tag{4.12}$$

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

$$-\Psi''_\infty + f'(H) \Psi_\infty = (\liminf_{\epsilon \rightarrow 0} \lambda) \Psi_\infty + \beta_k^0 H' \tag{4.13}$$

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

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

Therefore

$$\int_{\mathbf{R}} \Psi_\infty H' dt = 0. \tag{4.15}$$

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

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

Then (4.13) becomes

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

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). \square

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

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

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

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

which by (4.2) implies

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

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

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

of \mathcal{P}_{ξ} 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

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

Lemma 4.2 follows from (4.22). \square

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 $S(w_\xi + \phi_\xi) = 0$. 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 $0 < \zeta_1 < \zeta_2 < \dots < \zeta_N < 1, l_j > 0$, for $j = 1, 2, \dots, 2N$.

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

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

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

$$I(w_\xi) = \frac{\epsilon^2}{2} \int_0^1 |w'_{\xi,1}|^2 dx + \epsilon^2 \int_0^1 w'_{\xi,1} w'_{\xi,2} dx \quad (5.10)$$

$$+ \int_0^1 W(w_{\xi,1}) dx + \int_0^1 f(w_{\xi,1}) w_{\xi,2} dx + \frac{1}{2} \int_0^1 f'(w_{\xi,1}) w_{\xi,2}^2 dx \quad (5.11)$$

$$+ \frac{\sigma}{2} \int_0^1 |(-\Delta)^{-1/2} (w_{\xi,1} + w_{\xi,2} - a)|^2 dx + O(\epsilon^{3/2}) \quad (5.12)$$

$$= \frac{\epsilon^2}{2} \int_0^1 |w'_{\xi,1}|^2 dx + \int_0^1 W(w_{\xi,1}) dx \quad (5.13)$$

$$+ \epsilon^2 \int_0^1 w'_{\xi,1} w'_{\xi,2} dx + \int_0^1 f(w_{\xi,1}) w_{\xi,2} dx \quad (5.14)$$

$$+ \frac{1}{2} \int_0^1 f'(w_{\xi,1}) w_{\xi,2}^2 dx + \frac{\sigma}{2} \int_0^1 |(-\Delta)^{-1/2} (w_{\xi,1} + w_{\xi,2} - a)|^2 dx + O(\epsilon^{3/2}) \quad (5.15)$$

$$= 2N\tau\epsilon + \frac{1}{2} \int_0^1 f'(w_{\xi,1}) w_{\xi,2}^2 dx \quad (5.16)$$

$$+ \frac{\sigma}{2} \int_0^1 (w_{\xi,1} + w_{\xi,2} - a) (-\Delta)^{-1} (w_{\xi,1} + w_{\xi,2} - a) dx + O(\epsilon^{3/2}) \quad (5.17)$$

$$= 2N\tau\epsilon + \frac{1}{2} \int_0^1 f'(w_{\xi,1}) w_{\xi,2}^2 dx - \frac{f'(0)}{2} \int_0^1 (w_{\xi,1} + w_{\xi,2} - a) w_{\xi,2} dx + O(\epsilon^{3/2}) \quad (5.18)$$

$$= 2N\tau\epsilon + \frac{1}{2} \int_0^1 (f'(w_{\xi,1}) - f'(0)) w_{\xi,2}^2 dx - \frac{f'(0)}{2} \int_0^1 (w_{\xi,1} - a) w_{\xi,2} dx + O(\epsilon^{3/2}) \quad (5.19)$$

$$= 2N\tau\epsilon - \frac{f'(0)}{2} \int_0^1 (w_{\xi,1} - a) w_{\xi,2} dx + O(\epsilon^{3/2}) \quad (5.20)$$

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

$$= 2N\tau\epsilon - \frac{f'(0)\epsilon}{2} \left[\int_0^1 \frac{w_{\xi,1}}{\epsilon^{1/2}} a_0 dx - 2 \int_0^1 \frac{w_{\xi,1}}{\epsilon^{1/2}} \left(\sum_{j=1}^N l_j G_D(x, \zeta_j) \right) dx - a_0^2 + 2a_0 \int_0^1 \left(\sum_{j=1}^N l_j G_D(x, \zeta_j) \right) dx \right] + O(\epsilon^{3/2}) \quad (5.22)$$

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

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

This proves the lemma. \square

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

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

and

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

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

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

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

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

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

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

Since p satisfies the linear differential equation

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

(5.30) and (5.31) imply that

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

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

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

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

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

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

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

This proves the lemma. \square

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

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

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

Next we write G_D as

$$G_D(x, y) = \Gamma(|x - y|) + R(x, y) \quad (5.38)$$

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

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

Then we calculate

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

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

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

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

Then if $k \neq j$

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

If $k = j$,

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

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

If $k \neq j$,

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

If $k = j$,

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

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

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

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

$$\mathbf{H} = \begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{C} \end{bmatrix}. \quad (5.48)$$

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. \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 $\epsilon \rightarrow 0$. 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 $(\tilde{\zeta}, \tilde{l}) \rightarrow (\zeta^0, l^0)$ as $\epsilon \rightarrow 0$. 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). \square

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

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

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

$$\frac{\coth \beta - \operatorname{csch} \beta}{\beta} = \frac{1}{2} - \frac{\beta^2}{24} + \dots \quad (6.2)$$

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

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

The last expression is minimized at

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

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

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

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, Sect. 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

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

Therefore

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

where the eigenvalues of \mathbf{A} are

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

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

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

is independent of j , proving (5.35).

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

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

where the jk entry of \mathbf{D} is

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

However from (5.39) we find that

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

is the Green function of

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

divided by D . Argument similar to [19, Sect. 7] shows that

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

which is diagonalized by

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

Then

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

where the μ_j 's are

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

Hence

$$\mathbf{Q}^T \mathbf{C} \mathbf{Q} = \begin{bmatrix} c_1 & 0 & \dots & 0 \\ 0 & c_2 & \dots & 0 \\ \dots & & & \\ 0 & 0 & \dots & c_N \end{bmatrix} \quad (\text{A.18})$$

where

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

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

We will use

$$\begin{bmatrix} \mathbf{P} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q} \end{bmatrix} \quad (\text{A.21})$$

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

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

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

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

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

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

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

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

Then

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

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

$$\mathbf{A} \mathbf{P} = [a_1 \mathbf{p}_1, a_2 \mathbf{p}_2, \dots, a_N \mathbf{p}_N], \quad (\text{A.27})$$

and

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

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

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

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

$$\sum_{k=1}^N e_{jk} = 0, \quad j = 1, 2, \dots, N. \quad (\text{A.30})$$

Thus f_{jj} defined in (A.24) are all 0 and (A.22) simplifies to

$$\mathbf{B} = \iota \mathbf{E}. \quad (\text{A.31})$$

So we find that

$$\mathbf{P}^T \mathbf{B} \mathbf{Q} = \begin{bmatrix} b_1 & 0 & \dots & 0 \\ 0 & b_2 & \dots & 0 \\ \dots & & & \\ 0 & 0 & \dots & b_N \end{bmatrix} \quad (\text{A.32})$$

where

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

Hence

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

which is indeed a matrix of diagonal 2×2 blocks

$$\begin{bmatrix} a_j & b_j \\ b_j & c_j \end{bmatrix} \quad (\text{A.35})$$

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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