Wriggled Lamellar Solutions and their Stability in the Diblock Copolymer Problem *

Xiaofeng Ren
Department of Mathematics and Statistics
Utah State University
Logan, UT 84322-3900, USA
and The Institute of Mathematical Sciences
The Chinese University of Hong Kong
Shatin, Hong Kong

Juncheng Wei †
Department of Mathematics
The Chinese University of Hong Kong
Shatin, Hong Kong

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Abstract

In a diblock copolymer system the free energy field depends nonlocally on the monomer density field. In addition there are two positive parameters in the constitutive relation. One of them is small with respect to which we do singular perturbation analysis. The second one is of order 1 with respect to which we do bifurcation analysis. Combining the two techniques we find wriggled lamellar solutions of the Euler-Lagrange equation of the total free energy. They bifurcate from the perfect lamellar solutions. The stability of the wriggled lamellar solutions is reduced to a relatively simple finite dimensional problem, which may be solved accurately by a numerical method. Our tests show that most of them are stable. The existence of such stable wriggled lamellar solutions explains why in reality the lamellar phase is fragile and it often exists in distorted forms.

Key words. distortion, bifurcation, singular perturbation, stability, wriggled lamellar solution, perfect lamellar solution, diblock copolymer
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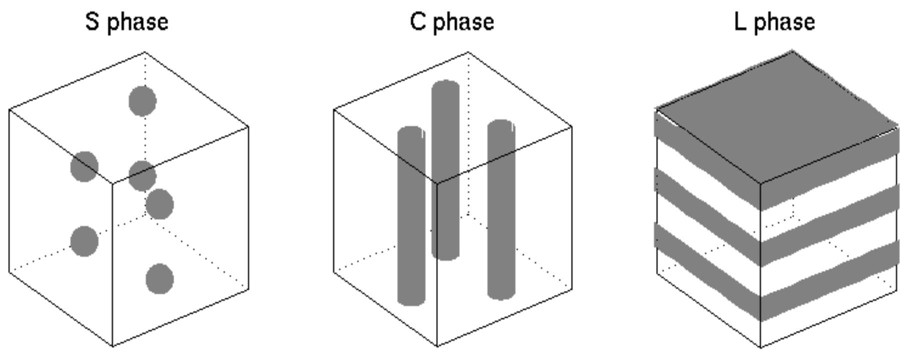

Figure 1: The spherical, cylindrical, and lamellar morphology phases commonly observed in diblock copolymer melts. The dark color indicates the concentration of type A monomer, and the white color indicates the concentration of type B monomer.

1 Introduction

Symmetry breaking distortion often appears for intrinsic reasons in systems of condensed matters that exhibit self-organization and pattern formation (Seul and Andelman [21], Tsori *et al* [23]). We study this phenomenon in diblock copolymers. A diblock copolymer is a soft material, characterized by fluid-like disorder on the molecular scale and a high degree of order at longer length scales. A molecule in a diblock copolymer melt is linear sub-chain of A monomers grafted covalently to another sub-chain of B monomers. Because of the repulsion between the unlike monomers, the different type sub-chains tend to segregate below some critical temperature, but as they are chemically bonded in chain molecules, even a complete 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 are formed. These micro-domains form morphology patterns/phases in a larger scale. The most commonly observed undistorted phases are the spherical, cylindrical and lamellar, depicted in Figure 1. Here we seek distorted, defective lamellar patterns, where the interfaces separating the microdomains, unlike the ones in Plot 3 of Figure 1, are wriggled.

We consider a scenario that a diblock copolymer melt is placed in a domain D and maintained at fixed temperature. D is scaled to have unit volume in space. Let $a \in (0,1)$ be the relative number of the A monomers in a chain molecule, and $b = 1 - a$ be the relative number of the B monomers in a chain. The relative A monomer density field u is an order parameter. $u \approx 1$ stands for high concentration of A monomers. The melt is incompressible so the relative B monomer density is $1-u$ and $u \approx 0$ stands for high concentration of B monomers.

Ohta and Kawasaki [10] introduced an equilibrium theory, in which the free energy of the system is a functional of the relative A monomer density:

$$I(u) = \int_D \{\frac{\epsilon^2}{2}|\nabla u|^2 + \frac{\epsilon\gamma}{2}|(-\Delta)^{-1/2}(u-a)|^2 + W(u)\}, \tag{1.1}$$

defined in $X_a = \{u \in W^{1,2}(D) : \overline{u} = a\}$, where $\overline{u} := \int_D u$ is the average of u on D. The original formula in [10] is given on the entire $\mathbf{R}^3$. The expression here on a bounded domain D first appeared in Nishiura and Ohnishi [8]. A mathematically more rigorous derivation is in Choksi and Ren [3]. The local function W is smooth and has the shape of a double well. It has the global minimum value 0 at two numbers: 0 and 1. To avoid unnecessary technical difficulties we assume that $W(p) = W(1-p)$. The two global minimum points are non-degenerate: $W''(0) = W''(1) \neq 0$.

The most unusual in (1.1) is the nonlocal expression $(-\Delta)^{-1/2}(u-a)$. It reflects the connectivity of polymer chains. $(-\Delta)^{-1/2}$ is the square root of the positive operator $(-\Delta)^{-1}$ from $\{w \in L^2(D) : \overline{w} = 0\}$ to itself. The integral of the nonlocal part in (1.1) may be rewritten as

$$\int_D |(-\Delta)^{-1/2}(u-a)|^2 = \int_D \int_D G_D(x,y)(u(x)-a)(u(y)-a)\, dxdy.$$

G_D is the Green function of $-\Delta$ with the Neumann boundary condition. It splits to a fundamental solution part and a regular part. The fundamental solution in $\mathbf{R}^3$ is $\frac{1}{4\pi|x-y|}$, a long range Coulomb type interaction, which is common in many important physical systems (Muratov [7]).

ϵ and γ are positive dimensionless parameters that depend on various physical quantities [3]. In the strong segregation region where morphology patterns form, ϵ is very small. γ is of order 1 when we choose the size of the sample to be comparable to the size of the microdomains [3]. We develop a particular two parameter perturbation method. We do singular perturbation analysis with respect to ϵ and bifurcation analysis with respect to γ. The challenge is to combine these two techniques to derive fine analytical results. Even though this mathematical method is tailored for the diblock copolymer problem, we believe that it may be applied to other ones with multiple parameters. Examples include the Seul-Andelman membrane problem [21, 11], charged Langmuir monolayers [1, 12], and smectic films [20].

The Euler-Lagrange equation of I is

$$-\epsilon^2\Delta u + f(u) - \overline{f(u)} + \epsilon\gamma(-\Delta)^{-1}(u-a) = 0, \quad \partial_\nu u = 0 \text{ on } \partial D. \tag{1.2}$$

f is the derivative of W. The term $\overline{f(u)}$ is equal to the Lagrange multiplier corresponding to the constraint $\overline{u} = a$. The equation (1.2) may also be written as an elliptic system:

$$\begin{cases} -\epsilon^2\Delta u + f(u) + \epsilon\gamma v = \text{Const.} \\ -\Delta v = u - a \\ \partial_\nu u = \partial_\nu v = 0 \text{ on } \partial D \\ \overline{u} - a = \overline{v} = 0 \end{cases}. \tag{1.3}$$

Here Const. is the Lagrange multiplier.

In Ren and Wei [13] a family of lamellar solutions is found. When $D = (0,1)$, for each positive integer K there exists a 1-dimensional local minimizer of I if ϵ is sufficiently small [1]. This 1-D local minimizer may be extended trivially to a 3-D solution of (1.2) on a box. Such a solution, illustrated in Plot 1 of Figure 2, models the lamellar phase, Plot 3 of Figure 1, only if it is stable in the sense that it is a local minimizer of I in 3-D. A local minimizer in 3-D is called a *meta-stable* state of the physical system. It survives mild thermal fluctuation.

However in Ren and Wei [17] it is shown that such 1-D solutions are not necessarily 3-D local minimizers. Detailed spectral information at each 1-D solution is found [2]. In summary a 1-D local

[1] See Theorem 2.1.
[2] See Theorem 3.1.

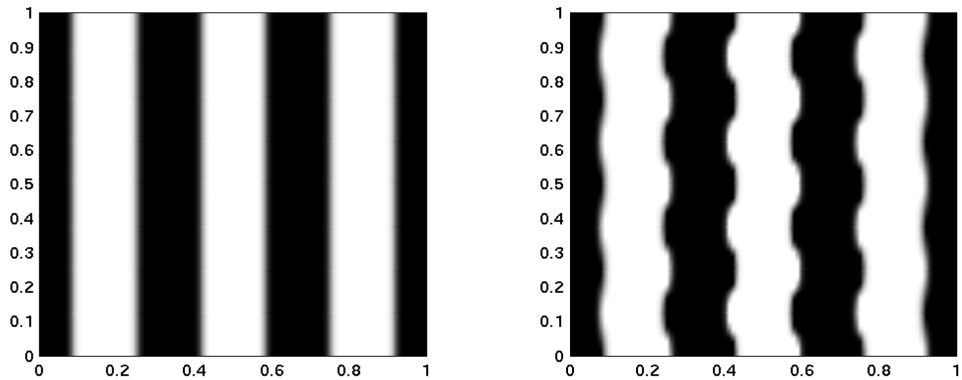

Figure 2: A perfect lamellar solution and a wriggled lamellar solution. In the dark regions the solutions are close to 1 and in the light regions the solutions are close to 0.

minimizer is a 3-D local minimizer only if K is sufficiently large or γ is sufficiently small. Moreover the 1-D global minimizer, which is one of the 1-D local minimizers with the optimal number of interfaces $K_{opt} \approx (\frac{a^2 b^2 \gamma}{3\tau})^{1/3}$, where τ is defined in (2.2), has a delicate stability property. It actually lies near the *borderline* that separates the stable 1-D solutions from the unstable 1-D solutions.

All this suggests that the lamellar phase is only a meta-stable, transient state of the material. Thermal fluctuation will eventually destroy this phase. In reality one often observes the lamellar phase in distorted forms. We predict based on the model (1.1) that a defective, wriggled lamellar pattern (Figure 2, Plot 2) exists in diblock copolymers. We point out that the wriggled lamellar pattern is typically observed in systems with competing interactions [21].

The existence of wriggled lamellar solutions is shown by a bifurcation analysis. Each perfect lamellar solution u_γ with K interfaces is stable when γ is sufficiently small. The spectrum of the second variation of I at u_γ, which consists of real eigenvalues only, lies to the right of 0. If we increase γ, the spectrum moves to the left. When γ reaches a critical value γ_{B}, the principal (the smallest) eigenvalue in the spectrum becomes 0. A new solution branch bifurcates out of $u_{\gamma_{\mathrm{B}}}$. This is a wriggled lamellar solution (Figure 2, Plot 2). If we further increase γ, then another eigenvalue of u_γ, which is not the principal eigenvalue, may become 0, and another new solution also of a wriggled lamellar pattern bifurcates from u_γ. However wriggled lamellar solutions that bifurcate from larger eigenvalues are unstable and physically less interesting.

Whether the wriggled lamellar solution associated with the principal eigenvalue of $u_{\gamma_{\mathrm{B}}}$ is stable is a subtle question. It is relatively easy to see that the bifurcation diagram has the shape of a pitchfork (Figure 3). The stability of the wriggled solution depends on the direction of the fork. Here we face a formidable problem. The direction is determined by the sign of a number which turns out to be terribly small (of ϵ^5 order, Lemma 5.2). To find this number we have to expand the "trivial solution" $u_{\gamma_{\mathrm{B}}}$, its principal eigenfunction corresponding to the 0 eigenvalue, and the third function $g'(0)$ defined in (5.4), with respect to ϵ. As we prove Lemma 5.2, these expansions have to be carefully managed. All the lower order terms up to ϵ^4 vanish. In the end we arrive at a quantity $S(a, K)$ that depends on a, and K only. The bifurcating solution is stable if $S(a, K) > 0$ and unstable if $S(a, k) < 0$. $S(a, K)$ may be accurately calculated by a simple numerical method. Our tests, reported in Section 5, show that for most values of a and K the wriggled lamellar solution bifurcating out of the principal eigenvalue is stable.

The paper is organized as follows. In Section 2 we recall some properties of the perfect lamellar solutions u_γ. Section 3 contains some spectral information of the second variation of I at u_γ. The existence of the wriggled lamellar solutions is in Theorem 4.1. The reduction of their stability to the positivity of $S(a, K)$ culminates in Theorem 5.4. The lengthy calculations that prove Lemma 5.2 are in Appendices B and C.

To avoid clumsy notations a quantity's dependence on ϵ is usually suppressed. For example we write u, the lamellar solution, instead of u_ϵ. On the other hand we often emphasize a quantity's independence of ϵ with a superscript 0. For example the limit of a lamellar solution u as $\epsilon \to 0$ is denoted by u^0. In estimates C is always a positive constant independent of ϵ. Its value may vary from line to line. The L^2 inner product is denoted by $\langle \cdot, \cdot \rangle$ and the L^p norm by $\| \cdot \|_p$.

To simplify the formulation of our results, we take $D = (0,1) \times (0,1)$ to be a 2-D square instead of a 3-D box. Generalization to 3-D is trivial.

References on the mathematical aspects of the block copolymer theory include, in addition to the ones cited already, Ohnishi *et al* [9], Choksi [2], Fife and Hilhorst [5], Henry [6], Ren and Wei [15, 14], on diblock copolymers, and Ren and Wei [16, 18] on triblock copolymers.

2 The perfect lamellar solution u_γ

The perfect lamellar solutions that serve as "trivial solutions" in the bifurcation theory are constructed in [13] by the Γ-limit theory. The findings there are summarized in the following theorem.

Theorem 2.1 (Ren and Wei [13]) *In 1-D for each positive integer K the functional*

$$I_1(u) := \int_0^1 \{ \frac{\epsilon^2}{2} (\frac{du}{dx})^2 + \frac{\epsilon\gamma}{2} |(-\frac{d^2}{dx^2})^{-1/2} (u-a)|^2 + W(u) \} \, dx,$$

in $\{u \in W^{1,2}(0,1) : \overline{u} = a\}$, has a local minimizer u near u^0, under the L^2 norm, when ϵ is sufficiently small. It satisfies the Euler-Lagrange equation

$$-\epsilon^2 u'' + f(u) - \overline{f(u)} + \epsilon\gamma G_0[u-a] = 0, \ u'(0) = u'(1) = 0,$$

and has the properties

$$\lim_{\epsilon \to 0} \|u - u^0\|_2 = 0, \ \text{and} \ \lim_{\epsilon \to 0} \epsilon^{-1} I_1(u) = \tau K + \frac{\gamma}{2} \int_0^1 |(-\frac{d^2}{dx^2})^{-1/2} (u^0 - a)|^2 \, dx.$$

Let H be the solution of

$$-H'' + f(H) = 0 \text{ in } \mathbf{R}, \ H(-\infty) = 0, \ H(\infty) = 1, \ H(0) = 1/2. \tag{2.1}$$

The constant τ in the theorem is defined by

$$\tau := \int_{\mathbf{R}} (H'(t))^2 \, dt. \tag{2.2}$$

τ is often called the surface tension in the literature. u^0 is a step function of K jump discontinuity points, defined to be

$$u^0(x) = 1 \text{ on } (0, x_1^0),\ 0 \text{ on } (x_1^0, x_2^0),\ 1 \text{ on } (x_2^0, x_3^0),\ 0 \text{ on } (x_3^0, x_4^0),\ 1 \text{ on } (x_4^0, x_5^0), ...$$

with (recall $b = 1 - a$)

$$x_1^0 = \frac{a}{K},\ x_2^0 = \frac{1+b}{K},\ x_3^0 = \frac{2+a}{K},\ x_4^0 = \frac{3+b}{K},\ x_5^0 = \frac{4+a}{K}, ... \tag{2.3}$$

G_0 is the solution operator of $-v'' = g$, $v'(0) = v'(1) = \overline{v} = 0$, i.e. $v = G_0[g] = (-\frac{d^2}{dx^2})^{-1} g$.

There is another K-interface 1-D local minimizer whose limiting value as $\epsilon \to 0$ is 0 instead of 1 on the first interval $(0, b/K)$. It is just $1 - \tilde{u}$ where $\tilde{u}$ is a solution constructed in Theorem 2.1, but with $\overline{\tilde{u}} = b$ instead. $1 - \tilde{u}$ has the same properties as u does, so we focus on u. u is found periodic in the following sense.

Theorem 2.2 (Ren and Wei [17]) *Let u be a 1-D local minimizer constructed in Theorem 2.1. When ϵ is small, for every $x \in (0, 1/K)$,*

$$u(x) = u(\frac{2}{K} - x) = u(x + \frac{2}{K}) = u(\frac{4}{K} - x) = u(x + \frac{4}{K}) = ... = \begin{cases} u(1-x) & \text{if } K \text{ is even} \\ u(x + \frac{K-1}{K}) & \text{if } K \text{ is odd} \end{cases}.$$

Moreover when ϵ is small, u is the unique local minimizer of I_1 in an L^2 neighborhood of u^0. If u on $((j-1)/K, j/K)$ for some $j = 1, 2, ..., K$ is scaled to a function on $(0, 1)$, then it is exactly a one-layer local minimizer of I_1 with ϵ and γ replaced by $\tilde{\epsilon} = \epsilon K$ and $\tilde{\gamma} = \gamma / K^3$.

Let us denote this u of K interfaces by u_γ, to emphasize its dependence on γ. We need asymptotic expansions of u_γ in terms of ϵ. According to [17, Lemma A.1] there exist exactly K points x_j, $j = 1, 2, ..., K$, in $(0, 1)$ so that $u(x_j) = 1/2$. These K points identify the interfaces of u. Theorem 2.2 implies that $x_2 = \frac{2}{K} - x_1$, $x_3 = \frac{4}{K} - x_2$, $x_4 = \frac{6}{K} - x_3$, etc. The zeroth order approximation of u_γ is

$$s(x) = H(-\frac{x - x_1}{\epsilon}) + H(\frac{x - x_2}{\epsilon}) + H(-\frac{x - x_3}{\epsilon}) - 1 + ... + \begin{cases} H(\frac{x - x_K}{\epsilon}) & \text{if } K \text{ is even} \\ H(-\frac{x - x_K}{\epsilon}) - 1 & \text{if } K \text{ is odd} \end{cases}. \tag{2.4}$$

The ϵ order outer expansion term is z^0, defined to be

$$z^0(x) = -\frac{\gamma(v^0(x) - v^0(x_j^0))}{f'(0)}, \quad v^0 = (-\frac{d^2}{dx^2})^{-1}(u^0 - a). \tag{2.5}$$

and the ϵ order inner expansion term is 0. Because of the periodicity, $v^0(x_j^0)$ is independent of j and z^0 is well defined. The ϵ^2 order inner expansion term is P, where P is the solution of

$$-P'' + f'(H)P = -\gamma (v^0)'(x_j^0) t,\ P \perp H'. \tag{2.6}$$

There are two different P's depending on whether j is odd or even. But they just differ by a sign, and it is always easy to tell from the context which one is referred to.

Lemma 2.3 (Ren and Wei [17]) *Let z be defined by $u_\gamma = s + \epsilon z$.*

1. $\|z - z^0\|_\infty = O(\epsilon)$.

2. *There exists a constant* $C > 0$ *independent of* ϵ *so that* $|\epsilon^{-1} z(x_j + \epsilon t)| \le C(1 + |t|)$ *for all* $t \in (-\frac{x_j}{\epsilon}, \frac{1-x_j}{\epsilon})$. $\epsilon^{-1} z(x_j + \epsilon \cdot)$ *converges to* P *in* $C^2_{loc}(\mathbf{R})$.

Proof. See [17, Lemmas 2.4 and 2.5]. □

It is proved in [17] that u_γ is a non-degenerate 1-D local minimizer in the sense that the 1-D spectrum at u_γ lies to the right of the origin [3]. This allows us to apply the implicit function theorem to conclude that u_γ depends on γ smoothly. Next we estimate $\frac{du_\gamma}{d\gamma}$. Define

$$h_j(x) = H'(\frac{x - x_j}{\epsilon}) + e.s. \tag{2.7}$$

where $e.s.$ is an exponentially small correction term. It is chosen so that $h_j(0) = h_j(1) = h_j'(0) = h_j'(1) = 0$, $\|h_j' - \epsilon^{-1} H''(\frac{\cdot - x_j}{\epsilon})\|_\infty = O(\epsilon^{-C/\epsilon})$, and $\|h_j'' - \epsilon^{-2} H'''(\frac{\cdot - x_j}{\epsilon})\|_\infty = O(\epsilon^{-C/\epsilon})$. Decompose

$$\frac{du_\gamma}{d\gamma} = \sum_j c(h_j - \overline{h_j}) + \epsilon \psi \tag{2.8}$$

where $h_j - \overline{h_j} \perp \psi$ for each j. Here that c is the same in front of all $h_j - \overline{h_j}$ is a consequence of Theorem 2.2.

Lemma 2.4 1. $c \to c_0 := -\frac{v^0(x_j^0)}{K f'(0)}$.

2. $\psi = O(1)$, *and near each* x_j, $\psi(x_j + \epsilon \cdot) \to R$ *in* $C^2_{loc}(\mathbf{R})$, *where* R *is the solution of*

$$-R'' + f'(H) R = -\frac{v^0(x_j^0)}{f'(0)} f'(H), \ \ R \perp H'.$$

3. *Near each* x_j, $\epsilon^{-1}(\psi(x_j + \epsilon \cdot) - R) \to \gamma^{-1} P + b_0$ *in* $C^2_{loc}(\mathbf{R})$ *where* b_0 *is the solution of*

$$-b_0'' + f'(H) b_0 = -c^0 f''(H) H_t P + Const., \ \ b_0 \perp H_t.$$

The proof of this lemma is technical. We include it in Appendix A.

The 1-D local minimizer u_γ of I_1 is now viewed as a function on D, through extension to the second dimension trivially, so $u_\gamma(x, y) = u_\gamma(x)$. It is a solution of (1.2) and $I_1(u_\gamma) = I(u_\gamma)$. In 2-D it has straight interfaces. We call it a perfect lamellar solution of (1.2).

3 The 2-D spectrum at u_γ

The linearized operator at u_γ is

$$L_\gamma \varphi := -\epsilon^2 \Delta \varphi + f'(u_\gamma)\varphi - \overline{f'(u_\gamma)\varphi} + \epsilon \gamma (-\Delta)^{-1} \varphi, \ \ \varphi \in W^{2,2}(D), \ \ \partial_\nu \varphi = 0 \text{ on } \partial D, \ \overline{\varphi} = 0. \tag{3.1}$$

[3] See Part 2 of Theorem 3.1.

This is an unbounded self-adjoint operator defined densely on $\{\phi \in L^2(D) : \overline{\phi} = 0\}$ whose spectrum consists of real eigenvalues only.

For an eigen pair (λ, φ) of L_γ separation of variables shows that $\varphi(x,y) = \phi_m(x)\cos(m\pi y)$ where m is a non-negative integer. Hence the eigenvalues λ are naturally classified by m. We therefore denote a λ that is associated with m by λ_m. We have the following reduced eigenvalue problems for (λ_m, ϕ_m).

1. When $m = 0$,

$$-\epsilon^2\phi_0'' + f'(u_\gamma)\phi_0 - \overline{f'(u_\gamma)\phi_0} + \epsilon\gamma G_0[\phi_0] = \lambda_0\phi_0, \quad \phi_0'(0) = \phi_0'(1) = \overline{\phi_0} = 0. \tag{3.2}$$

2. When $m \neq 0$,

$$-\epsilon^2(\phi_m'' - m^2\pi^2\phi_m) + f'(u_\gamma)\phi_m + \epsilon\gamma G_m[\phi_m] = \lambda_m\phi_m, \quad \phi_m'(0) = \phi_m'(1) = 0. \tag{3.3}$$

Here G_m are the solution operators of the differential equations

$$-X'' = \phi_0, \quad X'(0) = X'(1) = 0, \ \overline{X} = 0, \text{ if } m = 0, \tag{3.4}$$

$$-X'' + m^2\pi^2 X = \phi_m, \quad X'(0) = X'(1) = 0, \text{ if } m \neq 0, \tag{3.5}$$

i.e. $G_m[\phi_m] = X$. We often identify the operators G_m with the Green functions of (3.4) and (3.5).

Theorem 3.1 (Ren and Wei [17]) [4] *The eigenvalues λ of L are classified into λ_m by m which is a non-negative integer. The following 3 statements hold when ϵ is sufficiently small.*

1. *There exists $M(K)$ depending on K but not ϵ so that when $|m| \geq M(K)$, $\lambda_m \geq C\epsilon^2$ for some $C > 0$ independent of ϵ.*

2. *When $m = 0$, there are K small positive λ_0's. One of them is of order ϵ whose only eigenfunction is approximately $\sum_j (h_j(x) - \overline{h_j})$. The other $K - 1$ λ_0's are of order ϵ^2. Their only eigenfunctions are approximately $\sum_j c_j^0 h_j(x)$ for some vectors c^0 satisfying $\sum_j c_j^0 = 0$. The remaining λ_0's are positive and bounded below by a positive constant independent of ϵ.*

3. *When $m \neq 0$ and $|m| < M(K)$, there are K λ_m's of order ϵ^2, which are not necessarily positive, whose only eigenfunctions are approximately $\sum_j c_j^0 h_j(x)\cos(m\pi y)$. The remaining λ_m's are positive and bounded below by a positive constant independent of ϵ. Only when K is sufficiently large or γ is sufficiently small, all the eigenvalues of L are positive and u is stable.*

The eigenvalues λ_0 in Part 2 of Theorem 3.1 are just the 1-D eigenvalues of u_γ. That they are positive is consistent with the fact that u_γ is a local minimizer of I_1. Bifurcations occur at 0 eigenvalues, so we are more interested in the λ_m's of Part 3. In [17, Sections 6 and 7] we obtained asymptotic expansions of the K pairs (λ_m, ϕ_m) in Part 3. When $m \geq 1$,

$$\lambda_m = \epsilon^2\left(\frac{\gamma}{\tau}\left(\Lambda - \frac{ab}{K}\right) + m^2\pi^2\right) + o(\epsilon^2), \ \phi_m = \sum_j c_j h_j + \epsilon^2\phi_m^\perp. \tag{3.6}$$

[4] [17, Theorem 1.1] is formulated for a 3-D box. The similar conclusions hold true for the 2-D square D here.

In (3.6) ϕ_m is decomposed to $\sum_j c_j h_j$ in the subspace spanned by h_j, $j=1,2,...,K$, and $\epsilon^2\phi_m^\perp$ in the orthogonal complement of the subspace. Moreover $\|\phi_m^\perp\|_2 = O(|c|)$ [5]. As $\epsilon\to 0$, $c_j \to c_j^0$. Here (Λ, c^0) are the K eigenpairs of the K by K matrix $[G_m(x_j^0, x_k^0)]$. $[G_m(x_j^0, x_k^0)]$ is diagonalized in [17, Section 7]. When $K=1$, it has, for each $m\geq 1$, one eigenvalue pair

$$\Lambda = \frac{1}{m\pi(\tanh(m\pi a)+\tanh(m\pi b))},\ c^0 \propto 1. \tag{3.7}$$

When $K=2$, there are two eigenpairs

$$\begin{aligned}\Lambda &= \frac{1}{m\pi(\coth(m\pi a)+\cot(m\pi b)-\text{csch}\,(m\pi a)+\text{csch}\,(m\pi b))}, \quad c^0 \propto (-1,1),\\ \Lambda &= \frac{1}{m\pi(\coth(m\pi a)+\cot(m\pi b)-\text{csch}\,(m\pi a)-\text{csch}\,(m\pi b))}, \quad c^0 \propto (1,1).\end{aligned} \tag{3.8}$$

When $K\geq 3$, there are K eigenpairs

$$\Lambda = \frac{1}{d-q},\ c^0. \tag{3.9}$$

Here q is one of the K eigenvalues of the triagonal matrix

$$Q = \begin{bmatrix} \alpha & \beta & & & \\ \beta & 0 & \alpha & & \\ & \alpha & 0 & \beta & \\ & & \beta & 0 & \alpha \\ & & & \cdots & \end{bmatrix} \tag{3.10}$$

where

$$\alpha = m\pi\text{csch}\,\frac{2m\pi a}{K},\ \beta = m\pi\text{csch}\,\frac{2m\pi b}{K},\ d = m\pi(\coth\frac{2m\pi a}{K} + \coth\frac{2m\pi b}{K}),$$

and c^0 is a corresponding eigenvector of Q.

In this paper we improve $\|\phi_m^\perp\|_2 = O(|c|)$ to $\|\phi_m^\perp\|_\infty = O(|c|)$, and find the limiting behavior of $\phi_m^\perp$ near each x_j. Define Π to be the solution of

$$-\Pi'' + f'(H)\Pi = \frac{\gamma}{\tau}(\Lambda - \frac{ab}{K})H' + \text{Const.},\quad \Pi \perp H', \tag{3.11}$$

in $\mathbf{R}$. Recall P from (2.6).

Lemma 3.2 *1.* $\|\phi_m^\perp\|_\infty = O(|c|)$.

2. At each x_j, $\phi_m^\perp(x_j+\epsilon\cdot)$ converges in $C^2_{loc}(\mathbf{R})$ to $c_j^0(P'+\Pi)$.

Proof. We define an operator L_m so that the left side of (3.3) is $L_m\phi_m$ [6]. $\phi_m^\perp$ satisfies the equation

$$L_m\phi_m^\perp - \lambda_m\phi_m^\perp = \sum_j c_j\{-m^2\pi^2 h_j - \frac{1}{\epsilon^2}(f'(u_\gamma)-f'(H))h_j - \gamma G_m[\frac{h_j}{\epsilon}] + \frac{\lambda_m}{\epsilon^2}h_j\}. \tag{3.12}$$

[5]See [17, Formula (6.55)].

[6]This L_m differs from the one in [17] slightly.

We claim that the right side of (3.12) is $O(|c|)$. The first term inside $\{\}$ on the right side is obviously $O(1)$. The last term is $O(1)$ by (3.6). The third term is $O(1)$ because $G_m[\frac{h_j}{\epsilon}] \to G_m(x, x_j^0)$ as $\epsilon \to 0$. The least obvious is the second term. It is $O(1)$ by Lemma 2.3.

Suppose that Part 1 of Lemma 3.2 is false. Let $\psi = \frac{\phi_m^\perp}{\|\phi_m^\perp\|_\infty}$. ψ satisfies

$$L_m \psi = o(1). \tag{3.13}$$

Without the loss of generality we let $x_* \in [0,1]$ so that $\psi(x_*) = \max|\psi| = 1$. Then $x_* - x_j = O(\epsilon)$ for some x_j. If this is not the case, (3.13) can not be satisfied at x_* since

$$L_m\psi(x_*) = -\epsilon^2(\psi''(x_*) - m^2\pi^2\psi(x_*)) + f'(u_\gamma(x_*))\psi(x_*) + \epsilon\gamma G_m[\psi](x_*) \geq f'(0) + o(1).$$

Define $\Psi(t) = \psi(x_j + \epsilon t)$. As $\epsilon \to 0$, Ψ converges in $C^2_{loc}(\mathbf{R})$ to a non-zero solution Ψ_∞ of

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

Therefore $\Psi_\infty \propto H'$. But $\psi \perp h_j$ implies that $\Psi_\infty \perp H'$. Hence $\Psi_\infty = 0$, a contradiction.

To prove Part 2 we let $\Phi^\perp(t) = \phi_m^\perp(x_j + \epsilon t)$. From (3.12) we find that $\Phi^\perp \to \Phi_\infty^\perp$ which is a solution of

$$-(\Phi_\infty^\perp)'' + f'(H)\Phi_\infty^\perp = c_j^0(f''(H)H'P + \frac{\gamma}{\tau}(\Lambda - \frac{ab}{K})H' + \gamma\Lambda). \tag{3.14}$$

By differentiating the equation for P we find

$$-(P')'' + f'(H)P' = -f''(H)H'P - \frac{\gamma ab}{K}.$$

So $\Phi_\infty^\perp$ and $c_j^0(P' + \Pi)$ satisfy the same equation (3.14). Moreover $\phi_m^\perp \perp h_j$ implies $\Phi_\infty^\perp \perp H'$. Hence $\Phi_\infty^\perp = c_j^0(P' + \Pi)$. □

4 Bifurcation at $(\gamma_{\rm B}, u_{\rm B})$

We use γ as a bifurcation parameter. Let $\lambda(\gamma)$ be one of the K eigenvalues of order ϵ^2 found in Part 3 of Theorem 3.1, associated with a positive integer m. Generically this eigenvalue is simple. To have multiplicity there would be another $m' \neq m$ so that $\lambda(\gamma) = \lambda_{m'}$ for a $\lambda_{m'}$ associated with m'. Because of (3.6) the latter case happens rarely, so we assume that $\lambda(\gamma)$ is simple. It is continued smoothly to a curve of simple eigenvalues $\lambda(\gamma)$ of L_γ as γ varies. Let $\gamma_{\rm B}$ be a particular value of γ so that $\lambda(\gamma_{\rm B}) = 0$. The existence of such $\gamma_{\rm B}$ follows from (3.6). The sign of $\lambda(\gamma)$ is determined, to the leading order term, by $\frac{\gamma}{\tau}(\Lambda - \frac{ab}{K}) + m^2\pi^2$. This quantity is positive when γ is small and negative when γ is large. See [17, Section 7] for more details. Denote the eigenfunction associated with $\lambda(\gamma_{\rm B})$ by $\varphi_{\rm B}(x,y) = \phi_{\rm B}(x)\cos(m\pi y)$. We write $u_{\rm B} := u_{\gamma_{\rm B}}$ and $L_{\rm B} := L_{\gamma_{\rm B}}$ for simplicity. Let

$$X := \{w \in W^{2,2}(D):\ \partial_\nu w = 0 \text{ on } \partial D,\ \overline{w} = 0\},\quad Y := \{z \in L^2(D):\ \overline{z} = 0\}. \tag{4.1}$$

Here X is a dense subspace of Y. Y is an Hilbert space with the usual inner product $\langle\cdot,\cdot\rangle$ inherited from $L^2(D)$.

A nonlinear map $F : (0,\infty) \times X \to Y$ is defined by

$$F(\gamma, w) := -\epsilon^2\Delta(u_\gamma + w) + f(u_\gamma + w) - \overline{f(u_\gamma + w)} + \epsilon\gamma(-\Delta)^{-1}(u_\gamma + w - a). \tag{4.2}$$

Obviously the "trivial branch" $(\gamma, 0)$ is a solution branch of $F(\gamma, w) = 0$. It corresponds to the K-interface, perfect lamellar solution u_γ of (1.2), parameterized by γ. We look for another solution branch, a bifurcating branch, $(\gamma(s), w(s))$ of F. It gives another solution $u_{\gamma(s)} + w(s)$ of (1.2).

Theorem 4.1 *At $\gamma = \gamma_{\rm B}$ another solution branch $(\gamma(s), w(s))$ bifurcates from the "trivial branch" $(\gamma, 0)$. Here $w(s) = s\varphi_{\rm B} + sg(s)$ where the parameter s is in a neighborhood of 0 with $\gamma(0) = \gamma_{\rm B}$ and $w(0) = 0$. Moreover $g(s) \in X$ satisfies $g(s) \perp \varphi_{\rm B}$ and $g(0) = 0$.*

Note that $u_{\gamma(s)} + w(s)$ is approximately $u_{\gamma(s)}(x) + s\phi_{\rm B}(x)\cos(m\pi y)$ since $g(s)$ is a smaller term compared to $\varphi_{\rm B}(x, y) = \phi_{\rm B}(x)\cos(m\pi y)$. Plot 2 of Figure 2 is made based on this observation.

Proof. We appeal to the standard "Bifurcation from simple eigenvalue" theorem [7]. Denote the Fréchet derivatives of F with respect to γ by D_1 and with respect to w by D_2. We need to verify the following three properties.

1. $D_2F(\gamma_{\rm B}, 0)$, which is just $L_{\rm B} : X \to Y$, has a one dimensional kernel, spanned by $\varphi_{\rm B}$.
2. $\mathcal{R}(D_2F(\gamma_{\rm B}, 0))$, the range of $D_2F(\gamma_{\rm B}, 0)$, has co-dimension 1.
3. $D_1D_2F(\gamma_{\rm B}, 0)\varphi_{\rm B}$ is not in $\mathcal{R}(D_2F(\gamma_{\rm B}, 0))$.

Property 1. follows from the simplicity assumption of $\lambda(\gamma)$. To prove 2. we claim that there exists a positive constant $c(\epsilon, \gamma_{\rm B})$ depending on ϵ and $\gamma_{\rm B}$ so that

$$\|\psi\|_2 \leq c(\epsilon, \gamma_{\rm B})\|L_{\rm B}\psi\|_2, \text{ for all } \psi \perp \varphi_{\rm B}, \ \psi \in X. \tag{4.3}$$

Suppose (4.3) is false. There would exist a sequence $\psi_n \in X$, $\psi_n \perp \varphi_{\rm B}$, $\|\psi_n\| = 1$ so that $\|L_{\rm B}\psi_n\|_2 \to 0$. Let $\psi_n \to \psi_*$ weakly in $L^2(D)$. Then $\psi_* \perp \varphi_{\rm B}$. For every $\omega \in X$

$$\langle \psi_*, L_{\rm B}\omega \rangle = \lim_{n\to\infty} \langle \psi_n, L_{\rm B}\omega \rangle = \lim_{n\to\infty} \langle L_{\rm B}\psi_n, \omega \rangle = 0.$$

By the self-adjointness of $L_{\rm B}$, $\psi_* \in X$ and $L_{\rm B}\psi_* = 0$. Hence $\psi_* = 0$ from property 1. Rewrite $L_{\rm B}\psi_n$ as

$$-\epsilon^2 \Delta\psi_n = -f'(u_{\rm B})\psi_n + \overline{f'(u_{\rm B})\psi_n} - \epsilon\gamma_{\rm B}(-\Delta)^{-1}\psi_n + L_{\rm B}\psi_n.$$

Since $\|\psi_n\|_2 = 1$ and $\|L_{\rm B}\psi_n\|_2 \to 0$, the right side is bounded in $L^2(D)$. The elliptic regularity theory asserts that ψ_n is pre-compact in $L^2(D)$. Hence $\psi_n \to 0$ in $L^2(D)$. This is inconsistent with the fact $\|\psi_n\| = 1$. Hence (4.3) holds.

We now prove 2. by showing $\mathcal{R}(L_{\rm B}) = \{\varphi_{\rm B}\}^\perp$. The self-adjointness of $L_{\rm B}$ and 1. imply that every $\psi \in \mathcal{R}(L_{\rm B})^\perp$ is $\varphi_{\rm B}$ multiplied by a constant. It suffices to show that $\mathcal{R}(L_{\rm B})$ is closed. Take $\omega_n \in \mathcal{R}(L_{\rm B})$ so that $\omega_n \to \omega_*$ in $L^2(D)$. Let $\psi_n \in X$, $\psi_n \perp \varphi_{\rm B}$ such that $L_{\rm B}\psi_n = \omega_n$. Since ω_n is a Cauchy sequence, by (4.3) ψ_n is also a Cauchy sequence. Let $\psi_n \to \psi_*$ in $L^2(D)$. Note that $L_{\rm B}$ is a closed operator since it is self-adjoint. Hence $\psi_* \in X$ and $L_{\rm B}\psi_* = \omega_*$. This proves 2.

To prove 3. note that the linear map $D_1D_2F(\gamma_{\rm B}, 0) : X \to Y$ is

$$\psi \to f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\psi - \overline{f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\psi} + \epsilon(-\Delta)^{-1}\psi. \tag{4.4}$$

[7] See [22, Theorem 13.5, page 173].

Since $\mathcal{R}(L_{\rm B}) = \{\varphi_{\rm B}\}^\perp$, it suffices to show

$$\langle D_1 D_2 F(\gamma_{\rm B}, 0)\varphi_{\rm B}, \varphi_{\rm B}\rangle \neq 0, \text{ i.e. } \int_D \{f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\varphi_{\rm B}^2 + \epsilon\varphi_{\rm B}(-\Delta)^{-1}\varphi_{\rm B}\} \neq 0. \tag{4.5}$$

This fact is established in the next lemma. □

Lemma 4.2 *When ϵ is sufficiently small,*

$$\int_D \{f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\varphi_{\rm B}^2 + \epsilon\varphi_{\rm B}(-\Delta)^{-1}\varphi_{\rm B}\} = -\frac{\epsilon^3|c^0|^2\tau m^2\pi^2}{2\gamma_{\rm B}} + o(\epsilon^3|c^0|^2) < 0.$$

Here τ is given in (2.2), and c^0 is in (3.7-3.9), a non-zero vector.

Proof. Note that $\varphi_{\rm B}(x,y) = \phi_{\rm B}(x)\cos(m\pi y)$ and $(-\Delta)^{-1}\varphi_{\rm B}(x,y) = G_m[\phi_{\rm B}](x)\cos(m\pi y)$. Hence after integrating out the y variable we deduce

$$\int_D \{f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\varphi_{\rm B}^2 + \epsilon\varphi_{\rm B}(-\Delta)^{-1}\varphi_{\rm B}\} = \int_0^1 \{\frac{1}{2}f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\phi_{\rm B}^2 + \frac{\epsilon}{2}G_m[\phi_{\rm B}]\phi_{\rm B}\}\,dx. \tag{4.6}$$

By Lemmas 2.4, 3.2, we find

$$\begin{aligned}
\int_0^1 f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\phi_{\rm B}^2 &= \int_0^1 f''(u_{\rm B})(\sum_j c(h_j - \overline{h_j}) + \epsilon R + \epsilon^2(\gamma^{-1}P + b_0))\phi_{\rm B}^2 + o(\epsilon^3) \\
&= \int_0^1 f''(u_{\rm B})(\sum_j (ch_j + \epsilon^2(\gamma^{-1}P + b_0))\phi_{\rm B}^2 + o(\epsilon^3|c|^2) \\
&= \int_0^1 f''(u_{\rm B})(\sum_j (ch_j + \epsilon^2(\gamma^{-1}P + b_0))\phi_{\rm B}^2 + o(\epsilon^3|c|^2) \\
&= \epsilon^2\int_0^1 f''(u_{\rm B})(\gamma^{-1}P)\phi_{\rm B}^2 + o(\epsilon^3|c|^2).
\end{aligned}$$

We have used the fact that P is odd and b_0, H_t and Π are even. Hence we arrive at

$$\int_0^1 f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\phi_{\rm B}^2 = \epsilon^3\int_{\mathbf{R}} f''(H)\gamma^{-1}P(\sum_j c_j^2)(H')^2\,dt + o(\epsilon^3|c|^2) = -\frac{\epsilon^3|c^0|^2 ab}{K} + o(\epsilon^3|c^0|^2)$$

where the last equation follows after we differentiate the equation for $\gamma^{-1}P$:

$$-(\gamma^{-1}P)''' + f'(H)(\gamma^{-1}P)' + f''(H)H'(\gamma^{-1}P) = -\frac{ab}{K},$$

multiply by H', and integrate: $\int_{\mathbf{R}} f''(H)\gamma^{-1}P(H')^2\,dt = -ab/K$. By Lemma 3.2 we obtain

$$\begin{aligned}
\int_0^1 \epsilon G_m[\phi_{\rm B}]\phi_{\rm B} &= \epsilon^3\int_0^1 (\sum_j c_j G_m[\frac{h_j}{\epsilon}])(\sum_k c_k\frac{h_k}{\epsilon}) + o(\epsilon^3|c|^2) \\
&= \epsilon^3\sum_{j,k} c_j c_k G_m(x_k, x_j) + o(\epsilon^3|c|^2) \ = \ \epsilon^3\Lambda|c^0|^2 + o(\epsilon^3|c^0|^2).
\end{aligned}$$

Here Λ is an eigenvalue of the K by K matrix $G_m(x_k^0, x_j^0)$ and c^0 is a corresponding eigenvector, satisfying $\lim_{\epsilon\to 0} c_j = c_j^0$.

Hence the right side of (4.6) becomes

$$\frac{\epsilon^3|c^0|^2}{2}(\Lambda - \frac{ab}{K}) + o(\epsilon^3|c^0|^2).$$

To determine the sign of this quantity we recall (3.6):

$$\lambda(\gamma_{\rm B}) = \epsilon^2[\frac{\gamma_{\rm B}}{\tau}(\Lambda - \frac{ab}{K}) + m^2\pi^2] + o(\epsilon^2).$$

But here $\lambda(\gamma_{\rm B}) = 0$. Hence

$$\Lambda - \frac{ab}{K} = -\frac{\tau m^2\pi^2}{\gamma_{\rm B}} + o(1).$$

This proves the lemma. $\square$

5 Stability of the bifurcating solutions

The eigenvalue $\lambda(\gamma)$ of the "trivial" branch u_γ corresponds to an eigenvalue $\lambda_*(s)$ of the bifurcating solution $u_{\gamma(s)} + w(s)$. The sign of $\lambda_*(s)$ may be determined from the shape of $\gamma(s)$. Thus we proceed to compute $\gamma'(0)$ and $\gamma''(0)$. However the overall stability of $u_{\gamma(s)} + w(s)$ is interesting only when $\lambda(\gamma)$ is the principal, i.e. the smallest, eigenvalue of L_γ. Otherwise, both u_γ and $u_{\gamma(s)} + w(s)$ are unstable. For the moment when studying the shape of $\gamma(s)$, we do not assume that $\lambda(\gamma)$ is the principal eigenvalue. We will do so later in Theorem 5.4.

Place $w(s) = s\varphi_{\rm B} + sg(s)$ into $F(\gamma, w) = 0$ and divide by s:

$$-\epsilon^2\Delta(\frac{u_{\gamma(s)}}{s} + \varphi_{\rm B} + g(s)) + \frac{f(u_{\gamma(s)} + w(s))}{s} + \epsilon\gamma(s)(-\Delta)^{-1}(\frac{u_{\gamma(s)} - a}{s} + \varphi_{\rm B} + g(s)) = \text{Const.} \quad (5.1)$$

where Const. refers to the term coming from the average of f, which is independent of (x, y). Here we do not need its exact value. On the other hand divide the equation (1.2) of $u_{\gamma(s)}$ by s and subtract the result from (5.1):

$$-\epsilon^2\Delta(\varphi_{\rm B} + g(s)) + \frac{f(u_{\gamma(s)} + w(s)) - f(u_{\gamma(s)})}{s} + \epsilon\gamma(s)(-\Delta)^{-1}(\varphi_{\rm B} + g(s)) = \text{Const.} \quad (5.2)$$

Differentiate (5.2) with respect to s and set $s = 0$ afterwards:

$$L_{\rm B}g'(0) + \gamma'(0)\{f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\varphi_{\rm B} + \epsilon(-\Delta)^{-1}\varphi_{\rm B}\} + \frac{1}{2}f''(u_{\rm B})\varphi_{\rm B}^2 = \text{Const..} \quad (5.3)$$

Then we multiply (5.3) by $\varphi_{\rm B}$ and integrate over D:

$$\gamma'(0)\int_D\{f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\varphi_{\rm B}^2 + \epsilon\varphi_{\rm B}(-\Delta)^{-1}\varphi_{\rm B}\} = -\int_D\frac{1}{2}f''(u_{\rm B})\varphi_{\rm B}^3. \quad (5.4)$$

Clearly the right side of (5.4) is 0 since $\varphi_{\rm B}(x, y) = \phi_{\rm B}(x)\cos(m\pi y)$ and integration with respect to y yields 0. Lemma 4.2 then implies

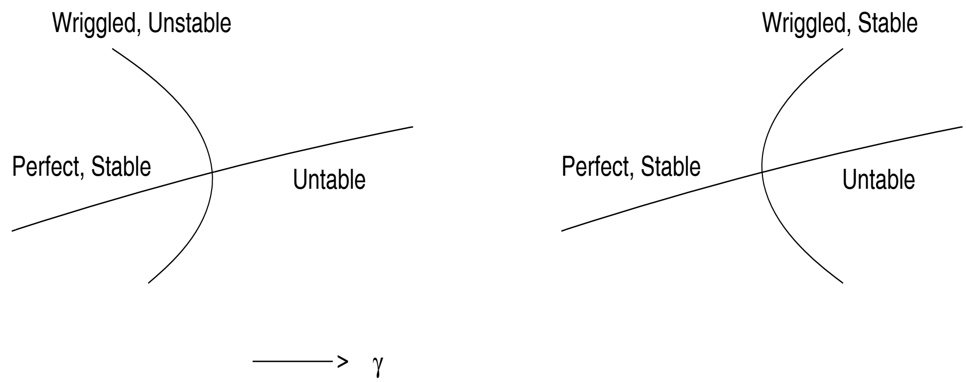

Figure 3: The two possible diagrams of wriggled lamellar solutions bifurcating out of perfect lamellar solutions. The bifurcating solutions are unstable in the first case where $\gamma''(0) < 0$, and stable in the second case where $\gamma''(0) > 0$.

Corollary 5.1 $\gamma'(0) = 0$.

Consequently the equation (5.3) is simplified to

$$L_{\rm B} g'(0) = -\frac{1}{2} f''(u_{\rm B}) \varphi_{\rm B}^2 + \text{Const.}, \quad g'(0) \perp \varphi_{\rm B}. \tag{5.5}$$

The right side of (5.5) is perpendicular to $\varphi_{\rm B}$ since the integration of the right side multiplied by $u_{\rm B}$ with respect to y yields 0, so there is a solution of $g'(0)$. $g'(0) \perp \varphi_{\rm B}$ follows from $g(s) \perp \varphi_{\rm B}$ in Theorem 4.1, so $g'(0)$ is uniquely determined.

Corollary 5.1 implies that the bifurcation digram has the shape of a pitchfork. There are two possibilities illustrated in Figure 3. To determine which of the two cases occurs, we need to find $\gamma''(0)$. Differentiate (5.2) with respect to s twice and set $s = 0$ afterwards:

$$L_{\rm B} g''(0) + \gamma''(0)\{f''(u_{\rm B}) \frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}} \varphi_{\rm B}^2 + \epsilon(-\Delta)^{-1}\varphi_{\rm B}\} + 2f''(u_{\rm B})\varphi_{\rm B} g'(0) + \frac{1}{3} f'''(u_{\rm B})\varphi_{\rm B}^3 = \text{Const.}. \tag{5.6}$$

We have used Corollary 5.1 in deriving (5.6). Again we multiply (5.6) by $\varphi_{\rm B}$ and integrate:

$$\gamma''(0) \int_D \{f''(u_{\rm B}) \frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}} \varphi_{\rm B}^2 + \epsilon\varphi_{\rm B}(-\Delta)^{-1}\varphi_{\rm B}\} = -\int_D \{2f''(u_{\rm B})\varphi_{\rm B}^2 g'(0) + \frac{1}{3} f'''(u_{\rm B})\varphi_{\rm B}^4\}. \tag{5.7}$$

The integral on the left side of (5.7) has been calculated in Lemma 4.2. We now need to know the right side.

Lemma 5.2

$$-\int_D \{2f''(u_{\rm B})\varphi_{\rm B}^2 g'(0) + \frac{1}{3} f'''(u_{\rm B})\varphi_{\rm B}^4\} =$$

$$-\epsilon^5 m\pi\gamma_{\rm B} \sum_{j=1}^K c_j^4 \left[\frac{2+\cosh(2m\pi)}{8\sinh(2m\pi)} + \frac{\cosh(2m\pi(1-2x_j^0))}{8\sinh(2m\pi)} + \frac{\cosh(m\pi(1-2x_j^0))}{4\sinh(m\pi)} - \frac{5(m\pi)^3\tau}{8\gamma_{\rm B}} \right] + o(\epsilon^5|c|^4).$$

The proof of Lemma 5.2 is formidable. We have to expand the quantity to the ϵ^5 order term, because all the lower order terms up to ϵ^4 vanish. Our main idea is to expand $u_{\rm B}, \phi_{\rm B}, 2g'(0)$ as $(...)+\epsilon^2(...)$ near each interface x_j and then show that the quantity in Lemma 5.2 depends "locally" on these expansions near x_j. This is a very long computation. We do not know if there is a simpler proof. We include it in Appendices B and C. The reader may skip it at a first reading. Combining Lemmas 4.2 and 5.2 we obtain

Corollary 5.3 *As* $\epsilon \to 0$, $\epsilon^{-2}\gamma''(0) \to$

$$\frac{2({\gamma_{\rm B}}^0)^2}{|c^0|^2 m\pi\tau}\sum_{j=1}^{K}(c_j^0)^4\left[\frac{2+\cosh(2m\pi)}{8\sinh(2m\pi)}+\frac{\cosh(2m\pi(1-2x_j^0))}{8\sinh(2m\pi)}+\frac{\cosh(m\pi(1-2x_j^0))}{4\sinh(m\pi)}-\frac{5(m\pi)^3\tau}{8{\gamma_{\rm B}}^0}\right]$$

where ${\gamma_{\rm B}}^0 = \lim_{\epsilon\to 0}\gamma_{\rm B}$ *and* $\frac{{\gamma_{\rm B}}^0}{\tau}$ *is determined from* $\dfrac{{\gamma_{\rm B}}^0}{\tau} = \dfrac{m\pi}{\frac{ab}{K}-\Lambda}$.

To study the overall stability of $u_{\gamma(s)} + w(s)$ we now assume that at $\gamma = \gamma_{\rm B}$, the principle eigenvalue $\lambda(\gamma_{\rm B})$ of $u_{\rm B}$ is 0, and this eigenvalue is associated with a particular m. There are K eigenvalues of order ϵ^2 associated with this particular m. Here the 0 eigenvalue is the smallest. Hence Λ now is the smallest eigenvalue of $[G_m(x_j^0, x_k^0)]$. According to [17, Section 7]

$$\begin{aligned}
\Lambda &= \frac{1}{m\pi(\tanh(m\pi a)+\tanh(m\pi b))} \quad \text{if } K=1,\\
\Lambda &= \frac{1}{m\pi(\coth(m\pi a)+\cot(m\pi b)-\operatorname{csch}(m\pi a)+\operatorname{csch}(m\pi b))} \quad \text{if } K=2, \qquad (5.8)\\
\Lambda &= \frac{1}{d+\sqrt{\alpha^2+\beta^2+2\alpha\beta\cos\theta}}, \quad \theta = 2\pi/K, \quad \text{if } K\geq 3.
\end{aligned}$$

Define

$$S(a,K) := \sum_{j=1}^{K}\left(\frac{c_j^0}{|c^0|}\right)^4\left[\frac{2+\cosh(2m\pi)}{8\sinh(2m\pi)}+\frac{\cosh(2m\pi(1-2x_j^0))}{8\sinh(2m\pi)}+\frac{\cosh(m\pi(1-2x_j^0))}{4\sinh(m\pi)}-\frac{5(m\pi)^3\tau}{8{\gamma_{\rm B}}^0}\right] \qquad (5.9)$$

where ${\gamma_{\rm B}}^0/\tau$ is determined as in Corollary 5.3 and m is associated with the principal eigenvalue 0. Note that $S(a,K)$ depends on a and K only. It does not depend on τ. Since τ depends on the shape of W, $S(a,K)$ is independent of the exact shape of W. Then Corollary 5.3 implies

$$\lim_{\epsilon\to 0}\epsilon^{-2}\gamma''(0) = \frac{2({\gamma_{\rm B}}^0)^2|c^0|^2}{m\pi\tau}S(a,K). \qquad (5.10)$$

Theorem 5.4 *When* ϵ *is sufficiently small, the bifurcating solution* $u_{\gamma(s)} + w(s)$ *of* K *wriggled interfaces is stable if* $S(a,K) > 0$ *and it is unstable if* $S(a,K) < 0$.

Proof. We first find $\lambda'(\gamma_{\rm B})$. Differentiate the equation $L_\gamma\varphi = \lambda\varphi$ with respect to γ:

$$-\epsilon^2\Delta\varphi_\gamma + f'(u_\gamma)\varphi_\gamma + \epsilon\gamma(-\Delta)^{-1}\varphi_\gamma + f''(u_\gamma)\frac{du_\gamma}{d\gamma}\varphi_\gamma + \epsilon(-\Delta)^{-1}\varphi = \lambda\varphi_\gamma + \lambda'(\gamma)\varphi + \text{Const.}.$$

Set $\gamma = \gamma_{\rm B}$ in the equation, multiply the equation by $\varphi_{\rm B}$, and integrate over D:

$$\int_D \{f''(u_{\rm B})\frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_{\rm B}}\varphi_{\rm B}^2 + \epsilon\varphi_{\rm B}(-\Delta)^{-1}\varphi_{\rm B}\} = \lambda'(\gamma_{\rm B})\int_D \varphi_{\rm B}^2.$$

The left side is calculated in Lemma 4.2. The integral on the right side is

$$\int_D \varphi_{\rm B}^2 = \int_D (\sum_j c_j h_j)^2 \cos^2(m\pi y)\,dxdy + o(\epsilon|c|^2) = \frac{\epsilon\tau}{2}\sum_j c_j^2 + o(\epsilon|c|^2).$$

Therefore

$$\lambda'(\gamma_{\rm B}) = -\frac{\epsilon^2 m^2\pi^2}{\gamma_{\rm B}} + o(\epsilon^2) < 0. \tag{5.11}$$

According to Crandall and Rabinowitz [4, Theorem 1.16], which generalizes an earlier result of Sattinger [19], near $s=0$, $\lambda_*(s)$ and $-s\gamma'(s)\lambda'(\gamma_{\rm B})$ have the same zeros, and

$$\lim_{s\to 0,\ \lambda_*(s)\neq 0} \frac{-s\gamma'(s)\lambda'(\gamma_{\rm B})}{\lambda_*(s)} = 1. \tag{5.12}$$

Here $\lambda_*(s)$ is the principle eigenvalue of the bifurcating solution $u_{\gamma(s)}+w(s)$. Whether the bifurcating solution is stable depends on whether $\lambda_*(s)$ is positive. The theorem follows from (5.10), (5.11), and (5.12). □

Let us use Theorem 5.4 to work out some examples. The quantity $S(a,K)$ may be accurately calculated following these numerical steps.

1. For each positive integer m find Λ from (5.8).

2. With this Λ find ${\gamma_{\rm B}}^0/\tau$ from the formula in Corollary 5.3. If one obtains a non-positive ${\gamma_{\rm B}}^0/\tau$, this means that eigenvalues associated with this m are positive for any γ and this m does not yield any wriggled lamellar solution. Discard such m.

3. Minimize the positive ${\gamma_{\rm B}}^0/\tau$ with respect to the remaining m. The minimum is achieved at the particular m associated to the principal eigenvalue of $u_{\rm B}$. Find c^0 from Q of (3.10), using this m and its corresponding Λ.

4. Use this particular m and the corresponding ${\gamma_{\rm B}}^0/\tau$ and c^0 to find $S(a,K)$ from (5.9).

Tables 1, 2 and 3 report our numerical calculations based on this method for the cases $a = 1/2$, $1/8$, and $7/8$. In each table the first column is the number of the interfaces in the perfect lamellar solution $u_{\rm B}$. The second column gives the value of m associated with the principal eigenvalue 0 of $u_{\rm B}$. Note that m does not increase as fast as K does. The third column has the value of ${\gamma_{\rm B}}^0/\tau$. We will explain the fourth in a moment. The fifth column has the value of $S(a,K)$. The last column indicates the stability of the bifurcating solution with K wriggled interfaces.

We have deliberately chosen $a = 1/8$ and $a = 7/8$ because they are somehow "symmetric". With the exception of $K = 2$, the ${\gamma_{\rm B}}^0/\tau$'s are identical in Tables 2 and 3 for the same value of K. Moreover the $S(a,K)$ values are the same in the two tables when K is odd. All these symmetries and asymmetries can be explained from the formula (5.8) for Λ and the matrix (3.10) of Q.

There is something interesting about the perfect lamellar solution $u_{\rm B}$ whose principal eigenvalue is 0 where bifurcation occurs. In [17, Section 8] it is shown that the 1-D global minimizer (the

K	m	${\gamma_{\rm B}}^0/\tau$	K_{opt}	$S(1/2, K)$	Stability
1	1	1.2906e+02	2	-2.0964e-03	Unstable
2	2	8.6349e+02	3	-2.1740e-02	Unstable
3	3	2.7193e+03	4	-3.3075e-02	Unstable
4	3	5.3823e+03	5	1.0764e-02	Stable
5	3	9.7086e+03	6	2.1578e-02	Stable
6	4	1.6165e+04	7	1.2129e-02	Stable
7	4	2.4091e+04	8	1.5804e-02	Stable
8	4	3.4492e+04	9	1.6739e-02	Stable
9	4	4.7728e+04	10	1.6541e-02	Stable
10	4	6.4156e+04	11	1.5885e-02	Stable

Table 1: The stability of the wriggled lamellar solutions that bifurcate from the principal eigenvalues of the perfect lamellar solutions, when $a = b = 1/2$.

K	m	${\gamma_{\rm B}}^0/\tau$	K_{opt}	$S(1/8, K)$	Stability
1	3	1.7317e+03	2	-1.5234e-01	Unstable
2	5	1.3418e+04	4	-8.9872e-03	Unstable
3	2	1.0218e+04	3	5.7102e-02	Stable
4	3	2.3798e+04	5	5.1520e-02	Stable
5	3	4.3553e+04	6	3.4174e-02	Stable
6	3	7.3607e+04	7	2.9597e-02	Stable
7	4	1.1373e+05	8	2.4505e-02	Stable
8	4	1.6489e+05	9	2.2058e-02	Stable
9	4	2.3061e+05	10	1.9979e-02	Stable
10	4	3.1284e+05	11	1.8189e-02	Stable

Table 2: The stability of the wriggled lamellar solutions that bifurcate from the principal eigenvalues of the perfect lamellar solutions, when $a = 1/8$.

K	m	${\gamma_B}^0/\tau$	K_{opt}	$S(7/8, K)$	Stability
1	3	1.7317e+03	2	-1.5234e-01	Unstable
2	2	3.4949e+03	2	4.0940e-02	Stable
3	2	1.0218e+04	3	5.7102e-02	Stable
4	3	2.3798e+04	5	2.6416e-02	Stable
5	3	4.3553e+04	6	3.4174e-02	Stable
6	3	7.3607e+04	7	2.9798e-02	Stable
7	4	1.1373e+05	8	2.4505e-02	Stable
8	4	1.6489e+05	9	2.2092e-02	Stable
9	4	2.3061e+05	10	1.9979e-02	Stable
10	4	3.1284e+05	11	1.8196e-02	Stable

Table 3: The stability of the wriggled lamellar solutions that bifurcate from the principal eigenvalues of the perfect lamellar solutions, when $a = 7/8$.

global minimizer of I_1 in Theorem 2.1, also a perfect lamellar solution on D after trivial extension), which is one of the 1-D local minimizers, has the number of interfaces K_{opt} which minimizes (among positive integers N) $\tau N + \gamma a^2 b^2/(6N^2)$. If we take $\gamma = \gamma_B$ so that the K-interface, perfect lamellar solution u_B has 0 principal eigenvalue, we find the 1-D global minimizer corresponding to γ_B. The number of interfaces K_{opt} of this 1-D global minimizer is reported in the fourth columns in Tables 1, 2, and 3. For most a and K the 1-D global minimizer has one more interface than u_B does. In some other cases the 1-D global minimizer is exactly u_B.

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References

[1] D. Andelman, F. Broçhard, and J.-F. Joanny. Phase transitions in Langmuir monolayers of polar molecules. *J. Chem. Phys.*, 86(6):3673–3681, 1987.

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

[3] R. Choksi and X. Ren. On the derivation of a density functional theory for microphase separation of diblock copolymers. *J. Statist. Phys.*, to appear.

[4] M.G. Crandall and P.H. Rabinowitz. Bifurcation, perturbation of simple eigenvalues, and linearized stability. *Arch. Rational Mech. Anal.*, 52(2):161–180, 1973.

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

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

[7] C.B. Muratov. Theory of domain patterns in systems with long-range interactions of Coulomb type. *Phys. Rev. E*, 66:066108, 2002.

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

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

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

[11] X. Ren and J. Wei. The soliton-stripe pattern in the Seul-Andelman membrane. preprint.

[12] X. Ren and J. Wei. Soliton-stripe patterns in charged Langmuir monolayers. preprint.

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

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

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

[16] X. Ren and J. Wei. Triblock copolymer theory: Free energy, disordered phase and weak segregation. *Physica D*, 178:103–117, 2003.

[17] X. Ren and J. Wei. On the spectra of 3-D lamellar solutions of the diblock copolymer problem. *SIAM J. Math. Anal.*, to appear.

[18] X. Ren and J. Wei. Triblock copolymer theory: Ordered ABC lamellar phase. *J. Nonlinear Sci.*, to appear.

[19] D.H. Sattinger. Stability of bifurcating solutions by Leray-Schauder degree. *Arch. Rational Mech. Anal.*, 43:154–166, 1971.

[20] J.V. Selinger, Z.-G. Wang, R.F. Bruinsma, and C.M. Knobler. Chiral symmetry breaking in Langmuir monolayers and smectic films. *Phys. Rev. Lett.*, 70(8):1139–1142, 1993.

[21] M. Seul and D. Andelman. Domain shapes and patterns: The phenomenology of modulated phases. *Science*, 267:476–483, 1995.

[22] J. Smoller. *Shock Waves and Reaction-Diffusion Equations*. Springer-Verlag, New York Heidelberg Berlin, 1983.

[23] Y. Tsori, D. Andelman, and M. Schick. Defects in lamellar diblock copolymers: Chevron- and Ω-shaped boundaries. *Phys. Rev. E*, 61(3):2848–2858, 2000.

A Proof of Lemma 2.4

Proof. We differentiate the 1-D Euler-Lagrange equation in Theorem 2.1 with respect to γ to deduce

$$-\epsilon^2(\frac{du_\gamma}{d\gamma})'' + f'(u_\gamma)\frac{du_\gamma}{d\gamma} - \overline{f'(u_\gamma)\frac{du_\gamma}{d\gamma}} + \epsilon\gamma G_0[\frac{du_\gamma}{d\gamma}] = -\epsilon G_0[u_\gamma - a]. \tag{A.1}$$

Let us define an operator L_0 so the left side of (A.1) is $L_0\frac{du_\gamma}{d\gamma}$. Rewrite (A.1) as

$$c\sum_j L_0(h_j - \overline{h_j}) + \epsilon L_0\psi = -\epsilon G_0[u-a]. \tag{A.2}$$

Note that

$$L_0(h_j - \overline{h_j}) = (f'(u_\gamma) - f'(H))h_j + \epsilon\gamma G_0[h_j - \overline{h_j}] + (\overline{f'(u_\gamma)} - f'(u_\gamma))\overline{h_j} - \overline{f'(u_\gamma)h_j} + e.s.. \tag{A.3}$$

We claim that

$$\|\psi\|_\infty = O(1)(1+|c|). \tag{A.4}$$

According to [17, (4.29)], $L_0(h_j - \overline{h_j}) = O(\epsilon)$. Hence we deduce from (A.2)

$$L_0\psi = O(1)(1+|c|). \tag{A.5}$$

If (A.4) is false, let $\omega = \frac{\psi}{\|\psi\|_\infty}$, which satisfies

$$L_0\omega = o(1). \tag{A.6}$$

Assume without the loss of generality at some $x_* \in [0,1]$, $\omega(x_*) = \max|\omega| = 1$. We show that $x_* - x_j = O(\epsilon)$ for some x_j. Otherwise at x_* (A.6) implies

$$o(1) = L_0\omega(x_*) \geq f'(u_\gamma(x_*))\omega(x_*) - \overline{(f'(u_\gamma) - f'(0))\omega} + O(\epsilon) = f'(0) + o(1),$$

which is impossible. Define $\Omega(t) = \omega(x_j + \epsilon t)$, which satisfies

$$-\Omega'' + f'(u_\gamma)\Omega = o(1) \tag{A.7}$$

on $(-x_j/\epsilon, (1-x_j)/\epsilon)$ by (A.6). As $\epsilon \to 0$, $\Omega \to \Omega_\infty$ in $C^2_{loc}(\mathbf{R})$. Ω_∞ is non-zero and satisfies

$$-\Omega_\infty'' + f'(H)\Omega_\infty = 0.$$

Therefore $\Omega_\infty \propto H'$. On the other hand $\psi \perp h_j$ implies $\Omega_\infty \perp H'$. Hence $\Omega_\infty = 0$, a contradiction. This proves (A.4).

Multiply (A.2) by $h_k - \overline{h_k}$ and integrate:

$$c\sum_j \langle L_0(h_j - \overline{h_j}), h_k - \overline{h_k}\rangle + \epsilon\langle\psi, L_0(h_k - \overline{h_k})\rangle = -\epsilon\langle G_0[u_\gamma - a], h_k - \overline{h_k}\rangle. \tag{A.8}$$

It is proved in [17, (4.35)] that

$$\langle L_0(h_j - \overline{h_j}), h_k - \overline{h_k}\rangle = -\frac{\epsilon^3\gamma ab\delta_{jk}}{K} + \epsilon^3\gamma G_0(x_j, x_k) + \epsilon^2\overline{f'(u_\gamma)} + o(\epsilon^3), \tag{A.9}$$

where $\delta_{jk} = 0$ if $j = k$ and $= 0$ otherwise, and proved in [17, (4.30)] that

$$\|L_0(h_j - \overline{h_j})\|_1 = O(\epsilon^2). \tag{A.10}$$

Following (A.9) and (A.10), (A.8) becomes

$$c\sum_j\{-\frac{\epsilon^3\gamma ab\delta_{jk}}{K} + \epsilon^3\gamma G_0(x_j, x_k) + \epsilon^2\overline{f'(u_\gamma)}\} + o(\epsilon^3)|c| + O(\epsilon^3)(1+|c|) = -\epsilon^2 v(x_k) + o(\epsilon^2). \tag{A.11}$$

Comparing the leading order ϵ^2 terms on the both sides of (A.11), we conclude that $c = O(1)$ and $\lim_{\epsilon\to 0} c = c_0 := -\frac{v^0(x_k^0)}{Kf'(0)}$. This proves Part 1.

The above argument (A.11) also shows that

$$c = -\frac{v^0(x_k^0)}{Kf'(0)} + O(\epsilon). \tag{A.12}$$

Rewrite (A.2) as

$$\begin{aligned} L_0\psi &= -G_0[u-a] - \frac{c}{\epsilon}\sum_j L_0(h_j - \overline{h_j}) && \text{(A.13)} \\ &= -\frac{c}{\epsilon}[\sum_j (f'(u_\gamma) - f'(H))h_j + f'(u_\gamma)\overline{h_j} + \gamma\epsilon G_0[h_j - \overline{h_j}] \\ &\quad -(G_0[u-a] + Kc\overline{f'(u_\gamma)}\,\overline{h_j}). && \text{(A.14)} \end{aligned}$$

The limit of $\psi(x_j + \epsilon\cdot)$ satisfies the limit of (A.14) in the t-coordinate:

$$-R'' + f'(H)R = -\frac{v^0(x_k^0)}{f'(0)}f'(H) + \text{Const.} \tag{A.15}$$

This is because in the right side of (A.3) the third term is of the leading ϵ order (See [17, Section 4] for details). Multiply (A.15) by H_t and integrate to find Const. $= 0$. This proves Part 2.

To prove Part 3, we note that we can write $R = -\frac{v^0(x_j^0)}{f'(0)} + d_0 H_t$, where d_0 is such that $R \perp H_t$. This is the inner expansion of ψ. We have to glue the inner expansion and outer expansion of ψ. The outer expansion of ψ is $\frac{v}{f'(0)}$. We now choose

$$R_\epsilon = \sum_j (\frac{\hat{c}\overline{h_j}}{\epsilon} + \hat{d}h_j - \frac{v}{f'(0)})\chi(\frac{x - x_j}{\sqrt{\epsilon}}) + \frac{v}{f'(0)} \tag{A.16}$$

where $\chi(s)$ is a cut-off function such that $\chi(s) = 1$ for $s \le 1$ and $\chi(s) = 0$ for $s \ge 2$, and the constants $\hat{c}$ and $\hat{d}$ are chosen such that $\int R_\epsilon h_j = 0, \int R_\epsilon = 0$. By (A.12), we have

$$\hat{c} = Kc + O(\epsilon), \quad \hat{d} = d_0 + O(\epsilon).$$

It is then easy to calculate that

$$L_0 R_\epsilon = -\sum_j G_0[u-a](1 - \chi(\frac{x - x_j}{\sqrt{\epsilon}})) - \frac{\hat{c}}{\epsilon}\sum_j f'(u_\gamma)\overline{h_j} + \epsilon\,\text{Const.} + o(\epsilon). \tag{A.17}$$

Set now

$$\psi = R_\epsilon + \epsilon b_\epsilon$$

Then b_ϵ satisfies

$$\begin{aligned} L_0 b_\epsilon &= \frac{c}{\epsilon^2}\sum_j (f' - f'(u))h_j - \frac{c\gamma}{\epsilon}\sum_j \gamma G_0[h_j - \overline{h_j}] \\ &\quad -\frac{1}{\epsilon}\sum_j (G_0[u-a]\chi(\frac{x-x_j}{\sqrt{\epsilon}}) - v(x_j)) + \text{Const.} + o(1). \end{aligned} \tag{A.18}$$

Since $\int b_\epsilon h_j = 0, \int b_\epsilon = 0$, we see from (A.18) that b_ϵ is bounded and hence we pass to the limit in (A.18). The limiting equation of (A.18) becomes

$$\hat{b}'' - f'(H)\hat{b} = -(v^0)'(x_j^0)t + c_0 f''(H)H_t P + \text{Const.}, \hat{b} \perp H_t, \tag{A.19}$$

where $\hat{b}(t) = \lim_{\epsilon\to 0} b_\epsilon(x_j + \epsilon t)$. Multiplying (A.19) by H_t, we see that the Const. in (A.19) must be $-c_0\int_{\mathbf{R}} f''(H)H_t^2 P$. It then follows that $\hat{b} = \frac{1}{\gamma}P + b_0$, where b_0 is defined in Lemma 2.4. This gives Part 3. □

B Expansion of $2g'(0)$

In Appendices B and C we use the following simplified notations:

$$u := u_{\rm B},\ v := G_0[u_{\rm B} - a],\ \gamma := \gamma_{\rm B},\ \phi := \phi_{\rm B},\ \omega := \phi_{\rm B}^{\perp},\ f' := f'(H),\ f'' := f''(H),\ \text{etc.} \tag{B.1}$$

The vector c_j in the expansion of ϕ satisfies $|c| = 1$.

Define a linear operator $\mathcal{L}$ by

$$\mathcal{L}U := U'' - f'U \tag{B.2}$$

where U is defined on $\mathbf{R}$. Then

$$\mathcal{L}H_t = 0, \tag{B.3}$$

$$\mathcal{L}H_{tt} = f''H_t^2, \tag{B.4}$$

$$\mathcal{L}H_{ttt} = 3f''H_tH_{tt} + f'''H_t^3. \tag{B.5}$$

Let $u = H(t) + \epsilon^2 p$. Then p satisfies

$$\epsilon^2 p'' - f'p = \frac{1}{\epsilon^2}[\gamma\epsilon G_0[u-a] - \text{Constant}] + \epsilon^2 f''\frac{p^2}{2} + O(\epsilon^4). \tag{B.6}$$

By Lemma 2.3 as $\epsilon \to 0, p(x_j + \epsilon\cdot) \to P$ in $C^2_{loc}(\mathbf{R})$, where P satisfies

$$\mathcal{L}P + \gamma(v^0)'(x_j^0)t = 0. \tag{B.7}$$

Note that $P(t)$ is an odd function (and hence $P \perp H_t$). It is easy to compute that

$$\mathcal{L}P_t = f''H_tP - \gamma(v^0)'(x_j^0), \tag{B.8}$$

$$\mathcal{L}P_{tt} = (f''H_t)_tP + 2f''H_tP_t, \tag{B.9}$$

$$\mathcal{L}P_{ttt} = (f''H_t)_{tt}P + 3(f''H_t)_tP + 3f''H_tP_{tt}. \tag{B.10}$$

Recall Lemma 3.2. In the decomposition

$$\phi(x) = \sum_{j=1}^{K} c_j h_j + \epsilon^2 \omega, \; h_j \perp \omega \tag{B.11}$$

ω satisfies

$$\begin{aligned} &\epsilon^2 \omega'' - \epsilon^2 (m\pi)^2 \omega - f'(u)\omega - \epsilon\gamma G_m[\omega] \\ = \quad & -\frac{1}{\epsilon^2} \sum_{j=1}^{K} c_j [(f' - f'(u))h_j - \epsilon^2 (m\pi)^2 h_j] + \frac{\gamma}{\epsilon} \sum_{k=1}^{K} c_k G_m[h_k]. \end{aligned} \tag{B.12}$$

We further expand (B.12):

$$\begin{aligned} \epsilon^2 \omega'' - f'\omega \quad = \quad & \sum_{j=1}^{K} c_j [f'' H_t p - m^2 \pi^2 H_t] \; + \frac{\gamma}{\epsilon} \sum_{k=1}^{K} c_k G_m[h_k] \\ & + \gamma\epsilon G_m[\omega] + \epsilon^2 [f'' p\omega + m^2\pi^2 \omega + f''' H_t \frac{p^2}{2}] + O(\epsilon^3). \end{aligned} \tag{B.13}$$

As $\epsilon \to 0$, we have $\omega(x_j + \epsilon \cdot) \to c_j^0 \Omega$ in $C^2_{loc}(\mathbf{R})$, where Ω satisfies

$$\mathcal{L}\Omega = f'' H_t P - (m\pi)^2 H_t + \text{Const.}, \; \Omega \text{ is even and } \Omega \perp H_t. \tag{B.14}$$

Hence

$$\mathcal{L}\Omega_t = f'' H_t \Omega + (f'' H_t)_t P + f'' H_t P_t - (m\pi)^2 H_{tt}. \tag{B.15}$$

Finally, we calculate $2g'(0)$. Since $\varphi_{\mathrm{B}}^2 = \phi^2(x)\cos^2(m\pi y)$, we decompose the solution of (5.5) into

$$2g'(0)(x,y) = \frac{g_1(x)}{2} + \frac{g_2(x)\cos(2m\pi y)}{2} \tag{B.16}$$

where g_1 and g_2 are solutions of the following two equations.

$$\epsilon^2 g_1'' - f'(u) g_1 - \epsilon\gamma G_0[g_1] = f''(u)\phi^2 - \overline{f''(u)\phi^2}, \;\; g_1'(0) = g_1'(1) = \overline{g_1} = 0; \tag{B.17}$$

$$\epsilon^2 (g_2'' - 4m^2\pi^2 g_2) - f'(u) g_2 - \epsilon\gamma G_{2m}[g_2] = f''(u)\phi^2, \; g_2'(0) = g_2'(1) = 0. \tag{B.18}$$

Both equations are uniquely solvable, since the eigenvalues of the two operators in (B.17) and (B.18) are non-zero (the zero eigenvalue is associated with m), i.e. both operators are invertible.

We write

$$2g'(0) = \psi_1 + \epsilon^2 \psi_2 \tag{B.19}$$

where

$$\psi_1(x,y) = \sum_j c_j^2 H_{tt}(\frac{x - x_j}{\epsilon}) \cos^2(m\pi y), \; \psi_2 = \frac{g_{11}}{2} + \frac{g_{21}}{2} \cos(2m\pi y). \tag{B.20}$$

Here

$$g_1 = \sum_j c_j^2 H_{tt}(\frac{x - x_j}{\epsilon}) + \epsilon^2 g_{11}, \; g_2 = \sum_j c_j^2 H_{tt}(\frac{x - x_j}{\epsilon}) + g_{21}. \tag{B.21}$$

The equation for g_{11} is

$$\begin{aligned}
&\epsilon^2 g_{11}'' - f'(u)g_{11} - \epsilon\gamma G_0[g_{11}] \\
= &\ \frac{\gamma c_j^2}{\epsilon} G_0[H_{tt}] + \frac{1}{\epsilon^2}[f''(u)\phi_m^2 - c_j^2 f'' H_t^2 - \overline{f''(u)\phi_m^2}] \\
= &\ \frac{\gamma c_j^2}{\epsilon} G_0[H_{tt}] + c_j^2 f''' H_t^2 p + 2f'' H_t c_j \omega + c_j^2 f'' H_{tt} p \\
&+\epsilon^2 [c_j^2 f^{(4)} H_t^2 \frac{p^2}{2} + c_j^2 f''' H_{tt} \frac{p^2}{2} + 2c_j f''' H_t p\omega + f''\omega^2] + O(\epsilon^4) + C_1 \qquad \text{(B.22)}
\end{aligned}$$

where $C_1 = \epsilon^{-2}\overline{f''(u)\phi_m^2}$. By (B.15), it is easy to see that

$$C_1 = \frac{1}{\epsilon^2}\int_0^1 f''(u)\phi_m^2 = \frac{1}{\epsilon^2}\sum_{j=1}^K f''(H+\epsilon^2 p)c_j^2 H_t^2 + o(1) = o(1). \qquad \text{(B.23)}$$

Similarly the equation for g_{21} is

$$\begin{aligned}
&\epsilon^2 g_{21}'' - 4m^2\pi^2 g_{21} - f'(u)g_{21} - \epsilon\gamma G_{2m}[g_{21}] \\
= &\ 4m^2\pi^2 c_j^2 H_{tt} + \frac{\gamma c_j^2}{\epsilon} G_{2m}[H_{tt}] + c_j^2 f''' H_t^2 p + 2f'' H_t c_j \omega + c_j^2 f'' H_{tt} p \\
&+\epsilon^2 [c_j^2 f^{(4)} H_t^2 \frac{p^2}{2} + c_j^2 f''' H_{tt} \frac{p^2}{2} + 2c_j f''' H_t p\omega + f''\omega^2] + O(\epsilon^4). \qquad \text{(B.24)}
\end{aligned}$$

We state the following lemma.

Lemma B.1 *As $\epsilon \to 0$, near x_j we have $g_{11}(x_j + \epsilon\cdot) \to (c_j^0)^2 G_{11}, g_{21}(x_j + \epsilon\cdot) \to (c_j^0)^2 G_{21}$, where G_{11} satisfies*

$$\mathcal{L}G_{11} = f''' H_t^2 P + 2f'' H_t \Omega + f'' H_{tt} P, \ G_{11} \textit{is odd}$$

and G_{21} satisfies

$$\mathcal{L}G_{21} = f''' H_t^2 P + 2f'' H_t \Omega + f'' H_{tt} P + (2m\pi)^2 H_{tt}, \ G_{21} \textit{is odd.}$$

Proof. We only prove the convergence of g_{11}. The convergence of g_{21} is similar. To this end, let us decompose

$$g_{11} = \sum_{j=1}^K \alpha_j (h_j - \overline{h_j}) + G_{11} + \hat{g}_{11}$$

where $\hat{g}_{11} \perp h_j, j = 1, ..., K$ and $\int_0^1 \hat{g}_{11} = 0$. The key is to show that $\alpha_j = o(1)$. This is similar to the proof of (3) of Lemma 2.4.

Simple calculations show that $\hat{g}_{11}$ satisfies

$$\epsilon^2 \hat{g}_{11}'' - f'(u)\hat{g}_{11} - \epsilon\gamma G_0[\hat{g}_{11}] = O(\epsilon^2 \sum_{j=1}^K |\alpha_j|) + o(1)$$

Since $\hat{g}_{11} \perp h_j, j = 1, ..., K, \int \hat{g}_{11} = 0$, standard arguments show that

$$\hat{g}_{11} = O(\sum_{j=1}^{K} |\alpha_j|\epsilon^2) + o(1). \tag{B.25}$$

We multiply (B.22) by h_j and integrate over $(0,1)$, to find

$$\begin{aligned}
\epsilon C_1 + \alpha_j \int_0^1 (f' - f'(u))H_t^2 &= \int_0^1 [c_j^2 f''' H_t^2 p + 2c_j f'' H_t \omega + c_j^2 f'' H_{tt} p] H_t + o(\epsilon^3) \\
&= \int_0^1 [c_j^2 f''' H_t^2 p + c_j^2 f'' H_{tt} p] H_t + 2c_j \int_0^1 \mathcal{L} H_{tt} \omega + o(\epsilon^3) \\
&= \int_0^1 [c_j^2 f''' H_t^2 p + 3c_j^2 f'' H_{tt} p] H_t + o(\epsilon^3) \\
&= c_j^2 \int_0^1 (\mathcal{L} H_{ttt}) p + o(\epsilon^3) \;=\; o(\epsilon^3).
\end{aligned}$$

Thus we obtain the first identity

$$C_1 + \epsilon^2 \alpha_j \int_{\mathbf{R}} f'' P H_t^2 = o(\epsilon^2). \tag{B.26}$$

Next, we integrate the equation (B.22) over $(0,1)$ and make use of (B.25) to deduce that

$$0 = \int_0^1 f'(u) g_{11} = \int_0^1 f'(u)(\sum_j \alpha_j (h_j - \overline{h_j}) + \hat{g}_{11}).$$

So we obtain the second identity

$$\sum_j \alpha_j f'(0) = o(1). \tag{B.27}$$

Substituting (B.27) into (B.26), we have that

$$C_1 = o(\epsilon^2),\;\; \alpha_j = o(1) \tag{B.28}$$

and hence $\hat{g}_{11} = o(1)$. □

C Proof of Lemma 5.2

In this appendix we omit $\sum_j$ most of the time. When c_j appears in a quantity, $\sum_j$ is usually implied. We use the notation $A \approx B$ for $A - B = o(\epsilon^5)$.

Define a linear operator S by

$$S\psi := \epsilon^2 \Delta\psi - f'(u)\psi + \epsilon\gamma\Delta^{-1}\psi. \tag{C.1}$$

where ψ is a function on D. Recall ψ_1 and ψ_2 defined in (B.20). Note

$$\begin{aligned} S\psi_1 &= c_j^2\{(f'-f'(u))H_{tt}\cos^2(m\pi y)+f''H_t^2\cos^2(m\pi y) \\ &\quad -2\epsilon^2(m\pi)^2H_{tt}\cos(2m\pi y)+\epsilon\gamma\Delta^{-1}(H_{tt}\cos^2(m\pi y))\}. \end{aligned} \tag{C.2}$$

$$\begin{aligned} S\psi_2 &= 2(m\pi)^2c_j^2H_{tt}\cos(2m\pi y)-\frac{\gamma c_j^2}{\epsilon}\Delta^{-1}(H_{tt}\cos^2(m\pi y)) \\ &\quad +\frac{1}{\epsilon^2}(f''(u)\phi^2-c_j^2f''H_t^2)\cos^2(m\pi y)+\frac{c_j^2}{\epsilon^2}(f'(u)-f')H_{tt}\cos^2(m\pi y). \end{aligned} \tag{C.3}$$

Then

$$\begin{aligned} \int_D f''(u)\varphi^2(2g'(0)) &= \int_D (S(2g'(0)))(2g'(0)) \\ &= \int_D (S\psi_1)\psi_1+2\epsilon^2\int_D(S\psi_2)\psi_1+\epsilon^4\int_D(S\psi_2)\psi_2 \ := \ I_1+I_2+I_3 \end{aligned} \tag{C.4}$$

where the last equation defines I_1, I_2 and I_3. To prove Lemma 5.2 we compute

$$\int_D f''(u)\phi^2(2g'(0))+\frac{1}{3}\int_D f'''(u)\phi^4 = I_1+I_2+I_3+\frac{1}{3}\int_D f'''(u)\phi^4. \tag{C.5}$$

We start with I_2. From (C.3) we obtain

$$\begin{aligned} I_2 &\approx 4\epsilon^3(m\pi)^2c_j^4\int_{\mathbf{R}}H_{tt}^2\int_0^1\cos^2(m\pi y)\cos(2m\pi y) \\ &\quad -2\epsilon\gamma c_j^4\int_D(\Delta^{-1}(H_{tt}\cos^2(m\pi y)))H_{tt}\cos^2(m\pi y) \\ &\quad +2\epsilon c_j^2\int_{\mathbf{R}}(f''(u)\phi^2-c_j^2f''H_t^2)H_{tt}\int_0^1\cos^4(m\pi y) \\ &\quad +2\epsilon c_j^4\int_{\mathbf{R}}(f'(u)-f')H_{tt}^2\int_0^1\cos^4(m\pi y) \\ &\approx \epsilon^3(m\pi)^2c_j^4\int_{\mathbf{R}}H_{tt}^2+\epsilon\gamma c_j^4\int_0^1(2G_0+G_{2m})[H_{tt}]\frac{H_{tt}}{4} \\ &\quad +\frac{3\epsilon c_j^2}{4}\int_{\mathbf{R}}(f''(u)\phi^2-c_j^2f''H_t^2)H_{tt}+\frac{3\epsilon c_j^4}{4}\int_{\mathbf{R}}(f'(u)-f')H_{tt}^2. \end{aligned} \tag{C.6}$$

The last two terms in (C.6) are estimated as follows:

$$\begin{aligned} &\frac{3\epsilon}{4}\int_{\mathbf{R}}(f''(u)\phi^2-c_j^2f''H_t^2)H_{tt} \\ &\approx \frac{3\epsilon^3}{4}\int_{\mathbf{R}}(c_j^2f'''pH_t^2+2c_jf''H_t\omega+\epsilon^2f''\omega^2+2\epsilon^2c_jf'''p\omega+\epsilon^2c_j^2f^{(4)}\frac{p^2}{2}H_t^2)H_{tt}, \\ &\frac{3\epsilon}{4}\int_{\mathbf{R}}(f'(u)-f')H_{tt}^2 \\ &\approx \frac{3\epsilon^3}{4}\int_{\mathbf{R}}(f''H_{tt}^2p+\epsilon^2f'''H_{tt}^2\frac{p^2}{2}). \end{aligned} \tag{C.7}$$

Substitute (C.7) to (C.6) we obtain

$$
\begin{aligned}
I_2 \approx\ & \epsilon^3 (m\pi)^2 c_j^4 \int_{\mathbf{R}} H_{tt}^2 + \epsilon\gamma c_j^4 \int_0^1 (2G_0 + G_{2m})[H_{tt}] \frac{H_{tt}}{4} \\
& + \frac{3\epsilon^3 c_j^3}{4} \int_{\mathbf{R}} (c_j f''' H_t^2 H_{tt} p + c_j f'' H_{tt}^2 p + 2 f'' H_t H_{tt} \omega) \\
& + \frac{3\epsilon^5 c_j^2}{4} \int_{\mathbf{R}} (f'' H_{tt} \omega^2 + 2 c_j f''' H_t H_{tt} p\omega + c_j^2 (f^{(4)} H_t^2 H_{tt} + f''' H_{tt}^2) \frac{p^2}{2}). \qquad \text{(C.8)}
\end{aligned}
$$

On the other hand

$$
\begin{aligned}
\frac{1}{3}\int_D f'''(u)\varphi^4 &= \frac{1}{8}\int_0^1 f'''(H+\epsilon^2 p)(c_j H_t + \epsilon^2\omega)^4 \\
&\approx \frac{\epsilon c_j^4}{8}\int_{\mathbf{R}} f''' H_t^4 + \frac{\epsilon^3 c_j^3}{8}\int_{\mathbf{R}} (c_j f^{(4)} H_t^4 p + 4 f''' H_t^3 \omega) \\
&\quad + \frac{\epsilon^5 c_j^2}{8}\int_{\mathbf{R}} (c_j^2 f^{(5)} H_t^4 \frac{p^2}{2} + 4 c_j f^{(4)} H_t^3 p\omega + 6 f''' H_t^2 \omega^2).
\end{aligned}
$$

We combine the last with (C.8) to deduce

$$
\begin{aligned}
& I_2 + \frac{1}{3}\int_D f'''(u)\varphi^4 \\
\approx\ & \frac{\epsilon c_j^4}{8}\int_{\mathbf{R}} f''' H_t^4 + \epsilon^3 (m\pi)^2 c_j^4 \int_{\mathbf{R}} H_{tt}^2 + \epsilon\gamma c_j^4 \int_0^1 (2G_0 + G_{2m})[H_{tt}] \frac{H_{tt}}{4} \\
& + \frac{\epsilon^3 c_j^3}{8}\int_{\mathbf{R}} \{c_j (f^{(4)} H_t^4 + 6 f''' H_t^2 H_{tt} + 6 f'' H_{tt}^2) p + 4 (f''' H_t^3 + 3 f'' H_t H_{tt})\omega\} \\
& + \frac{\epsilon^5 c_j^2}{8}\int_{\mathbf{R}} \{(6 f''' H_t^2 + 6 f'' H_{tt})\omega^2 + c_j (4 f^{(4)} H_t^3 + 12 f''' H_t H_{tt}) p\omega \\
& \quad + c_j^2 (f^{(5)} H_t^4 + 6 f^{(4)} H_t^2 H_{tt} + 6 f''' H_{tt}^2) \frac{p^2}{2}\}. \qquad \text{(C.9)}
\end{aligned}
$$

One term in the integral after $\frac{\epsilon^3 c_j^3}{8}$ is simplified using (B.5) and (B.13):

$$
\begin{aligned}
& \int_{\mathbf{R}} (f''' H_t^3 + 3 f'' H_t H_{tt})\omega \\
=\ & \int_{\mathbf{R}} (\mathcal{L} H_{ttt})\omega = \int_{\mathbf{R}} (\mathcal{L}\omega) H_{ttt} = \int_{\mathbf{R}} \{(f'(u) - f') H_{ttt}\omega + (\omega'' - f'(u)\omega) H_{ttt}\} \\
=\ & \epsilon^2 \int_{\mathbf{R}} f'' H_{ttt} p\omega + \epsilon^2 (m\pi)^2 \int_{\mathbf{R}} H_{ttt}\omega + \epsilon\gamma \int_0^1 G_m[\omega] H_{ttt} - (m\pi)^2 c_j \int_{\mathbf{R}} H_{tt}^2 \\
& + \frac{\gamma c_j}{\epsilon}\int_0^1 G_m[H_t] H_{ttt} + c_j \int_{\mathbf{R}} (f'' H_t H_{ttt} p + \epsilon^2 f''' H_t H_{ttt} \frac{p^2}{2}) + o(\epsilon^2). \qquad \text{(C.10)}
\end{aligned}
$$

Here we have dropped $\int_0^1 G_m[\omega] H_{ttt} = \int_0^1 G_m[H_{ttt}]\omega = o(\epsilon)$. Substituting (C.10) to (C.9) we deduce

$$
I_2 + \frac{1}{3}\int_D f'''(u)\varphi^4
$$

$$\approx \frac{\epsilon c_j^4}{8}\int_{\mathbf{R}} f''' H_t^4 + \frac{\epsilon^3(m\pi)^2 c_j^4}{2}\int_{\mathbf{R}} H_{tt}^2 + \frac{\epsilon^5(m\pi)^2 c_j^4}{2}\int_{\mathbf{R}} H_{ttt}\omega$$
$$+\epsilon\gamma c_j^4 \int_0^1 \{(2G_0+G_{2m})[H_{tt}]\frac{H_{tt}}{4} + G_m[H_t]\frac{H_{ttt}}{2}\}$$
$$+\frac{\epsilon^3 c_j^4}{8}\int_{\mathbf{R}} (f^{(4)}H_t^4 + 6f'''H_t^2 H_{tt} + 6f''H_{tt}^2 + 4f''H_t H_{ttt})p$$
$$+\frac{\epsilon^5 c_j^2}{8}\int_{\mathbf{R}} \{(6f'''H_t^2 + 6f''H_{tt})\omega^2 + c_j(4f^{(4)}H_t^3 + 12f'''H_t H_{tt} + 4f''H_{ttt})p\omega$$
$$+c_j^2(f^{(5)}H_t^4 + 6f^{(4)}H_t^2 H_{tt} + 4f'''H_t H_{ttt} + 6f'''H_{tt}^2)\frac{p^2}{2}\}. \quad \text{(C.11)}$$

Next we compute I_1. From (C.2) we deduce

$$I_1 \approx \frac{3\epsilon c_j^4}{8}\int_{\mathbf{R}} f''H_t^2 H_{tt} + \frac{3\epsilon c_j^4}{8}\int_{\mathbf{R}} (f' - f'(u))H_{tt}^2 - \frac{\epsilon^3(m\pi)^2 c_j^4}{2}\int_{\mathbf{R}} H_{tt}^2$$
$$+\epsilon\gamma c_j^4 \int_D (\Delta^{-1}(H_{tt}\cos^2(m\pi y))(H_{tt}\cos^2(m\pi y))$$
$$\approx \frac{3\epsilon c_j^4}{8}\int_{\mathbf{R}} f''H_t^2 H_{tt} - \frac{3\epsilon^3 c_j^4}{8}\int_{\mathbf{R}} f''H_{tt}^2 p - \frac{3\epsilon^5 c_j^4}{8}\int_{\mathbf{R}} f'''H_{tt}^2\frac{p^2}{2} - \frac{\epsilon^3(m\pi)^2 c_j^4}{2}\int_{\mathbf{R}} H_{tt}^2$$
$$-\epsilon\gamma c_j^4 \int_0^1 (2G_0+G_{2m})[H_{tt}]\frac{H_{tt}}{8}. \quad \text{(C.12)}$$

(C.12) is added to (C.11). The ϵ order terms and the $\epsilon^3(m\pi)^2$ terms cancel out:

$$I_1 + I_2 + \frac{1}{3}\int_D f'''(u)\varphi^4$$
$$\approx \frac{\epsilon^5(m\pi)^2 c_j^3}{2}\int_{\mathbf{R}} H_{ttt}\omega + \epsilon\gamma c_j^4\int_0^1 \{(2G_0+G_{2m})[H_{tt}]\frac{H_{tt}}{8} + G_m[H_t]\frac{H_{ttt}}{2}\}$$
$$+\frac{\epsilon^3 c_j^4}{8}\int_{\mathbf{R}} (f^{(4)}H_t^4 + 6f'''H_t^2 H_{tt} + 3f''H_{tt}^2 + 4f''H_t H_{ttt})p$$
$$+\frac{\epsilon^5 c_j^2}{8}\int_{\mathbf{R}} \{(6f'''H_t^2 + 6f''H_{tt})\omega^2 + c_j(4f^{(4)}H_t^3 + 12f'''H_t H_{tt} + 4f''H_{ttt})p\omega$$
$$+c_j^2(f^{(5)}H_t^4 + 6f^{(4)}H_t^2 H_{tt} + 4f'''H_t H_{ttt} + 3f'''H_{tt}^2)\frac{p^2}{2}\}. \quad \text{(C.13)}$$

The integral after $\frac{\epsilon^3 c_j^4}{8}$ is, by (B.6),

$$\int_{\mathbf{R}} (f^{(4)}H_t^4 + 6f'''H_t^2 H_{tt} + 3f''H_{tt}^2 + 4f''H_t H_{ttt})p$$
$$= \int_{\mathbf{R}} (\mathcal{L}H_{tttt})p = \int_{\mathbf{R}} (\mathcal{L}p)H_{tttt}$$
$$= \frac{\gamma}{\epsilon}\int_{\mathbf{R}} vH_{tttt} + \epsilon^2\int_{\mathbf{R}} f''H_{tttt}\frac{p^2}{2} + o(\epsilon^2) = \epsilon\gamma\int_{\mathbf{R}} v_{xx}H_{tt} + \epsilon^2\int_{\mathbf{R}} f''H_{tttt}\frac{p^2}{2} + o(\epsilon^2)$$

$$= \quad -\epsilon\gamma \int_{\mathbf{R}} (H + \epsilon^2 p - a) H_{tt} + \epsilon^2 \int_{\mathbf{R}} f'' H_{tttt} \frac{p^2}{2} \ = \ \epsilon\gamma \int_{\mathbf{R}} H_t^2 + \epsilon^2 \int_{\mathbf{R}} f'' H_{tttt} \frac{p^2}{2} + o(\epsilon^2).$$

Hence (C.13) becomes

$$\begin{aligned}
& I_1 + I_2 + \frac{1}{3}\int_D f'''(u)\varphi^4 \\
\approx \quad & \epsilon\gamma c_j^4 \int_0^1 \{(2G_0 + G_{2m})[H_{tt}]\frac{H_{tt}}{8} + G_m[H_t]\frac{H_{ttt}}{2}\} + \frac{\epsilon^4\gamma c_j^4}{8}\int_{\mathbf{R}} H_t^2 + \frac{\epsilon^5(m\pi)^2 c_j^3}{2}\int_{\mathbf{R}} H_{ttt}\omega \\
& + \frac{\epsilon^5 c_j^2}{8}\int_{\mathbf{R}} \{(6f''' H_t^2 + 6f'' H_{tt})\omega^2 + c_j(4f^{(4)}H_t^3 + 12 f''' H_t H_{tt} + 4 f'' H_{ttt}) p\omega \\
& \quad + c_j^2 (f^{(5)} H_t^4 + 6 f^{(4)} H_t^2 H_{tt} + 4 f''' H_t H_{ttt} + 3 f''' H_{tt}^2 + f'' H_{tttt})\frac{p^2}{2}\} \\
= \quad & \epsilon\gamma c_j^4 \int_0^1 \{(2G_0 + G_{2m})[H_{tt}]\frac{H_{tt}}{8} + G_m[H_t]\frac{H_{ttt}}{2}\} + \frac{\epsilon^4\gamma c_j^4}{8}\int_{\mathbf{R}} H_t^2 + \frac{\epsilon^5(m\pi)^2 c_j^3}{2}\int_{\mathbf{R}} H_{ttt}\omega \\
& + \frac{\epsilon^5 c_j^2}{8}\int_{\mathbf{R}} \{6(f''H_t)_t\omega^2 + 4c_j(f''Ht)_{tt} p\omega + c_j^2 (f''H_t)_{ttt}\frac{p^2}{2}\}.
\end{aligned} \tag{C.14}$$

Finally we compute I_3. By (C.3) we find

$$\begin{aligned}
& I_3 = \epsilon^4 \int_D (S\psi_2)\psi_2 \\
\approx \quad & \epsilon^4\{c_j^3 \int_D (c_j (f''H_t)_t p + 2f''H_t\omega)\cos^2(m\pi y)(\frac{g_{11}}{2} + \frac{g_{21}}{2}\cos(2m\pi y)) \\
& + 2(m\pi)^2 c_j^4 \int_D H_{tt}\cos(2m\pi)(\frac{g_{11}}{2} + \frac{g_{21}}{2}\cos(2m\pi y)) \\
& - \frac{\gamma c_j^4}{\epsilon}\int_D (\Delta^{-1}(H_{tt}\cos^2(m\pi y)))(\frac{g_{11}}{2} + \frac{g_{21}}{2}\cos(2m\pi y))\} \\
\approx \quad & \frac{\epsilon^5 (c_j^0)^4}{8}\int_{\mathbf{R}} ((f''(H_t)_t P + 2f''H_t\Omega)(2G_{11} + G_{21}) + \frac{\epsilon^5 (m\pi)^2 (c_j^0)^4}{2}\int_{\mathbf{R}} H_{tt} G_{21}
\end{aligned} \tag{C.15}$$

where we have used Lemma B.1. We have dropped the last integral of the second last line for it is of order $o(\epsilon^2)$. Combining (C.14) and (C.15) we arrive at

$$\begin{aligned}
& I_1 + I_2 + I_3 + \frac{1}{3}\int_D f'''(u)\varphi^4 \\
\approx \quad & \epsilon\gamma c_j^4 \int_0^1 \{(2G_0 + G_{2m})[H_{tt}]\frac{H_{tt}}{8} + G_m[H_t]\frac{H_{ttt}}{2}\} \\
& + \frac{\epsilon^4\gamma c_j^4}{8}\int_{\mathbf{R}} H_t^2 + \frac{\epsilon^5 (m\pi)^2 (c_j^0)^4}{2}\int_{\mathbf{R}} H_{tt}(G_{21} - \Omega_t) \\
& + \frac{\epsilon^5 (c_j^0)^4}{8}\int_{\mathbf{R}} \{6(f''H_t)_t\Omega^2 + 4(f''Ht)_{tt} P\Omega + (f''H_t)_{ttt}\frac{P^2}{2} + 3((f''H_t)_t P + 2f''H_t\Omega)\Gamma\}.
\end{aligned} \tag{C.16}$$

Here we have introduced

$$\Gamma := \frac{2G_{11} + G_{21}}{3}. \tag{C.17}$$

We simplify the last integral in (C.16). Let

$$\Omega = P_t + \Pi,\ \Gamma = P_{tt} + \Psi. \tag{C.18}$$

Note that by (3.11) and $\lambda(\gamma_{\rm B}) = 0$,

$$\mathcal{L}\Pi = (m\pi)^2 H_t + \text{Const.}, \quad \mathcal{L}\Psi = 2f'' H_t \Pi + \frac{4(m\pi)^2}{3} H_{tt}. \tag{C.19}$$

The integral after $\frac{\epsilon^5 (c_j^0)^4}{8}$ in (C.16) is

$$\int_{\mathbf{R}} \{ (f''H_t)_{ttt} \frac{P^2}{2} + 6(f''H_t)_t P_t^2 + 4(f''H_t)_{tt} P P_t + 3((f''H_t)_t P + 2f''H_t P_t) P_{tt} \} + \tag{C.20}$$

$$\int_{\mathbf{R}} \{4(f''H_t)_{tt} P\Pi + 12(f''H_t)_t P_t \Pi + 6(f''H_t)_t \Pi^2 + 3((f''H)_t P + 2f''H_t P_t)\Psi + 6f''H_t \Pi\Psi + 6f''H_t \Pi P_{tt}\}.$$

The first integral in (C.20) is 0 after integration by parts. To calculate the second integral note, by (B.9),

$$\begin{aligned} &\int_{\mathbf{R}} 3((f''H_t)_t P + 2f''H_t P_t)\Psi \\ &= 3\int_{\mathbf{R}} (\mathcal{L}P_{tt})\Psi = 3\int_{\mathbf{R}} (\mathcal{L}\Psi) P_{tt} = 6\int_{\mathbf{R}} f''H_t \Pi P_{tt} + 4(m\pi)^2 \int_{\mathbf{R}} H_{tt} P_{tt}, \end{aligned} \tag{C.21}$$

$$\begin{aligned} &\int_{\mathbf{R}} f''H_t \Pi\Psi \\ &= 6\int_{\mathbf{R}} (\mathcal{L}\Pi_t - (m\pi)^2 H_{tt}) \;=\; 6\int_{\mathbf{R}} (2f''H_t\Pi + \frac{4(m\pi)^2}{3} H_{tt})\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi \\ &= -6\int_{\mathbf{R}} (f''H_t)_t \Pi^2 + 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi. \end{aligned} \tag{C.22}$$

Substituting (C.21) and (C.22) into the second integral in (C.20) we find, with the help of (B.10) and (C.19),

$$\begin{aligned} (\text{C.20}) &= \int_{\mathbf{R}} (4(f'H_t)_{tt} P + 12(f''H_t)_t P_t + 12 f''H_t P_{tt})\Pi \qquad \text{(C.23)} \\ &\quad + 4(m\pi)^2 \int_{\mathbf{R}} H_{tt} P_{tt} + 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi \\ &= 4\int_{\mathbf{R}} (\mathcal{L}P_{ttt})\Pi + 4(m\pi)^2 \int_{\mathbf{R}} H_{tt} P_{tt} + 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi \\ &= 4(m\pi)^2 \int_{\mathbf{R}} H_t P_{ttt} + 4(m\pi)^2 \int_{\mathbf{R}} H_{tt} P_{tt} + 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi \\ &= 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi. \qquad \text{(C.24)} \end{aligned}$$

Substitute (C.24) back to (C.16) we find

$$I_1 + I_2 + I_3 + \frac{1}{3}\int_D f'''(u)\varphi^4$$

$$\approx \quad \epsilon\gamma c_j^4 \int_0^1 \{(2G_0+G_{2m})[H_{tt}]\frac{H_{tt}}{8} + G_m[H_t]\frac{H_{ttt}}{2}\} + \frac{\epsilon^4\gamma c_j^4}{8}\int_{\mathbf{R}} H_t^2$$
$$+\frac{\epsilon^5(m\pi)^2(c_j^0)^4}{2}\int_{\mathbf{R}} H_{tt}(G_{21}-\Omega_t+2\Pi_t-\frac{3}{2}\Psi). \quad \text{(C.25)}$$

Note that

$$\mathcal{L}(G_{21}-\Omega_t+2\Pi_t-\frac{3}{2}\Psi)$$
$$= 4(m\pi)^2 + f'''H_t^2P + 2f''H_t\Omega + f''H_{tt}P - 2f''H_t\Omega - (f''H_t)_tP + f''H_t\Pi + (m\pi)^2H_{tt}$$
$$+2f''H_t\Pi + 2(m\pi)^2H_{tt} - (\frac{3}{2})2f''H_t\Pi - (\frac{3}{2})\frac{4(m\pi)^2H_{tt}}{3}$$
$$= 5(m\pi)^2H_{tt}. \quad \text{(C.26)}$$

On the other hand we may solve the last equation to find

$$G_{21}-\Omega_t+2\Pi_t-\frac{3}{2}\Psi = \frac{5(m\pi)^2}{2}tH_t$$

since $\mathcal{L}(\frac{t}{2}H_t) = H_{tt}$. Hence the last integral in (C.25) is

$$\int_{\mathbf{R}} H_{tt}(G_{21}-\Omega_t+2\Pi_t-\frac{3}{2}\Psi) = \frac{5(m\pi)^2}{2}\int_{\mathbf{R}} tH_tH_{tt} = -\frac{5(m\pi)^2\tau}{4}.$$

Putting this back to (C.25) we deduce

$$I_1+I_2+I_3+\frac{1}{3}\int_D f'''(u)\varphi^4$$
$$\approx \quad \epsilon\gamma c_j^4 \int_0^1 \{(2G_0+G_{2m})[H_{tt}]\frac{H_{tt}}{8} + G_m[H_t]\frac{H_{ttt}}{2}\} + \frac{\epsilon^4\gamma c_j^4}{8}\int_{\mathbf{R}} H_t^2 - \frac{5\epsilon^5(m\pi)^2\tau(c_j^0)^4}{8} \quad \text{(C.27)}$$

We now compute the first term in (C.27). Note that

$$\int_0^1 G_0[H_{tt}]H_{tt} = \epsilon^3\int_{\mathbf{R}} H_t^2 + o(\epsilon^4), \quad \text{(C.28)}$$

since $G_0[H_{tt}] = \epsilon^2(\overline{H(\frac{\cdot - x_j}{\epsilon})} - H(\frac{\cdot - x_j}{\epsilon}))$.

Recall that G_{2m} is identified with the Green function of

$$-G''_{2m} + (2m\pi)^2G_{2m} = \delta(\cdot - y), \quad G'_{2m}(0,y) = G'_{2m}(1,y) = 0.$$

G_{2m} splits to the fundamental solution part and the regular part:

$$G_{2m}(x,y) = \frac{1}{4m\pi}e^{-2m\pi|x-y|} - R_{2m}(x,y).$$

Note that R_{2m} is smooth in both variables x and y. We write down $G_{2m}(x,y)$ explicitly:

$$G_{2m}(x,y) = \frac{\cosh(2m\pi(1-|x-y|)) + \cosh(2m\pi(1-x-y))}{4m\pi\sinh(2m\pi)}.$$

Thus

$$R_{2m}(x,y) = \frac{1}{4m\pi} e^{-2m\pi|x-y|} - \frac{\cosh(2m\pi(1-|x-y|)) + \cosh(2m\pi(1-x-y))}{4m\pi \sinh(2m\pi)}.$$

We need to compute

$$R_{2m,xy}(y,y) := \left.\frac{\partial^2 R_{2m}}{\partial x \partial y}\right|_{x=y} = -m\pi + \frac{m\pi \cosh(2m\pi) - 2m\pi \cosh(2m\pi(1-2y))}{\sinh(2m\pi)}. \tag{C.29}$$

Then we have

$$G_{2m}[H_{tt}](x) = \int_0^1 G_{2m}(x,y) H_{tt}(\frac{y-x_j}{\epsilon}) dy.$$

By simple computations, we have that

$$\begin{aligned} G_{2m}[H_{tt}](x_j+\epsilon t) &= \epsilon \int_{-x_j/\epsilon}^{(1-x_j)/e} G_{2m}(x_j+\epsilon t, x_j+\epsilon z) H_{tt}(z)\, dz \\ &= \epsilon \int_{\mathbf{R}} [\frac{1}{4m\pi} e^{-2m\pi\epsilon|t-z|} - R_{2m}(x_j+\epsilon t, x_j+\epsilon z)] H_{zz} dz + o(\epsilon^4). \end{aligned} \tag{C.30}$$

We expand $e^{-2m\pi\epsilon|t-z|}$ to deduce

$$\begin{aligned} \int_{\mathbf{R}} e^{-2m\pi\epsilon|t-z|} H_{zz}\, dz &= \int_{\mathbf{R}} (1 - 2m\pi\epsilon|t-z| + 2(m\pi\epsilon)^2|t-z|^3 + O(\epsilon^3|t-z|^3)) H_{zz}\, dz \\ &= -4m\pi\epsilon H(t) + 4(m\pi\epsilon)^2 t + O(\epsilon^3). \end{aligned}$$

Hence (C.30) becomes

$$G_{2m}[H_{tt}](x_j+\epsilon t) = -\epsilon^2 H(t) + m\pi\epsilon^3 t - \epsilon \int_{\mathbf{R}} R_{2m}(x_j+\epsilon t, x_j+\epsilon z) H_{zz}\, dz. \tag{C.31}$$

Next we expand $R_{2m}(x_j+\epsilon t, x_j+\epsilon z)$ so that

$$\int_0^1 G_{2m}[H_{tt}] H_{tt} = \epsilon^3 \int_{\mathbf{R}} H_t^2 - m\pi\epsilon^4 - \epsilon^4 R_{2m,xy}(x_j^0, x_j^0) + o(\epsilon^4). \tag{C.32}$$

For the term involving G_m, integrating by parts, we obtain

$$\int_0^1 G_m[H_t] H_{ttt} = -\int_0^1 G_m^D[H_{tt}] H_{tt}$$

where $G_m^D[H_{tt}]$ is the Green function of

$$-(G_m^D)'' + (m\pi)^2 G_m^D = \delta(\cdot - y), \quad G_m^D(0,y)(0) = G_m^D(1,y) = 0. \tag{C.33}$$

The superscript D emphasizes the Dirichlet boundary condition. Similar to the Neumann boundary case we find

$$\begin{aligned} G_m^D(x,y) &= \frac{\cosh(m\pi(1-|x-y|)) - \cosh(m\pi(1-x-y))}{2m\pi\sinh(m\pi)}, \\ R_m^D(x,y) &:= \frac{1}{2m\pi}e^{-m\pi|x-y|} - \frac{\cosh(m\pi(1-|x-y|)) - \cosh(m\pi(1-x-y))}{2m\pi\sinh(m\pi)}, \\ R_{m,xy}^D(y,y) &:= \left.\frac{\partial^2 R_m^D}{\partial x \partial y}\right|_{x=y} = -\frac{m\pi}{2} + \frac{m\pi\cosh(m\pi) + m\pi\cosh(m\pi(1-2y))}{2\sinh(m\pi)}. \end{aligned} \tag{C.34}$$

By the same argument leading to (C.32), we arrive at

$$\int_0^1 G_m[H_t]H_{ttt} = -\epsilon^3 \int_{\mathbf{R}} H_t^2 + \frac{\epsilon^4 m\pi}{2} + \epsilon^4 R_{m,xy}^D(x_j^0, x_j^0) + o(\epsilon^4). \tag{C.35}$$

Substituting (C.28), (C.32) and (C.35) into (C.27), we obtain

$$\begin{aligned} & I_1 + I_2 + I_3 + \frac{1}{3}\int_D f'''(u)\varphi^4 \\ \approx\ & \sum_{j=1}^K c_j^4 \left[\frac{\epsilon^5\gamma m\pi}{8} - \frac{\epsilon^5\gamma}{8} R_{2m,xy}(x_j^0, x_j^0) + \frac{\epsilon^5\gamma}{2} R_{m,xy}^D(x_j^0, x_j^0) - \frac{5\epsilon^5(m\pi)^4\tau}{8} \right] \\ \approx\ & \epsilon^5 m\pi\gamma \sum_{j=1}^K (c_j^0)^4 \left[\frac{2+\cosh(2m\pi)}{8\sinh(2m\pi)} + \frac{\cosh(2m\pi(1-2x_j^0))}{8\sinh(2m\pi)} + \frac{\cosh(m\pi(1-2x_j^0))}{4\sinh(m\pi)} - \frac{5(m\pi)^3\tau}{8\gamma} \right], \end{aligned}$$

using (C.29) and (C.34), (restoring the $\sum_j$ sign). This completes the proof. □