

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

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

October 5, 2005

Abstract

In a diblock copolymer system the free energy field depends non-locally 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 under a hypothesis regarding the simplicity of the principal eigenvalue, which is generically satisfied. The wriggled lamellar solutions 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
2000 Mathematics Subject Classification. 58E07, 35J55, 34D15, 45J05, 82D60

1 Introduction

Symmetry breaking distortions often appear for intrinsic reasons in systems of condensed matters that exhibit self-organization and pattern formation. 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 a 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

^{*}Abbreviated title. Wriggled Lamellar Solutions.

[†]Supported in part by a Direct Grant from CUHK and an Earmarked Grant of RGC of Hong Kong.

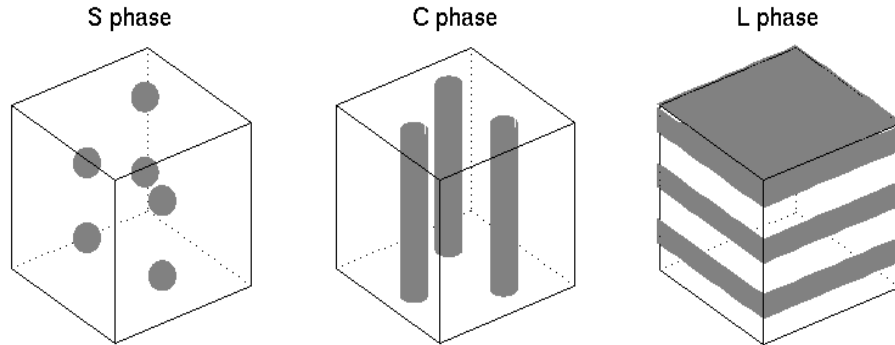


Figure 1: The spherical, cylindrical, and lamellar morphology phases commonly observed in diblock copolymer melts. The dark color indicates the concentration of type A monomer, and the white color indicates the concentration of type B monomer.

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 (Figure 2, Plot 2).

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

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

defined in $X_a = \{u \in W^{1,2}(D) : \bar{u} = a\}$, where $\bar{u} := \int_D u$ is the average of u on D . The original formula in [11] is given on the entire \mathbf{R}^3 . The expression here on a bounded domain D first appeared in Nishiura and Ohnishi [9]. 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 feature 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

$\{w \in L^2(D) : \bar{w} = 0\}$ to itself. The integral of the nonlocal part in (1.1) may be rewritten as

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

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]).

The dimensionless parameters ϵ and γ are positive and depend on various physical quantities [3]. In the strong segregation region where morphology patterns form, ϵ is very small. The second parameter 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 [25, 19], charged Langmuir monolayers [1, 16], and smectic films [24].

The Euler-Lagrange equation of I is

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

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

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

Here Const. is the Lagrange multiplier.

In Ren and Wei [12] 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 having K sharp interfaces if ϵ is sufficiently small (See Theorem 2.1). 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 [15] it is shown that such 1-D local minimizers are not necessarily 3-D local minimizers after trivial extension. Detailed spectral information at each 1-D solution is found (See Theorem 3.1, A similar analysis for the FitzHugh-Nagumo system was carried out by Nishiura [8]). In summary these 1-D local minimizers are not 3-D local minimizers unless 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

$$K_{opt} \approx \left(\frac{a^2 b^2 \gamma}{3\tau}\right)^{1/3}$$

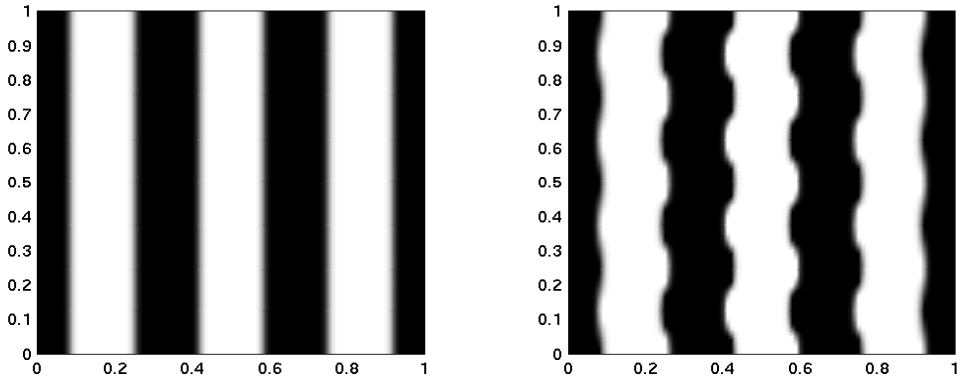


Figure 2: A perfect lamellar solution and a wriggled lamellar solution. In the dark regions the solutions are close to 1 and in the light regions the solutions are close to 0.

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 [25].

To simplify the presentation of our results, we consider wriggled lamellar solutions in 2-D. We take $D = (0, 1) \times (0, 1)$ to be a 2-D square instead of a 3-D box. The 1-D local minimizers are trivially extended to D . Generalization of our results to 3-D is straightforward.

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. Under the Hypothesis 4.1, which is generically satisfied, the principal eigenvalue is simple. Then a new solution branch bifurcates out of u_{γ_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_{γ_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 order ϵ^5 , Lemma 5.2). To find this number we have to expand the “trivial solution” u_{γ_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 $S(a, k) < 0$. The quantity $S(a, K)$ 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.

Our study of defects in diblock copolymers is partially motivated by the work of Tsori *et al* [27]. They considered two tilt lamellar patterns: chevron morphology and omega morphology. They used a model different from (1.1), which agrees well with experiment in the so called weak segregation regime. In this regime interfaces separating microdomains are not sharp compared to the size of the microdomains. In our work we deal with the strong segregation regime using (1.1). Here microdomains are separated by sharp interfaces. The calculations in [27] are restricted to an ansatz without solving the Euler-Lagrange equation of their free energy functional. The wriggled lamellar patterns we find are solutions of the Euler-Lagrange equation (1.2). Many of them are proved to be stable. They are therefore genuine meta-stable states of the system.

Moreover we are able to answer the question whether a 1-D global minimizer, mentioned earlier, is stable in 2-D. We will find cases where the 1-D global minimizer is stable and also cases where the 1-D global minimizer is unstable.

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 Hypothesis 4.1 that guarantees the simplicity of the principal eigenvalue is given in Section 4. Under this condition the existence of the wriggled lamellar solutions is given in Theorem 4.2. The reduction of their stability to the positivity of $S(a, K)$ culminates in Theorem 5.4. The stability of the 1-D global minimizer is discussed after 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 $\epsilon \rightarrow 0$ is denoted by u^0 . The parameter γ may vary in a compact interval of positive numbers. It is understood in this paper that all estimates are uniform in such γ . In estimates C is always a positive constant independent of ϵ and γ . 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 $\| \cdot \|_p$.

References on the mathematical aspects of the block copolymer theory include, in addition to the ones cited already, Ohnishi *et al* [10], Choksi [2], Fife and Hilhorst [5], Henry [6], Ren and Wei [14, 13, 20, 21, 22] on diblock copolymers, and Ren and Wei [17, 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 [12] by the Γ -limit theory. The findings there are summarized in the following theorem.

Theorem 2.1 (Ren and Wei [12]) *In 1-D for each positive integer K the functional*

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

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

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

and has the properties

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

Let H be the solution of

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

The constant τ in the theorem is defined by

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

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

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

with (recall $b = 1 - a$)

$$x_1^0 = \frac{a}{K}, \quad x_2^0 = \frac{1+b}{K}, \quad x_3^0 = \frac{2+a}{K}, \quad x_4^0 = \frac{3+b}{K}, \quad x_5^0 = \frac{4+a}{K}, \dots \quad (2.3)$$

G_0 is the solution operator of $-v'' = g$, $v'(0) = v'(1) = \bar{v} = 0$, 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 $\epsilon \rightarrow 0$ 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 $\tilde{u} = b$ instead. $1 - \tilde{u}$ has the same properties as u does, so we focus on u . u is periodic in the following sense.

Theorem 2.2 (Ren and Wei [15]) *Let u be a 1-D local minimizer constructed in Theorem 2.1. When ϵ is small, for every $x \in (0, 1/K)$,*

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

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 $j = 1, 2, \dots, K$ 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 [15, Lemma A.1] there exist exactly K points x_j , $j = 1, 2, \dots, K$, 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

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

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

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

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

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

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 [15]) *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 $|\epsilon^{-1}z(x_j + \epsilon t)| \leq C(1 + |t|)$ for all $t \in (-\frac{x_j}{\epsilon}, \frac{1-x_j}{\epsilon})$. $\epsilon^{-1}z(x_j + \epsilon \cdot)$ converges to P in $C_{loc}^2(\mathbf{R})$.*

Proof. See [15, Lemmas 2.4 and 2.5]. \square

It is proved in [15] 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 (See Part 2 of Theorem 3.1). This allows us to apply the implicit function theorem to conclude that u_γ depends on γ smoothly.

Next we estimate $du_\gamma/d\gamma$. The inner approximation is

$$q_j(x) = cH'\left(\frac{x - x_j}{\epsilon}\right) + \epsilon^2 R\left(\frac{x - x_j}{\epsilon}\right) \quad (2.7)$$

near each x_j . The constant c is chosen so that

$$\frac{du_\gamma}{d\gamma}(x_j) = cH'(0). \quad (2.8)$$

We will show in Appendix A that

$$\lim_{\epsilon \rightarrow 0} c = c_0 := -\frac{v^0(x_j^0)}{Kf'(0)}. \quad (2.9)$$

The function R is the solution of

$$-R'' + f'(H)R + c_0 f''(H)H'P + tv'(x_j) = \zeta, \quad R(0) = 0. \quad (2.10)$$

The constant ζ is chosen so that

$$\int_{\mathbf{R}} (c_0 f''(H)H'P + v(x_j) - \zeta)H' dt = 0 \quad (2.11)$$

for solvability. Because of the periodicity of u_γ , Theorem 2.2, neither c nor R depends on j . However they do depend on ϵ . Our argument here is a bit different from the formal matched asymptotics method. If we compare (2.10) to (2.6) we find that

$$\lim_{\epsilon \rightarrow 0} R = \frac{1}{\gamma} P + \tilde{R}, \quad (2.12)$$

where \tilde{R} is the solution of

$$-\tilde{R}'' + f'(H)\tilde{R} + c_0 f''(H)H'P = \zeta_0, \quad \tilde{R}(0) = 0 \quad (2.13)$$

where ζ_0 satisfies

$$\int_{\mathbf{R}} (c_0 f''(H)H'P + v^0(x_j^0) - \zeta)H' dt = 0. \quad (2.14)$$

The inner approximation (2.7) is used in the interval $(x_j - \epsilon^\alpha, x_j + \epsilon^\alpha)$ where α satisfies

$$\alpha \in \left(\frac{1}{2}, 1\right). \quad (2.15)$$

The outer approximation is denoted by q_o :

$$q_o = \frac{\eta - \epsilon\gamma r - \epsilon v}{f'(u_\gamma)} \quad (2.16)$$

where

$$r = G_0\left[\frac{du_\gamma}{d\gamma}\right], \quad v = G_0[u_\gamma - a]. \quad (2.17)$$

The outer approximation is used in

$$[0, 1] \setminus (\cup_{j=1}^K (x_j - 2\epsilon^\alpha, x_j + 2\epsilon^\alpha)). \quad (2.18)$$

The inner approximation is matched to the outer approximation in the matching intervals $(x_j - 2\epsilon^\alpha, x_j - \epsilon^\alpha)$ and $(x_j + \epsilon^\alpha, x_j + 2\epsilon^\alpha)$, $j = 1, 2, \dots, K$. Let χ_j be smooth cut-off functions so that

$$\chi_j(x) = \begin{cases} 0 & \text{if } x \notin (x_j - 2\epsilon^\alpha, x_j + 2\epsilon^\alpha) \\ 1 & \text{if } x \in (x_j - \epsilon^\alpha, x_j + \epsilon^\alpha) \end{cases},$$

and moreover $\chi_j' = O(\epsilon^{-\alpha})$ and $\chi_j'' = O(\epsilon^{-2\alpha})$ in $(x_j - 2\epsilon^\alpha, x_j - \epsilon^\alpha)$ and $(x_j + \epsilon^\alpha, x_j + 2\epsilon^\alpha)$. We glue the two approximations to form a uniform approximation

$$q = \sum_{j=1}^K \chi_j q_j + \left(1 - \sum_{j=1}^K \chi_j\right) q_o. \quad (2.19)$$

Lemma 2.4 $q - u = o(\epsilon^2)$.

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

3 The 2-D spectrum at u_γ

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).

The linearized operator of (1.2) at u_γ is

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

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 eigenpair (λ, φ) of L_γ separation of variables shows that $\varphi(x, y) = \phi_m(x) \cos(m\pi y)$ where m , a non-negative integer, is called the mode of φ . We 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 $m = 0$,

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

2. When $m \neq 0$,

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

Here G_m are the solution operators of the differential equations

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

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

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 [15]) *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 . The other $K - 1$ λ_0 's are of order ϵ^2 . The remaining λ_0 's are positive and bounded below by a positive constant independent of ϵ .*
3. *When $1 \leq m < M(K)$, there are K λ_m 's of order ϵ^2 , which are not necessarily positive. The remaining λ_m 's are positive and bounded below by a positive constant independent of ϵ . For every $\gamma > 0$ there exist $K_0 > 0$ and $\epsilon_0 > 0$ such that for $\epsilon < \epsilon_0$ and $K > K_0$ all the eigenvalues of L are positive and the solution u , of K interfaces, is stable; For every positive integer K there exist $\gamma_0 > 0$ and $\epsilon_0 > 0$ so that for $\epsilon < \epsilon_0$ and $\gamma < \gamma_0$ all the eigenvalues of L are positive and u is stable.*

Actually [15, Theorem 1.1] is formulated for a 3-D box. Here we have stated the simpler 2-D version.

The eigenvalues λ_0 in Part 2 of Theorem 3.1 are just the 1-D eigenvalues of u_γ . The asymptotic expansions of the λ_0 's are given in [15, Sections 4 and 5]. One of the small λ_0 's satisfies

$$\lim_{\epsilon \rightarrow 0} \epsilon^{-1} \lambda_0 > 0.$$

The other $K - 1$ small λ_0 's satisfy

$$\lim_{\epsilon \rightarrow 0} \epsilon^{-2} \lambda_0 > 0.$$

That these eigenvalues are positive is consistent with the fact that u_γ is a local minimizer of I_1 .

Bifurcation occurs at a zero eigenvalue, so we focus on the λ_m 's of Part 3, whose proof is in [15, Sections 6 and 7]. There we obtained asymptotic expansions of the K eigenpairs (λ_m, ϕ_m) of (3.3) satisfying $\lambda_m \rightarrow 0$ as $\epsilon \rightarrow 0$. Define

$$h_j(x) = H'\left(\frac{x-x_j}{\epsilon}\right)\chi\left(\frac{x-x_j}{\sqrt{\epsilon}}\right) = H'\left(\frac{x-x_j}{\epsilon}\right) + e.s. \quad (3.6)$$

where χ is a smooth, even cutoff function

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

Here $e.s.$ 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 $h_j(0) = h_j(1) = h_j'(0) = h_j'(1) = 0$, $\|h_j' - \epsilon^{-1} H''(\frac{\cdot - x_j}{\epsilon})\|_\infty = O(\epsilon^{-C/\epsilon})$, and $\|h_j'' - \epsilon^{-2} H'''(\frac{\cdot - x_j}{\epsilon})\|_\infty = O(\epsilon^{-C/\epsilon})$. When $m \geq 1$,

$$\lambda_m = \epsilon^2 \left(\frac{\gamma}{\tau} \left(\Lambda - \frac{ab}{K} \right) + m^2 \pi^2 \right) + o(\epsilon^2), \quad \phi_m = \sum_j c_j h_j + \epsilon^2 \phi_m^\perp. \quad (3.7)$$

As mentioned in the introduction, the estimate of λ_m in (3.7) is uniform in γ when γ varies in a compact interval of positive numbers. Here the Λ 's are the K eigenvalues 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 [15, Section 7]. When $K = 1$, it has, for each $m \geq 1$, one eigenpair (Λ, c^0) :

$$\Lambda = \frac{1}{m\pi(\tanh(m\pi a) + \tanh(m\pi b))}, \quad c^0 \propto 1. \quad (3.8)$$

When $K = 2$, there are two eigenpairs (Λ, c^0) :

$$\begin{aligned} \Lambda &= \frac{1}{m\pi(\coth(m\pi a) + \cot(m\pi b) - \operatorname{csch}(m\pi a) + \operatorname{csch}(m\pi b))}, & c^0 &\propto (-1, 1), \\ \Lambda &= \frac{1}{m\pi(\coth(m\pi a) + \cot(m\pi b) - \operatorname{csch}(m\pi a) - \operatorname{csch}(m\pi b))}, & c^0 &\propto (1, 1). \end{aligned} \quad (3.9)$$

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

$$\Lambda = \frac{1}{d - q}, \quad c^0. \quad (3.10)$$

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

$$Q = \begin{bmatrix} \alpha & \beta & & & \\ \beta & 0 & \alpha & & \\ & \alpha & 0 & \beta & \\ & & \beta & 0 & \alpha \\ & & & \dots & \end{bmatrix} \quad (3.11)$$

where

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

and c^0 is a corresponding eigenvector of Q .

In (3.7) ϕ_m is decomposed to $\sum_j c_j h_j$ in the subspace spanned by h_j , $j = 1, 2, \dots, K$, and $\epsilon^2 \phi_m^\perp$ in the orthogonal complement of the subspace. Moreover $\|\phi_m^\perp\|_2 = O(|c|)$ (See [15, Formula (6.4)]). As $\epsilon \rightarrow 0$, $c_j \rightarrow c_j^0$.

Within each mode m the K eigenvalues λ_m described in (3.7) are all different when ϵ is sufficiently small, because the K eigenvalues Λ of $[G_m(x_j^0, x_k^0)]$ are all different [15, Sections 5 and 7]. However this does not imply that each λ_m is a simple eigenvalue. It is possible that there exists a different mode m' such that a $\lambda_{m'}$ happens to equal λ_m . This problem will appear when we consider the simplicity of the principal eigenvalue in the next section.

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

$$-\Pi'' + f'(H)\Pi = \frac{\gamma}{\tau}(\Lambda - \frac{ab}{K})H' + \text{Const.}, \quad \Pi \perp H', \quad (3.12)$$

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 $C_{loc}^2(\mathbf{R})$ to $c_j^0(P' + \Pi)$.

Proof. We define an operator L_m so that the left side of (3.3) is $L_m \phi_m$. Note that this L_m differs from the one in [15] slightly. The function ϕ_m^\perp satisfies the equation

$$L_m \phi_m^\perp - \lambda_m \phi_m^\perp = \sum_j c_j \left\{ -m^2 \pi^2 h_j - \frac{1}{\epsilon^2} (f'(u_\gamma) - f'(H)) h_j - \gamma G_m \left[\frac{h_j}{\epsilon} \right] + \frac{\lambda_m}{\epsilon^2} h_j \right\}. \quad (3.13)$$

We claim that the right side of (3.13) is $O(|c|)$. The first term inside $\{\}$ on the right side is obviously $O(1)$. The last term is $O(1)$ by (3.7). The third term is $O(1)$ because $G_m[\frac{h_j}{\epsilon}] \rightarrow G_m(x, x_j^0)$ as $\epsilon \rightarrow 0$. 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

$$\psi = \frac{\phi_m^\perp}{\|\phi_m^\perp\|_\infty}.$$

Then ψ satisfies

$$L_m \psi = o(1). \quad (3.14)$$

There exists $x_* \in [0, 1]$ so that $|\psi(x_*)| = \max |\psi| = 1$. Without the loss of generality we assume $\psi(x_*) = 1$. Otherwise just change ψ to $-\psi$. Then $x_* - x_j = O(\epsilon)$ for some x_j . If this is not the case, (3.14) can not be satisfied at x_* since, by a maximum principle argument,

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

Here $\psi''(x_*) \leq 0$ because x_* is a maximum, and because of the Neumann boundary condition in case x_* is on the boundary. Define $\Psi(t) = \psi(x_j + \epsilon t)$. On the rescaled interval $(x_j/\epsilon, (1 - x_j)/\epsilon)$ Ψ satisfies

$$-\Psi_{tt} + \epsilon^2 m^2 \pi^2 \Psi + f'(u_\gamma)\Psi + \epsilon \gamma G_m[\psi](x_j + \epsilon t) = o(1), \quad \Psi'(-\frac{x_j}{\epsilon}) = \Psi'(\frac{1 - x_j}{\epsilon}) = 0,$$

On every bounded subinterval of \mathbf{R} , because Ψ is bounded and the terms $\epsilon^2 m^2 \pi^2 \Psi$, $f'(u_\gamma)\Psi$, and $\epsilon \gamma G_m[\psi](x_j + \epsilon t)$ are bounded, by the elliptic regularity theory Ψ is bounded in $W^{2,p}$ for any $p > 1$. A bootstrapping argument shows that Ψ is bounded in $C^{2,\alpha}$ on the subinterval.

As $\epsilon \rightarrow 0$, Ψ converges in $C_{loc}^2(\mathbf{R})$, along a subsequence of ϵ , to a bounded non-zero solution Ψ_∞ of

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

There are infinitely many solutions to the last equation. However only H' and its scalar multiples are bounded on \mathbf{R} . 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 $\Phi^\perp(t) = \phi_m^\perp(x_j + \epsilon t)$. By Part 1 we can pass the limit in (3.13) to find that $\Phi^\perp \rightarrow \Phi_\infty^\perp$ in $C_{loc}^2(\mathbf{R})$ which is a solution of

$$-(\Phi_\infty^\perp)'' + f'(H)\Phi_\infty^\perp = c_j^0(-f''(H)H'P + \frac{\gamma}{\tau}(\Lambda - \frac{ab}{K})H' + \text{Const.}). \quad (3.15)$$

By differentiating the equation for P we find

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

So Φ_∞^\perp and $c_j^0(P' + \Pi)$ satisfy the same equation (3.15). Moreover $\phi_m^\perp \perp h_j$ implies $\Phi_\infty^\perp \perp H'$. Hence $\Phi_\infty^\perp = c_j^0(P' + \Pi)$. \square

4 Bifurcation at (γ_B, u_B)

We use γ as a bifurcation parameter. Since we are mainly interested in stable wriggled solutions, we study bifurcation from the principal eigenvalue, i.e. the smallest eigenvalue, which we denote by $\lambda(\gamma)$. We must find γ_B so that $\lambda(\gamma_B) = 0$ and make sure that $\lambda(\gamma_B)$ is a simple eigenvalue. The following procedure easily finds the critical γ_B .

1. According to [15, Section 7], for each m the eigenvalues Λ of the matrix $[G_m(x_j^0, x_k^0)]$ are all different and the smallest one is

$$\Lambda_m = \frac{1}{m\pi(\tanh(m\pi a) + \tanh(m\pi b))} \quad \text{if } K = 1,$$

$$\begin{aligned}\Lambda_m &= \frac{1}{m\pi(\coth(m\pi a) + \cot(m\pi b) - \operatorname{csch}(m\pi a) + \operatorname{csch}(m\pi b))} \quad \text{if } K = 2, \\ \Lambda_m &= \frac{1}{d + \sqrt{\alpha^2 + \beta^2 + 2\alpha\beta \cos \theta}}, \quad \theta = 2\pi/K, \quad \text{if } K \geq 3.\end{aligned}\tag{4.1}$$

Recall that α , β and d are defined after (3.11).

2. For each $m \geq 1$ we define γ_m^0 to be the solution of

$$\frac{\gamma_m^0}{\tau} \left(\Lambda_m - \frac{ab}{K} \right) + m^2 \pi^2 = 0.\tag{4.2}$$

According to (3.7) at $\gamma = \gamma_m^0$, $\lambda_m = o(\epsilon^2)$ where

$$\lambda_m = \epsilon^2 \left(\frac{\gamma_m^0}{\tau} \left(\Lambda_m - \frac{ab}{K} \right) + m^2 \pi^2 \right) + o(\epsilon^2)$$

is the smallest eigenvalue of the mode m . The solution γ_m^0 may or may not be positive. If $\gamma_m^0 \leq 0$, this means that the mode m does not yield a zero eigenvalue for any $\gamma > 0$. We discard non-positive γ_m^0 .

3. We minimize the positive γ_m^0 's with respect to m . Because $\lim_{m \rightarrow \infty} \gamma_m^0 = \infty$, the minimum is achieved and is denoted by γ_B^0 . If m is the mode where $\gamma_m^0 = \gamma_B^0$ and m' is another mode such that $\gamma_{m'}^0 > \gamma_B^0$, then, since for m'

$$\Lambda_{m'} - \frac{ab}{K} < 0,$$

a consequence of $\gamma_{m'}^0$ being positive, we find that

$$\frac{\gamma_B^0}{\tau} \left(\Lambda_{m'} - \frac{ab}{K} \right) + (m')^2 \pi^2 > \frac{\gamma_{m'}^0}{\tau} \left(\Lambda_{m'} - \frac{ab}{K} \right) + (m')^2 \pi^2 = 0.$$

Hence at $\gamma = \gamma_B^0$ the smallest eigenvalue associated with a mode m of γ_B^0 vanishes up to order ϵ^2 while the greater eigenvalues associated with the mode m and the eigenvalues associated with the modes m' satisfying $\gamma_{m'}^0 > \gamma_B^0$ are positive and of order ϵ^2 . Then there exists γ_B such that $\lim_{\epsilon \rightarrow 0} \gamma_B = \gamma_B^0$ and at $\gamma = \gamma_B$ the principal eigenvalue $\lambda(\gamma_B)$ is zero.

The simplicity of $\lambda(\gamma_B)$ is more complex. For most a and τ , the minimum γ_B^0 of γ_m^0 , is achieved at one m . Then for sufficiently small ϵ , the mode of $\lambda(\gamma_B)$ is the unique m , and $\lambda(\gamma_B)$ is a simple eigenvalue.

However it is possible, for some particular a and τ that two modes, m and $m+1$, both minimize γ_m^0 , so γ_B^0 is achieved by two modes. This does not necessarily mean that the principal eigenvalue $\lambda(\gamma_B)$ has multiplicity two, because there is the effect of the $o(\epsilon^2)$ order term in (3.7). Nevertheless we can not exclude the possibility. Throughout the rest of the paper we impose the following condition which can be easily tested numerically for given a and τ .

Hypothesis 4.1 *The positive γ_m^0 's defined in (4.2) are minimized at a unique m .*

Being a simple eigenvalue now, $\lambda(\gamma_B)$ is continued smoothly to a curve of simple eigenvalues $\lambda(\gamma)$ of L_γ as γ varies. $\lambda(\gamma)$ is estimated in (3.7) which is valid uniformly in γ when γ varies in a neighborhood (such as $[\gamma_B/2, 2\gamma_B]$) of γ_B . Denote the eigenfunction associated with $\lambda(\gamma_B)$ by $\varphi_B(x, y) = \phi_B(x) \cos(m\pi y)$ where m from now on is the unique mode in Hypothesis 4.1. We write $u_B := u_{\gamma_B}$ and $L_B := L_{\gamma_B}$ for simplicity. Let

$$X := \{w \in W^{2,2}(D) : \partial_\nu w = 0 \text{ on } \partial D, \bar{w} = 0\}, \quad Y := \{z \in L^2(D) : \bar{z} = 0\}. \quad (4.3)$$

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

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

$$F(\gamma, w) := -\epsilon^2 \Delta(u_\gamma + w) + f(u_\gamma + w) - \overline{f(u_\gamma + w)} + \epsilon \gamma (-\Delta)^{-1}(u_\gamma + w - a). \quad (4.4)$$

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 4.2 *Under the Hypothesis 4.1, when ϵ is sufficiently small, at $\gamma = \gamma_B$ another solution branch $(\gamma(s), w(s))$ bifurcates from the ‘‘trivial branch’’ $(\gamma, 0)$. Here $w(s) = s\varphi_B + sg(s)$ where the parameter s is in a neighborhood of 0 with $\gamma(0) = \gamma_B$ and $w(0) = 0$. Moreover $\gamma : s \rightarrow \gamma(s) \in \mathbf{R}$ and $g : s \rightarrow g(s) \in X$ are both continuously differentiable and g satisfies $g(s) \perp \varphi_B$ and $g(0) = 0$.*

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

Proof. We appeal to the standard ‘‘Bifurcation from simple eigenvalue’’ theorem (See [26, Theorem 13.5, page 173]). 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. $D_2 F(\gamma_B, 0)$, which is just $L_B : X \rightarrow Y$, has a one dimensional kernel, spanned by φ_B .
2. $\mathcal{R}(D_2 F(\gamma_B, 0))$, the range of $D_2 F(\gamma_B, 0)$, has co-dimension 1.
3. $D_1 D_2 F(\gamma_B, 0)\varphi_B$ is not in $\mathcal{R}(D_2 F(\gamma_B, 0))$.

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

$$\|\psi\|_2 \leq c(\epsilon, \gamma_B) \|L_B \psi\|_2, \text{ for all } \psi \perp \varphi_B, \psi \in X. \quad (4.5)$$

Suppose (4.5) is false. There would exist a sequence $\psi_n \in X$, $\psi_n \perp \varphi_B$, $\|\psi_n\|_2 = 1$ so that $\|L_B \psi_n\|_2 \rightarrow 0$. Let $\psi_n \rightarrow \psi_*$ weakly in $L^2(D)$. Then $\psi_* \perp \varphi_B$. For every $\omega \in X$

$$\langle \psi_*, L_B \omega \rangle = \lim_{n \rightarrow \infty} \langle \psi_n, L_B \omega \rangle = \lim_{n \rightarrow \infty} \langle L_B \psi_n, \omega \rangle = 0.$$

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

$$-\epsilon^2 \Delta \psi_n = -f'(u_B) \psi_n + \overline{f'(u_B) \psi_n} - \epsilon \gamma_B (-\Delta)^{-1} \psi_n + L_B \psi_n.$$

Since $\|\psi_n\|_2 = 1$ and $\|L_B\psi_n\|_2 \rightarrow 0$, 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 $\psi_n \rightarrow 0$ in $L^2(D)$. This is inconsistent with the fact $\|\psi_n\|_2 = 1$. Hence (4.5) holds.

We now prove 2. by showing $\mathcal{R}(L_B) = \{\varphi_B\}^\perp$. The self-adjointness of L_B and 1. imply that every $\psi \in \mathcal{R}(L_B)^\perp$ is φ_B multiplied by a constant. It suffices to show that $\mathcal{R}(L_B)$ is closed. Take $\omega_n \in \mathcal{R}(L_B)$ so that $\omega_n \rightarrow \omega_*$ in $L^2(D)$. Let $\psi_n \in X$, $\psi_n \perp \varphi_B$ such that $L_B\psi_n = \omega_n$. Since ω_n is a Cauchy sequence, by (4.5) ψ_n is also a Cauchy sequence. Let $\psi_n \rightarrow \psi_*$ in $L^2(D)$. Note that L_B is a closed operator since it is self-adjoint. Hence $\psi_* \in X$ and $L_B\psi_* = \omega_*$. This proves 2.

To prove 3. note that the linear map $D_1D_2F(\gamma_B, 0) : X \rightarrow Y$ is

$$\psi \rightarrow f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \psi - \overline{f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \psi} + \epsilon(-\Delta)^{-1}\psi. \quad (4.6)$$

Since $\mathcal{R}(L_B) = \{\varphi_B\}^\perp$, it suffices to show

$$\langle D_1D_2F(\gamma_B, 0)\varphi_B, \varphi_B \rangle \neq 0, \text{ i.e. } \int_D \{f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \varphi_B^2 + \epsilon\varphi_B(-\Delta)^{-1}\varphi_B\} \neq 0. \quad (4.7)$$

This fact is established in the next lemma. \square

Lemma 4.3 *When ϵ is sufficiently small,*

$$\int_D \{f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \varphi_B^2 + \epsilon\varphi_B(-\Delta)^{-1}\varphi_B\} = -\frac{\epsilon^3|c^0|^2\tau m^2\pi^2}{2\gamma_B} + o(\epsilon^3|c^0|^2) < 0.$$

Here τ is given in (2.2), and c^0 is in (3.8-3.10), a non-zero vector.

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

$$\int_D \{f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \varphi_B^2 + \epsilon\varphi_B(-\Delta)^{-1}\varphi_B\} = \int_0^1 \left\{ \frac{1}{2} f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \phi_B^2 + \frac{\epsilon}{2} G_m[\phi_B] \phi_B \right\} dx. \quad (4.8)$$

By Lemmas 2.4, 3.2, we find

$$\begin{aligned} \int_0^1 f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \phi_B^2 &= \int_0^1 f''(u_B) \left(\sum_j (ch_j + \epsilon^2 R) \right) \phi_B^2 + o(\epsilon^3) \\ &= \int_0^1 f''(u_B) \left(\sum_j (ch_j + \epsilon^2(\gamma^{-1}P + \tilde{R})) \right) \phi_B^2 + o(\epsilon^3|c|^2) \\ &= \epsilon^2 \int_0^1 f''(u_B) (\gamma^{-1}P) \phi_B^2 + o(\epsilon^3|c|^2). \end{aligned}$$

We have used the fact that P is odd, and \tilde{R} and H_t are even. Hence we arrive at

$$\int_0^1 f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \phi_B^2 = \epsilon^3 \int_{\mathbf{R}} f''(H) \gamma^{-1}P \left(\sum_j c_j^2 \right) (H')^2 dt + o(\epsilon^3|c|^2) = -\frac{\epsilon^3|c^0|^2 ab}{K} + o(\epsilon^3|c^0|^2)$$

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

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

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 $\lim_{\epsilon \rightarrow 0} c_j = c_j^0$.

Hence the right side of (4.8) becomes

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

To determine the sign of this quantity we recall (3.7):

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

But here $\lambda(\gamma_B) = 0$. Hence

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

This proves the lemma. \square

Remark 4.4 *The proof of Theorem 4.2 does not use the fact that $\lambda(\gamma_B)$ is a principal eigenvalue. The theorem continues to hold if $\lambda(\gamma_B)$ is just a zero, simple eigenvalue, not necessarily principal. However the bifurcating solution from a non-principal eigenvalue is unstable, and hence less interesting to us.*

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 $\gamma''(0)$.

Place $w(s) = s\varphi_B + sg(s)$ into $F(\gamma, w) = 0$ and divide by s :

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

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):

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

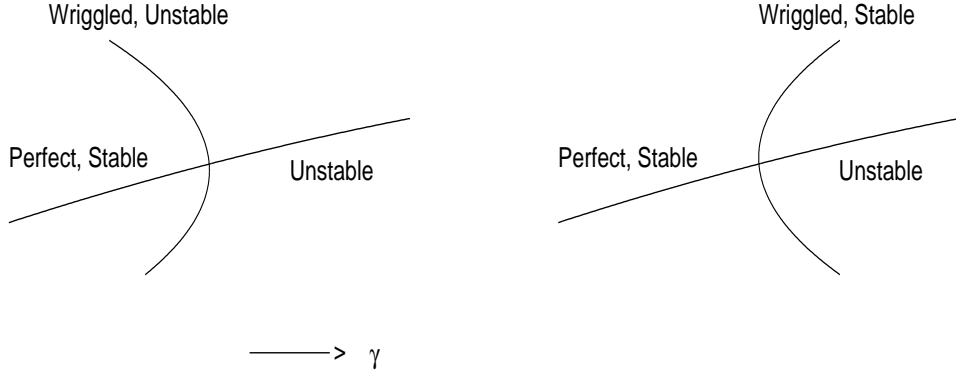


Figure 3: The two possible diagrams of wriggled lamellar solutions bifurcating out of perfect lamellar solutions. The bifurcating solutions are unstable in the first case where $\gamma''(0) < 0$, and stable in the second case where $\gamma''(0) > 0$.

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

$$L_B g'(0) + \gamma'(0) \left\{ f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \varphi_B + \epsilon(-\Delta)^{-1} \varphi_B \right\} + \frac{1}{2} f''(u_B) \varphi_B^2 = \text{Const..} \quad (5.3)$$

Then we multiply (5.3) by φ_B and integrate over D :

$$\gamma'(0) \int_D \left\{ f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \varphi_B^2 + \epsilon \varphi_B (-\Delta)^{-1} \varphi_B \right\} = - \int_D \frac{1}{2} f''(u_B) \varphi_B^3. \quad (5.4)$$

Clearly the right side of (5.4) is 0 since $\varphi_B(x, y) = \phi_B(x) \cos(m\pi y)$ and integration with respect to y yields 0. Lemma 4.3 then implies

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

Consequently the equation (5.3) is simplified to

$$L_B g'(0) = -\frac{1}{2} f''(u_B) \varphi_B^2 + \text{Const.}, \quad g'(0) \perp \varphi_B. \quad (5.5)$$

The right side of (5.5) is perpendicular to φ_B since the integration of the right side multiplied by u_B with respect to y yields 0, so there is a solution of $g'(0)$. $g'(0) \perp \varphi_B$ follows from $g(s) \perp \varphi_B$ in Theorem 4.2, so $g'(0)$ is uniquely determined.

Corollary 5.1 implies that the bifurcation diagram 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:

$$L_B g''(0) + \gamma''(0) \left\{ f''(u_B) \frac{du_\gamma}{d\gamma} \Big|_{\gamma=\gamma_B} \varphi_B^2 + \epsilon(-\Delta)^{-1} \varphi_B \right\} + 2f''(u_B) \varphi_B g'(0) + \frac{1}{3} f'''(u_B) \varphi_B^3 = \text{Const..} \quad (5.6)$$

We have used Corollary 5.1 in deriving (5.6). Again we multiply (5.6) by φ_B and integrate:

$$\gamma''(0) \int_D \{f''(u_B) \frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_B} \varphi_B^2 + \epsilon \varphi_B (-\Delta)^{-1} \varphi_B\} = - \int_D \{2f''(u_B) \varphi_B^2 g'(0) + \frac{1}{3} f'''(u_B) \varphi_B^4\}. \quad (5.7)$$

The integral on the left side of (5.7) has been calculated in Lemma 4.3. We now need to know the right side.

Lemma 5.2

$$- \int_D \{2f''(u_B) \varphi_B^2 g'(0) + \frac{1}{3} f'''(u_B) \varphi_B^4\} = -\epsilon^5 m\pi \gamma_B \sum_{j=1}^K c_j^4 \left[\frac{2 + \cosh(2m\pi)}{8 \sinh(2m\pi)} + \frac{\cosh(2m\pi(1 - 2x_j^0))}{8 \sinh(2m\pi)} + \frac{\cosh(m\pi(1 - 2x_j^0))}{4 \sinh(m\pi)} - \frac{3(m\pi)^3 \tau}{8\gamma_B} \right] + o(\epsilon^5 |c|^4).$$

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 $u_B, \phi_B, 2g'(0)$ as $(\dots) + \epsilon^2(\dots)$ 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 4.3 and 5.2 we obtain

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

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

where $\gamma_B^0 = \lim_{\epsilon \rightarrow 0} \gamma_B$ is given in Section 4.

Define

$$S(a, K) := \sum_{j=1}^K \left(\frac{c_j^0}{|c^0|} \right)^4 \left[\frac{2 + \cosh(2m\pi)}{8 \sinh(2m\pi)} + \frac{\cosh(2m\pi(1 - 2x_j^0))}{8 \sinh(2m\pi)} + \frac{\cosh(m\pi(1 - 2x_j^0))}{4 \sinh(m\pi)} - \frac{3(m\pi)^3 \tau}{8\gamma_B^0} \right]. \quad (5.8)$$

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

$$\lim_{\epsilon \rightarrow 0} \epsilon^{-2} \gamma''(0) = \frac{2(\gamma_B^0)^2 |c^0|^2}{m\pi \tau} S(a, K). \quad (5.9)$$

Theorem 5.4 Under Hypothesis 4.1 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 $\lambda'(\gamma_B)$. 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 $\gamma = \gamma_B$ in the equation, multiply the equation by φ_B , and integrate over D :

$$\int_D \{f''(u_B) \frac{du_\gamma}{d\gamma}|_{\gamma=\gamma_B} \varphi_B^2 + \epsilon \varphi_B (-\Delta)^{-1} \varphi_B\} = \lambda'(\gamma_B) \int_D \varphi_B^2.$$

The left side is calculated in Lemma 4.3. The integral on the right side is

$$\int_D \varphi_B^2 = \int_D (\sum_j c_j h_j)^2 \cos^2(m\pi y) dx dy + o(\epsilon|c|^2) = \frac{\epsilon\tau}{2} \sum_j c_j^2 + o(\epsilon|c|^2).$$

Therefore

$$\lambda'(\gamma_B) = -\frac{\epsilon^2 m^2 \pi^2}{\gamma_B} + o(\epsilon^2) < 0. \quad (5.10)$$

According to Crandall and Rabinowitz [4, Theorem 1.16], which generalizes an earlier result of Sattinger [23], near $s = 0$, $\lambda_*(s)$ and $-s\gamma'(s)\lambda'(\gamma_B)$ have the same zeros, and

$$\lim_{s \rightarrow 0, \lambda_*(s) \neq 0} \frac{-s\gamma'(s)\lambda'(\gamma_B)}{\lambda_*(s)} = 1. \quad (5.11)$$

Here $\lambda_*(s)$ is the principal 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 (5.9), (5.10), and (5.11). \square

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. Follow the procedure in Section 4 to find γ_B^0/τ and m .
2. Make certain that Hypothesis 4.1 is satisfied.
3. Find c^0 from Q corresponding to Λ of (4.1).
4. Find $S(a, K)$ from (5.8).

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_B . The second column gives the value of m associated with the principal eigenvalue 0 of u_B . Note that m does not increase as fast as K does. The third column has the value of γ_B^0/τ . 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 γ_B^0/τ '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 (4.1) for Λ and the matrix (3.11) of Q . In summary our problem is invariant under the reflection $u(x) \rightarrow u(1-x)$ with respect to $x = 1/2$, and the exchange $u(x) \rightarrow 1-u(x)$ of A and B monomers. When K is odd the perfect lamellar solution u_γ studied in Table 2 becomes u_γ in Table 3, and vice versa, after we perform the last two transformations. However this is not true when K is even.

There is an interesting relationship between the perfect lamellar solution u_B whose principal eigenvalue is 0, and the 1-D global minimizer. In [15, Section 8] it is shown that the 1-D global

K	m	γ_B^0/τ	K_{opt}	$S(1/2, K)$	Stability
1	1	1.2906e+02	2	5.7961e-02	Stable
2	2	8.6349e+02	3	1.4167e-02	Stable
3	3	2.7193e+03	4	5.4073e-03	Stable
4	3	5.3823e+03	5	2.5346e-02	Stable
5	3	9.7086e+03	6	2.8045e-02	Stable
6	4	1.6165e+04	7	1.9801e-02	Stable
7	4	2.4091e+04	8	2.0216e-02	Stable
8	4	3.4492e+04	9	1.9435e-02	Stable
9	4	4.7728e+04	10	1.8273e-02	Stable
10	4	6.4156e+04	11	1.7045e-02	Stable

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

K	m	γ_B^0/τ	K_{opt}	$S(1/8, K)$	Stability
1	3	1.7317e+03	2	-3.1473e-02	Unstable
2	5	1.3418e+04	4	2.7118e-02	Stable
3	2	1.0218e+04	3	6.0136e-02	Stable
4	3	2.3798e+04	5	5.5916e-02	Stable
5	3	4.3553e+04	6	3.5615e-02	Stable
6	3	7.3607e+04	7	3.0307e-02	Stable
7	4	1.1373e+05	8	2.5439e-02	Stable
8	4	1.6489e+05	9	2.2622e-02	Stable
9	4	2.3061e+05	10	2.0337e-02	Stable
10	4	3.1284e+05	11	1.8426e-02	Stable

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

K	m	γ_B^0/τ	K_{opt}	$S(7/8, K)$	Stability
1	3	1.7317e+03	2	-3.1473e-02	Unstable
2	2	3.4949e+03	2	4.9812e-02	Stable
3	2	1.0218e+04	3	6.0136e-02	Stable
4	3	2.3798e+04	5	2.8615e-02	Stable
5	3	4.3553e+04	6	3.5615e-02	Stable
6	3	7.3607e+04	7	3.0508e-02	Stable
7	4	1.1373e+05	8	2.5439e-02	Stable
8	4	1.6489e+05	9	2.2655e-02	Stable
9	4	2.3061e+05	10	2.0337e-02	Stable
10	4	3.1284e+05	11	1.8433e-02	Stable

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

minimizer (the 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.

It is known [15] that for any γ the 1-D global minimizer sits near the 2-D stability borderline. But it has not been determined whether the 1-D global minimizer is stable in 2-D. Now we show that the 1-D global minimizer is stable in 2-D for some γ and unstable for other γ .

First consider $\gamma = \gamma_B$. Then u_B is the borderline of 2-D stability. By examining the formulae (3.7) and (4.1) we find that for each γ the principal eigenvalue increases as K increases. If $\gamma = \gamma_B$ and K is the number of the interfaces of u_B whose principal eigenvalue is zero, then Tables 1-3 show that in most cases $K_{opt} = K + 1$, and hence the 1-D global minimizer is stable.

However in some cases, like the third row of Table 2, $K = K_{opt}$. Then u_B is the 1-D global minimizer. Since the principal eigenvalue of u_B is zero, the linear stability of u_B is undetermined. However if we consider γ in a small neighborhood of γ_B , then u_γ continues to be the 1-D global minimizer. But Figure 3 shows that when γ is slightly greater than γ_B the 1-D global minimizer is unstable in 2-D.

Acknowledgments. We thank Professors R. Kohn and C. Muratov for conversations on the subject of block copolymers during the 50th annual SIAM conference in Philadelphia. Thanks also go to Professor D. Sattinger for discussion on the bifurcation theory. The support from The Institute of Mathematical Sciences at The Chinese University of Hong Kong is much appreciated.

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A Proof of Lemma 2.4

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

$$-\epsilon^2 \Delta \left(\frac{du_\gamma}{d\gamma} \right) + f'(u_\gamma) \frac{du_\gamma}{d\gamma} - \eta + \epsilon \gamma G_0 \left[\frac{du_\gamma}{d\gamma} \right] + \epsilon v = 0. \quad (\text{A.1})$$

where

$$\eta = \overline{f'(u_\gamma) \frac{du_\gamma}{d\gamma}}. \quad (\text{A.2})$$

We first show that $du_\gamma/d\gamma = O(1)$ so that c defined in (2.8) is of order $O(1)$. By the periodicity of u_γ and $du_\gamma/d\gamma$ we consider (A.1) in one half period $(0, l)$ where $l = 1/K$. Decompose

$$\frac{du_\gamma}{d\gamma} = \beta \phi_0 + \phi_0^\perp, \quad \phi_0 \perp \phi_0^\perp, \quad (\text{A.3})$$

where ϕ_0 is the eigenfunction associated with the ϵ order eigenvalue λ_0 described in Part 2 of Theorem 3.1. Note that λ_0 is the only small eigenvalue of mode zero now. In [15, Section 4] it was shown that

$$\phi_0 = h_1 - \overline{h_1} + O(\epsilon). \quad (\text{A.4})$$

Denote the operator on the left side of (A.1) by L_0 . Then

$$L_0\phi_0^\perp = -\beta L_0\phi_0 - \epsilon v = -\beta\lambda_0 - \epsilon v = O(\epsilon|\beta|) + O(\epsilon).$$

This equation and the fact that $\phi_0 \perp \phi_0^\perp$ imply, as in the proof of Lemma 3.2, that

$$\phi_0^\perp = O(\epsilon|\beta|) + O(\epsilon). \quad (\text{A.5})$$

We rewrite (A.1) as $\beta L_0\phi_0 + L_0\phi_0^\perp = -\epsilon v$, multiply by ϕ_0 and integrate to deduce

$$\beta\lambda_0\|\phi_0\|_2^2 = -\epsilon \int_0^l v\phi_0 dx.$$

It follows from (A.4) that

$$\beta = O(1), \quad (\text{A.6})$$

and (A.5) in turn becomes

$$\phi_0^\perp = O(\epsilon). \quad (\text{A.7})$$

Therefore $du_\gamma/d\gamma = O(1)$. We can assume that along a subsequence of ϵ , $c \rightarrow c_0$. After we prove Lemma 2.4 we will find the value of c_0 . Then $c \rightarrow c_0$ along all $\epsilon \rightarrow 0$.

We now return to the whole interval $(0, 1)$ as we prove Lemma 2.4. We first construct a preliminary approximation $p = c \sum_j h_j$. The difference

$$\frac{du_\gamma}{d\gamma} - p$$

satisfies

$$-\epsilon^2 \Delta \left(\frac{du_\gamma}{d\gamma} - p \right) + f'(u_\gamma) \left(\frac{du_\gamma}{d\gamma} - p \right) = \eta + O(\epsilon). \quad (\text{A.8})$$

Together with the fact that

$$\frac{du_\gamma}{d\gamma}(x_j) = p(x_j),$$

we deduce that

$$\frac{du_\gamma}{d\gamma} - p = O(\epsilon) + O(|\eta|). \quad (\text{A.9})$$

If we multiply (A.8) by a h_i and integrate, then

$$\eta = O(\epsilon^2 \|\frac{du_\gamma}{d\gamma} - p\|_\infty) + O(\epsilon). \quad (\text{A.10})$$

We conclude from (A.9-A.10) that

$$\frac{du_\gamma}{d\gamma} - p = O(\epsilon), \quad \eta = O(\epsilon). \quad (\text{A.11})$$

and consequently (recall $r = G_0[du_\gamma/d\gamma]$)

$$r = O(\epsilon). \quad (\text{A.12})$$

We are now ready to consider the approximation q of $du_\gamma/d\gamma$. In the inner and matching regions

$$\begin{aligned}
& -\epsilon^2 \Delta q_j + f'(u_\gamma) q_j \\
&= -\epsilon^2 \Delta (cH'_j + \epsilon^2 R_j) + f'(u_\gamma) (cH'_j + \epsilon^2 R_j) \\
&= c(f'(u_\gamma) - f'(H))H'_j - \epsilon^2 (c_0 P H'_j f''(H) + tv'(x_j) - \zeta) + \epsilon^2 (f'(u_\gamma) - f'(H))R_j \\
&= \epsilon^2 (c - c_0) f''(H) P H'_j - \epsilon^2 (tv'(x_j) - \zeta) + \epsilon^2 (f'(u_\gamma) - f'(H))R_j \\
&= -\epsilon^2 (tv'(x_j) - \zeta) + o(\epsilon^2) + \epsilon^2 O(\epsilon|t|) \\
&= \epsilon^2 (\zeta - tv'(x_j)) + o(\epsilon^2).
\end{aligned}$$

Therefore with the help of $\alpha \in (1/2, 1)$

$$-\epsilon^2 \Delta q_j + f'(u_\gamma) q_j - \eta + \epsilon \gamma r + \epsilon v = -\eta + \epsilon \gamma r + \epsilon v(x_j) + \epsilon^2 \zeta + o(\epsilon^2). \quad (\text{A.13})$$

In the outer region, the definition of q_0 in (2.16) implies that

$$-\epsilon^2 \Delta q_o + f'(u_\gamma) q_o - \eta + \epsilon \gamma r + \epsilon v = O(\epsilon^3), \quad (\text{A.14})$$

because $\Delta q_o = O(\epsilon)$ on the outer region.

We now estimate the difference of q_j and q_o on a matching region. First from (2.10) we find

$$\epsilon^2 \Delta q_j = O(\epsilon^3).$$

Then (A.13) implies that

$$f'(u_\gamma) q_j - \eta + \epsilon \gamma r + \epsilon \gamma v = \sigma + o(\epsilon^2)$$

where

$$\sigma = -\eta + \epsilon \gamma r(x_j) + \epsilon v(x_j) + \epsilon^2 \zeta \quad (\text{A.15})$$

Comparing this to (2.16) we deduce that

$$q_j - q_o = O(|\sigma|) + o(\epsilon^2) \quad (\text{A.16})$$

on the matching regions $(x_j - 2\epsilon^\alpha, x_j - \epsilon^\alpha)$ and $(x_j + \epsilon^\alpha, x_j + 2\epsilon^\alpha)$. Then we consider q in the matching region. Here by (A.16)

$$\begin{aligned}
& -\epsilon^2 \Delta q + f'(u_\gamma) q - \eta + \epsilon \gamma r + \epsilon v \\
&= -\epsilon^2 \Delta q_o + f'(u_\gamma) q_o - \eta + \epsilon \gamma r + \epsilon v + O(\|q_j - q_o\|_\infty) \\
&= -\epsilon^2 \Delta q + O(|\sigma|) + o(\epsilon^2) \\
&= -\epsilon^2 \Delta q - \epsilon^2 \Delta (\chi_j (q_j - q_o)) + O(|\sigma|) + o(\epsilon^2) \\
&= -\epsilon^2 (\chi_j'' (q_j - q_o) + 2\chi_j' (q_j - q_o)' + \chi_j (q_j - q_o)'') + O(|\sigma|) + o(\epsilon^2) \\
&= O(|\sigma|) + o(\epsilon^2).
\end{aligned} \quad (\text{A.17})$$

If we let $g = u - q$, then (A.13), (A.14) and (A.17) imply that

$$-\epsilon^2 \Delta g + f'(u_\gamma) g = \begin{cases} \sigma + o(\epsilon^2) & \text{in an inner region} \\ O(|\sigma|) + o(\epsilon^2) & \text{in a matching region} \\ O(\epsilon^3) & \text{in the outer region} \end{cases} \quad (\text{A.18})$$

We deduce from (A.18) and $g(x_j) = 0$ that

$$g = O(|\sigma|) + o(\epsilon^2). \quad (\text{A.19})$$

On the other hand if we multiply (A.18) by H'_j and integrate, then

$$\int_0^1 [(f'(u_\gamma) - f'(H))gH'_j] dx = \epsilon\sigma_j + O(\epsilon^2|\sigma|) + o(\epsilon^3).$$

But the integral on the left side is $O(\epsilon^2\|g\|_\infty)$ from which we conclude that

$$\sigma = O(\epsilon\|g\|_\infty) + o(\epsilon^2). \quad (\text{A.20})$$

Inserting (A.20) to (A.19) we find that

$$g = o(\epsilon^2), \quad (\text{A.21})$$

proving Lemma 2.4; and moreover substituting (A.21) to (A.20) we deduce that

$$\sigma = o(\epsilon^2). \quad (\text{A.22})$$

Then we deduce

$$\eta = \epsilon v(x_j) + o(\epsilon). \quad (\text{A.23})$$

Because $\overline{du_\gamma/d\gamma} = 0$,

$$0 = \bar{q} + o(\epsilon^2) = \epsilon \int_0^1 \frac{v^0(x_j^0) - v^0(x)}{f'(0)} dx + c \int_0^1 \sum_j h_j + o(\epsilon) = \epsilon \left(\frac{v^0(x_j^0)}{f'(0)} + c_0 K \right) + o(\epsilon).$$

Thus we obtain the value for c_0 in (2.8).

B Expansion of $2g'(0)$

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

$$u := u_B, \quad v := G_0[u_B - a], \quad \gamma := \gamma_B, \quad \phi := \phi_B, \quad \omega := \phi_B^\perp, \quad f' := f'(H), \quad f'' := f''(H), \quad \text{etc.} \quad (\text{B.1})$$

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

Define a linear operator \mathcal{L} by

$$\mathcal{L}U := U'' - f'U \quad (\text{B.2})$$

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

$$\mathcal{L}H_t = 0, \quad (\text{B.3})$$

$$\mathcal{L}H_{tt} = f''H_t^2, \quad (\text{B.4})$$

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

Let $u = s + \epsilon^2 p$ where s is given in (2.4). Then p satisfies

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

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

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

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

$$\mathcal{L}P_t = f'' H_t P + \gamma(v^0)'(x_j^0), \quad (\text{B.8})$$

$$\mathcal{L}P_{tt} = (f'' H_t)_t P + 2f'' H_t P_t, \quad (\text{B.9})$$

$$\mathcal{L}P_{ttt} = (f'' H_t)_{tt} P + 3(f'' H_t)_t P_t + 3f'' H_t P_{tt}. \quad (\text{B.10})$$

Recall Lemma 3.2. Set the decomposition

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

for the zero principal eigenfunction ϕ . ω satisfies

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

We further expand (B.12):

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

As $\epsilon \rightarrow 0$, we have $\omega(x_j + \epsilon \cdot) \rightarrow c_j^0 \Omega$ in $C_{loc}^2(\mathbf{R})$ just as in the proof of Lemma 3.2, where Ω satisfies

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

Hence

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

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

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

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

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

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

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

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

where

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

Here

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

The equation for g_{11} is

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

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

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

Similarly the equation for g_{21} is

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

We state the following lemma.

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

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

and G_{21} satisfies

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

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

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

where $\hat{g}_{11} \perp h_j, j = 1, \dots, K$ and $\int_0^1 \hat{g}_{11} = 0$. The key is to show that $\alpha_j = o(1)$.

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

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

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

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

Thus we obtain the first identity

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

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

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

So we obtain the second identity

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

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

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

and hence $\hat{g}_{11} = o(1)$. \square

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

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

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

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

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

Then

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

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

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

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

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

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

$$\frac{3\epsilon}{4} \int_{\mathbf{R}} (f''(u)\phi^2 - c_j^2 f'' H_t^2) H_{tt}$$

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

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

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

On the other hand

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

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

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

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

$$\begin{aligned}
&\int_{\mathbf{R}} (f''' H_t^3 + 3f'' H_t H_{tt}) \omega \\
&= \int_{\mathbf{R}} (\mathcal{L} H_{ttt}) \omega = \int_{\mathbf{R}} (\mathcal{L} \omega) H_{ttt} = \int_{\mathbf{R}} \{(f'(u) - f') H_{ttt} \omega + (\omega'' - f'(u) \omega) H_{ttt}\}
\end{aligned}$$

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

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

$$\begin{aligned}
I_2 &+ \frac{1}{3} \int_D f'''(u) \varphi^4 \\
&\approx \frac{\epsilon c_j^4}{8} \int_{\mathbf{R}} f''' H_t^4 + \frac{\epsilon^3 (m\pi)^2 c_j^4}{2} \int_{\mathbf{R}} H_{tt}^2 + \frac{\epsilon^5 (m\pi)^2 c_j^4}{2} \int_{\mathbf{R}} H_{ttt} \omega \\
&\quad + \epsilon \gamma c_j^4 \int_0^1 \{(2G_0 + G_{2m})[H_{tt}] \frac{H_{tt}}{4} + G_m[H_t] \frac{H_{ttt}}{2}\} \\
&\quad + \frac{\epsilon^3 c_j^4}{8} \int_{\mathbf{R}} (f^{(4)} H_t^4 + 6f''' H_t^2 H_{tt} + 6f'' H_{tt}^2 + 4f'' H_t H_{ttt}) p \\
&\quad + \frac{\epsilon^5 c_j^2}{8} \int_{\mathbf{R}} \{(6f''' H_t^2 + 6f'' H_{tt}) \omega^2 + c_j (4f^{(4)} H_t^3 + 12f''' H_t H_{tt} + 4f'' H_{ttt}) p \omega \\
&\quad \quad + c_j^2 (f^{(5)} H_t^4 + 6f^{(4)} H_t^2 H_{tt} + 4f''' H_t H_{ttt} + 6f''' H_{tt}^2) \frac{p^2}{2}\}. \tag{C.11}
\end{aligned}$$

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

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

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

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

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

$$\begin{aligned}
& \int_{\mathbf{R}} (f^{(4)} H_t^4 + 6f''' H_t^2 H_{tt} + 3f'' H_{tt}^2 + 4f'' H_t H_{ttt}) p \\
&= \int_{\mathbf{R}} (\mathcal{L} H_{tttt}) p = \int_{\mathbf{R}} (\mathcal{L} p) H_{tttt} \\
&= \frac{\gamma}{\epsilon} \int_{\mathbf{R}} v H_{tttt} + \epsilon^2 \int_{\mathbf{R}} f'' H_{tttt} \frac{p^2}{2} + o(\epsilon^2) = \epsilon \gamma \int_{\mathbf{R}} v_{xx} H_{tt} + \epsilon^2 \int_{\mathbf{R}} f'' H_{tttt} \frac{p^2}{2} + o(\epsilon^2) \\
&= -\epsilon \gamma \int_{\mathbf{R}} (H + \epsilon^2 p - a) H_{tt} + \epsilon^2 \int_{\mathbf{R}} f'' H_{tttt} \frac{p^2}{2} = \epsilon \gamma \int_{\mathbf{R}} H_t^2 + \epsilon^2 \int_{\mathbf{R}} f'' H_{tttt} \frac{p^2}{2} + o(\epsilon^2).
\end{aligned}$$

Hence (C.13) becomes

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

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

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

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

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

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

Here we have introduced

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

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

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

Note that by (3.12) and $\lambda(\gamma_B) = 0$,

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

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

$$\begin{aligned}
&\int_{\mathbf{R}} \left\{ (f'' H_t)_{ttt} \frac{P^2}{2} + 6(f'' H_t)_t P_t^2 + 4(f'' H_t)_{tt} P P_t + 3((f'' H_t)_t P + 2f'' H_t P_t) P_{tt} \right\} + \\
&\int_{\mathbf{R}} \left\{ 4(f'' H_t)_{tt} P \Pi + 12(f'' H_t)_t P_t \Pi + 6(f'' H_t)_t \Pi^2 + 3((f'' H_t)_t P + 2f'' H_t P_t) \Psi + 6f'' H_t \Pi \Psi + 6f'' H_t \Pi P_{tt} \right\}.
\end{aligned} \tag{C.20}$$

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

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

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

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

$$(C.20) = \int_{\mathbf{R}} (4(f' H_t)_{tt} P + 12(f'' H_t)_t P_t + 12f'' H_t P_{tt}) \Pi \tag{C.23}$$

$$\begin{aligned}
& +4(m\pi)^2 \int_{\mathbf{R}} H_{tt}P_{tt} + 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi \\
= & 4 \int_{\mathbf{R}} (\mathcal{L}P_{ttt})\Pi + 4(m\pi)^2 \int_{\mathbf{R}} H_{tt}P_{tt} + 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi \\
= & 4(m\pi)^2 \int_{\mathbf{R}} H_tP_{ttt} + 4(m\pi)^2 \int_{\mathbf{R}} H_{tt}P_{tt} + 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi \\
= & 8(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Pi_t - 6(m\pi)^2 \int_{\mathbf{R}} H_{tt}\Psi. \tag{C.24}
\end{aligned}$$

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

$$\begin{aligned}
I_1 + I_2 + I_3 + \frac{1}{3} \int_D f'''(u)\varphi^4 \\
\approx & \epsilon\gamma c_j^4 \int_0^1 \{(2G_0 + G_{2m})[H_{tt}] \frac{H_{tt}}{8} + G_m[H_t] \frac{H_{ttt}}{2}\} + \frac{\epsilon^4 \gamma c_j^4}{8} \int_{\mathbf{R}} H_t^2 \\
& + \frac{\epsilon^5 (m\pi)^2 (c_j^0)^4}{2} \int_{\mathbf{R}} H_{tt}(G_{21} - \Omega_t + 2\Pi_t - \frac{3}{2}\Psi). \tag{C.25}
\end{aligned}$$

Note that

$$\begin{aligned}
\mathcal{L}(G_{21} - \Omega_t + 2\Pi_t - \frac{3}{2}\Psi) \\
= & 4(m\pi)^2 H_{tt} + f''' H_t^2 P + 2f'' H_t \Omega + f'' H_{tt} P - 2f'' H_t \Omega - (f'' H_t)_t P + f'' H_t \Pi - (m\pi)^2 H_{tt} \\
& + 2f'' H_t \Pi + 2(m\pi)^2 H_{tt} - (\frac{3}{2})2f'' H_t \Pi - (\frac{3}{2})\frac{4(m\pi)^2 H_{tt}}{3} \\
= & 3(m\pi)^2 H_{tt}. \tag{C.26}
\end{aligned}$$

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

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

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

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

Putting this back to (C.25) we deduce

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

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

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

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

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

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

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

Then we have

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

By simple computations, we have that

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

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

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

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

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

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

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

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

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

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

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

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

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

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