

Codimension one minimizers of highly amphiphilic mixtures[☆]Shibin Dai^{a,*}, Keith Promislow^b^a Department of Mathematics, The University of Alabama, Box 870350, Tuscaloosa, AL 35487-0350, USA^b Department of Mathematics, Michigan State University, East Lansing, MI 48824, USA

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ABSTRACT

We present a modified form of the Functionalized Cahn–Hilliard (FCH) functional which models highly amphiphilic systems in solvent. A molecule is highly amphiphilic if the energy of a molecule isolated within the bulk solvent molecule is prohibitively high. For such systems once the amphiphilic molecules assemble into a structure it is very rare for a molecule to exchange back into the bulk. The highly amphiphilic FCH functional has a well with limited smoothness and admits compactly supported critical points. In the limit of molecular length $\varepsilon \rightarrow 0$ we consider sequences with bounded energy whose support resides within an ε -neighborhood of a fixed codimension one interface. We show that the FCH energy is uniformly bounded from below, independent of $\varepsilon > 0$, and identify assumptions on tangential variation of sequences that guarantee the existence of subsequences that converge to a weak solution of a rescaled bilayer profile equation, and show that sequences with limited tangential variation enjoy a $\liminf$ inequality. For fixed codimension one interfaces we construct bounded energy sequences which converge to the bilayer profile and others with larger tangential variation which do not converge to the bilayer profile but whose limiting energy can violate the $\liminf$ inequality, depending upon the energy parameters.

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1. Introduction

Amphiphilic molecules play an essential role in the self assembly of nano-scale structures in solvent, in biological context they play an essential role in the formation of cell membranes and other organelles, and they are increasingly important in applications of synthetic chemistry. There are distinct approaches to model the free energy of amphiphilic mixtures that emphasize different scalings and assumptions on morphology. The classical sharp interface approximations include the Canham–Helfrich energy [1,2] which characterizes the free energy of a codimension one interface embedded in $\mathbb{R}^3$ in terms of its two curvatures. This is an appealingly simple formulation but does not readily handle singularities associated with topological change. Conventional phase field models based on the Cahn–Hilliard (CH) energy describe single layer interfaces, see [3–9] and references therein. Single-layer interfaces separate dissimilar phases which cannot be merged and describe the transition region around the boundary between the phases as if it were a high-energy void. For oil and water blends this is a very reasonable approximation, as a hydrophobic molecule generates a cavity when placed within water, [10] and see Fig. 1(left). Amphiphilic materials can create interfaces between similar fluids [11], see Fig. 1(right), or reside at interfaces between dissimilar fluids, such as oil and water. In this latter case they are

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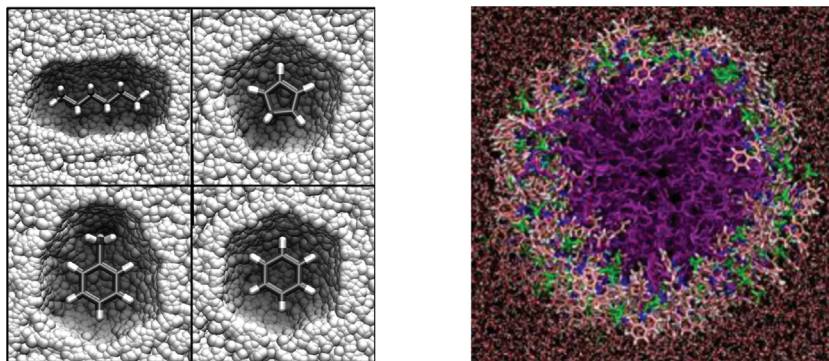


Fig. 1. (left) Results of molecular dynamics simulation showing shape of void induced in solvent phase in response to hydrophobic molecules of different shapes. Reprinted with permission from [10] Copyright (2012) American Chemical Society. (right) All atom simulation of packing of amphiphilic molecule (gray) at interface between external solvent molecules (reddish) and internal solvent (not imaged to show internal structure). Reproduced from [11] with permission from the Royal Society of Chemistry. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

also called surfactants and lower the overall mixture energy by packing the hydrophobic cavity. Modeling amphiphilic interfaces with single layer energies presents certain limitations, the first is that single layer models allow the transition region around the interface to change without material transport. Even when the total volume of the transition region is preserved by external constraint, transition volume removed at one point may reappear at another distant point without requiring transport of surfactant. In many applications transport of surfactant is the most significant rate limiting step, this is particularly true of highly amphiphilic molecules. A second limitation of single layer models is that the single layer interface cannot be punctured. The opening of holes in vesicles requires the introduction of additional order parameters for *each* vesicle, in particular the total number of vesicles must be predetermined [8].

The functionalized Cahn–Hilliard (FCH) free energy is a phenomenological model describing the free energy of amphiphilic mixtures [12–18], that supports codimension one bilayer interfaces that separate two identical phases by a thin region of a second phase – the amphiphilic material. Bilayer interfaces can be punctured and can form free edges and open structures. Gradient flows of the FCH free energy transport amphiphilic molecules either along the interface or through the bulk solvent phase. Over a bounded domain $\Omega \subset \mathbb{R}^n$, the conventional Cahn–Hilliard functional takes the form

$$E_\varepsilon(u) := \int_\Omega \left(\frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} W(u) \right) dx, \quad (1)$$

where u is the relative concentration of the two phases, the double well potential $W : \mathbb{R} \mapsto \mathbb{R}$ has two equal-depth minimizers at $u = 0$ and $u = u_+ > 0$ corresponding to the two phases, and $\varepsilon > 0$ is a small parameter characterizing the width of the void region between the phases. The weak functionalization form of the FCH functional can be scaled as

$$F_\varepsilon(u) := \int_\Omega \left\{ \frac{1}{2\varepsilon} \left(-\varepsilon \Delta u + \frac{1}{\varepsilon} W'(u) \right)^2 - \left(\frac{\eta_1 \varepsilon}{2} |\nabla u|^2 + \frac{\eta_2}{\varepsilon} W(u) \right) \right\} dx. \quad (2)$$

The first term on the left-hand side of (2) is the square of the variational derivative of a Cahn–Hilliard type energy and its volume integral captures distance of the configuration u from a critical point of the underlying Cahn–Hilliard type functional – these critical points represent the optimal packings of the amphiphilic molecules. The double well has unequal depth minima, $W(0) = 0 > W(u_+)$. The parameters $\eta_1 > 0$ and $\eta_2 \in \mathbb{R}$ model the strength of hydrophilic interactions and the aspect ratio of the amphiphilic molecule respectively. For fixed $\varepsilon > 0$ and mass amphiphilic mass fraction $M := \int_\Omega u dx$ the functional F_ε is bounded from below with a negative lower bound that diverges to negative infinity as $\varepsilon \rightarrow 0$ [19].

A key experimental quantity is the exchange rate which governs the probability of an amphiphilic molecule being ejected from an interface and returning to the bulk solvent. This rate is governed by the difference in free energies of a molecule when it is in the interface and when it is in the bulk. The insertion rate, that is, the propensity of an amphiphilic molecule in the bulk to be absorbed onto an interface, typically varies inversely to the exchange rate. These two processes mediate the exchange of surfactant materials between disjoint interfaces. The experimental literature shows that the exchange rate decays exponentially with the length of the hydrophobic moiety [20], diminishing effectively to zero for sufficiently diblocks with sufficiently long hydrophobic regions. These “highly amphiphilic” surfactants have a prohibitively large solvation energy and produce structures that have almost no measurable exchange of amphiphilic molecules with the bulk. The structures they form act like isolated islands in a sea of solvent. Important classes of amphiphilic are considered to be highly amphiphilic, these include most lipids which are characterized by a small hydrophilic head and longer, double-branched hydrophobic tail.

Analysis of mass-preserving gradient flows of the FCH functional has focused on the stability and asymptotic dynamics of codimension one bilayers and codimension two filamentous pore structures. The analysis shows that the temporal rate of surfactant exchange is inversely proportional to the second derivative of the double well at the pure solvent phase, $W''(0)$. This is relatively transparent from the form of the FCH free energy (2), for which direct calculation shows that a spatially constant distribution $u \equiv c$ has an energy

$$F_\varepsilon(c) = \frac{1}{2}\varepsilon^{-3}c^2|\Omega| \cdot |W''(0)|^2 + O(\varepsilon^{-3}c^3). \quad (3)$$

Moreover interfaces decay exponentially in space to the bulk constant value at a rate inversely proportional to $\varepsilon\sqrt{W''(0)}$. The exchange rate of an interfacial structure depends primarily upon its codimension. The differing exchange rates between structures of different codimension generically leads to growth of structures whose codimension has the lowest associated exchange rate at the expense of those structures with higher exchange rates [13–18]. To model highly amphiphilic molecules we drive the exchange rate to zero by considering a double well which is smooth for $u > 0$ but only $C^{1+\alpha}$ in a neighborhood of $u = 0$. This generates minimizers of the FCH that are potentially compactly supported, with no mechanism to exchange surfactant molecules between disjoint structures.

In experimental situations the amphiphilic materials typically occupy a small fraction of the total volume of the domain. Indeed, to produce an $O(1)$ surface area of codimension one bilayer requires an $O(\varepsilon)$ volume of amphiphile. Given the compactly supported nature of the critical points of the FCH energy it is natural to consider distributions $u \in H^2(\Omega)$ of amphiphile whose support lies in a small subset Ω_ε within the total domain Ω . Considering the boundary $\partial\Omega$ of the domain to be unfavorable for amphiphilic molecules, for example a clean glass beaker, it is natural to impose no-contact, no-flux boundary conditions

$$u = 0, \quad \frac{\partial u}{\partial \nu} = 0, \quad (4)$$

where ν is the outer normal of $\partial\Omega$. These boundary conditions indicate that amphiphilic structures lie in Ω and away from the boundary $\partial\Omega$. We further require the local regularity assumption

$$W(u) \sim u^r \text{ for some } 3/2 < r < 2 \text{ as } u \rightarrow 0^+, \quad (5)$$

and the growth rate assumptions

$$C_1|u|^p + C_2 \leq W(u) \leq C_1|u|^p + C_3, \quad (6)$$

$$|W'(u)| \leq C_1 p |u|^{p-1} + C'_3, \quad (7)$$

$$C_1 p |u|^p + C_4 \leq W'(u)u. \quad (8)$$

for some constants $C_1 > 0$ and $C_2, C_3, C'_3, C_4 \in \mathbb{R}$ and all $u \in \mathbb{R}$. Here

$$2 \leq p < \infty \quad \text{if } n = 2 \quad \text{and} \quad 2 \leq p < \frac{2n-2}{n-2} \quad \text{if } n \geq 3. \quad (9)$$

Specifically for $n = 3$, we require $2 \leq p < 4$. These conditions imply that

$$W(0) = W'(0) = 0, \quad W''(0^+) = +\infty.$$

The requirement $r > 3/2$ guarantees that the solvent-free profile, $u \equiv 0$, is a critical point of F_ε , and the requirement $r < 2$ signals the highly amphiphilic nature of the surfactant and guarantees the existence of compactly supported bilayer profiles corresponding to critical points of F_ε . The growth rate requirements on p are technical considerations to establish the existence of minimizers, the value of p has little impact on the model and no physical significance. A generic example of a double well satisfying these requirements is

$$W(u) = \chi(u)|u|^r \left((u - u_+)^2 + \tau \left(u - \frac{1+r}{r} u_+ \right) \right) + C_5(1 - \chi(u))|u|^p, \quad (10)$$

where $\chi : \mathbb{R} \mapsto \mathbb{R}$ is a C^∞ cut-off function which is 1 on $[-1, 2u_+]$ and zero outside a compact set. The parameter $C_5 > 0$ is chosen large enough to guarantee that W' has no zeros outside of $[0, u_+]$. The parameter τ controls the depth of the right well: $W(u_+) = -\frac{\tau}{r}|u_+|^{1+r} < 0$ for $\tau > 0$.

Remark 1.1. Finding local minimizers of F_ε under the restriction that $u \geq 0$ is both analytically and numerically challenging as the variational derivative of F_ε involves W'' which is not well defined at 0. One approach is to use variational inequalities, as outlined in [21]. While the model here differs from those considered for the Cahn–Hilliard equation with degenerate mobility [22–28], the mechanism that prevents interaction through the bulk is fundamentally distinct. For degenerate mobility molecules in the bulk are frozen in place and cannot move. In the model presented here molecules in the bulk phase would readily move and be rapidly and permanently absorbed in finite time; once depleted there is no mechanism to replenish the bulk density and bulk diffusion ceases.

1.1. Summary of main results

This discussion motivates the introduction of “geometrically localized critical points”, u_ε of F_ε over the set of functions in $H^2(\Omega)$ whose support is contained within an open subset Ω_ε compactly contained in Ω . These critical points are constructed in Section 2 for fixed values of $\varepsilon > 0$. In Section 3 for fixed $\ell > 0$ we take Ω_ε to be the $\varepsilon\ell$ neighborhood of a fixed codimension one interface Γ compactly embedded in Ω , and analyze behaviors of sequences of functions $\{u_{\varepsilon_k}\}_{k=1}^\infty$ with masses $\{m_{\varepsilon_k}\}_{k=1}^\infty$ whose energies $\{F_{\varepsilon_k}(u_{\varepsilon_k})\}_{k=1}^\infty$ are uniformly bounded as $\varepsilon_k \rightarrow 0$ as $k \rightarrow \infty$. We call these *codimension-one ℓ -bounded sequences* with respect to Γ , and establish upper bounds on their plane and tangential derivatives. In Theorem 3.1, under the assumption of slightly stronger bounds on the tangential derivatives, (42), we establish the existence of a subsequence which converges to a weak solution of the codimension one bilayer equation

$$U_{zz} = W'(U), \quad (11)$$

on a rescaled domain Ω_1 where z is ε -scaled distance to Γ . In Section 4, in Theorem 4.1 we establish a lim inf inequality that holds for all codimension-one ℓ bounded sequences that satisfy a yet slightly stronger bound, (66), on the tangential derivatives. The lim inf inequality provides a lower bound in terms of a sup of codimension-one energy, $\mathcal{G}_1$, defined in (63), evaluated at the weak solutions of the bilayer equation, see Corollary 4.2. Moreover for general codimension-one interface Γ we construct codimension-one ℓ -bounded sequences composed of solutions of the bilayer equation which converge in a strong sense to the codimension-one energy $\mathcal{G}_1$, achieving the lower bound. However, for the same interfaces, we construct a second family of codimension-one ℓ bounded sequences composed of superpositions of codimension n critical points, called micelles when $n = 3$, with disjoint, compact support. These sequences do not satisfy the enhanced bounds on the tangential derivatives, and do not have a subsequence converging to the bilayer equation, but their energies converge to a limit that may be lower than the associated codimension one limit, depending upon the choice of the functionalization parameters η_1 and η_2 and the size of the curvatures of Γ .

2. Geometrically localized minimizers of F_ε

Compactly supported solutions and positive solutions for reaction–diffusion equations have been of interest for theoretical and application reasons, see [29] and references therein. In [29] it has been shown that if the domain Ω is sufficiently large, then a class of low regularity reaction–diffusion equations admits compactly supported positive solutions, which can be interpreted as compactly supported positive critical points for free energies of the form (1), with $\varepsilon = 1$ and a nonsmooth potential

$$W_{\alpha,\lambda}(u) = \frac{1}{\alpha+1}|u|^{\alpha+1} - \frac{\lambda}{2}u^2,$$

for any $0 < \alpha < 1$, and $\lambda > \lambda_1$, where $\lambda_1 > 0$ is the first eigenvalue for the Laplace operator with Dirichlet boundary conditions. In our context a large domain is equivalent to a sufficiently small value of ε . Although the potential $W_{\alpha,\lambda}$ approaches negative infinity as $|u| \rightarrow \infty$, it shares the same strong absorption property as our non-smooth potential W , namely, $W'_{\alpha,\lambda}(0) = 0$, $W''_{\alpha,\lambda}(0^+) = +\infty$.

In this section, we will show that for any subset $\Omega_\varepsilon \subset \Omega$ such that $\partial\Omega_\varepsilon$ is C^1 , F_ε has a minimizer u_ε over the class of nonnegative functions in $H^2(\Omega)$ with support inside of Ω_ε subject to a prescribed total mass of the lipid phase,

$$\int_{\Omega_\varepsilon} u \, dx = m_\varepsilon. \quad (12)$$

Since $F_\varepsilon(0) = 0$, we need only consider the integral of the FCH energy density over the subset Ω_ε , denoted by $F_\varepsilon|_{\Omega_\varepsilon}$, over all u in the admissible set

$$\mathcal{A}_\varepsilon := \left\{ u \in H_0^2(\Omega_\varepsilon) : u \geq 0 \text{ in } \Omega_\varepsilon, \int_{\Omega_\varepsilon} u \, dx = m_\varepsilon \right\}. \quad (13)$$

To construct u_ε , we first derive a lower bound of $F_\varepsilon|_{\Omega_\varepsilon}$ over all $u \in H_0^2(\Omega_\varepsilon)$. The proof is a modification of that [19], which incorporates the positivity assumption that allows an explicit formulation of the lower bound on ε . We highlight the key steps of the calculation.

Lemma 2.1. Suppose W is a double well potential satisfying (5) and the growth assumptions (6)–(8) with $p \geq 2$ (but not necessarily the upper bound in (9)), then for ε sufficiently small and $\eta_2 < p\eta_1$ there exist constants $A_1, A_2 > 0$ depending only on $\eta_1, \eta_2, p, C_1, C_3$, and C_4 , such that for any $u \in H_0^2(\Omega_\varepsilon)$

$$F_\varepsilon|_{\Omega_\varepsilon}(u) \geq \int_{\Omega_\varepsilon} \left\{ \frac{1}{4\varepsilon} \left(\frac{\delta E_\varepsilon}{\delta u} \right)^2 + \frac{\eta_1\varepsilon}{2} |\nabla u|^2 + \frac{A_1}{\varepsilon} |u|^p \right\} dx - \frac{A_2}{\varepsilon} |\Omega_\varepsilon|. \quad (14)$$

Proof. The L^2 variational derivative of E_ε takes the form

$$\frac{\delta E_\varepsilon}{\delta u} = -\varepsilon \Delta u + \frac{1}{\varepsilon} W'(u), \quad (15)$$

and we may write

$$\int_{\Omega_\varepsilon} \frac{\delta E_\varepsilon}{\delta u} u \, dx = \int_{\Omega_\varepsilon} \varepsilon |\nabla u|^2 + \frac{1}{\varepsilon} W'(u) u. \quad (16)$$

Then

$$\begin{aligned} F_\varepsilon|_{\Omega_\varepsilon}(u) &= \int_{\Omega_\varepsilon} \left\{ \frac{1}{2\varepsilon} \left(\frac{\delta E_\varepsilon}{\delta u} \right)^2 - \frac{\eta_1 \varepsilon}{2} |\nabla u|^2 - \frac{\eta_2}{\varepsilon} W(u) \right\} dx \\ &= \int_{\Omega_\varepsilon} \left\{ \frac{1}{2\varepsilon} \left(\frac{\delta E_\varepsilon}{\delta u} \right)^2 - \eta_1 \frac{\delta E_\varepsilon}{\delta u} u + \eta_1 \left(\varepsilon |\nabla u|^2 + \frac{1}{\varepsilon} W'(u) u \right) \right. \\ &\quad \left. - \frac{\eta_1 \varepsilon}{2} |\nabla u|^2 - \frac{\eta_2}{\varepsilon} W(u) \right\} dx. \end{aligned} \quad (17)$$

Since

$$\eta_1 \frac{\delta E_\varepsilon}{\delta u} u \leq \frac{1}{4\varepsilon} \left(\frac{\delta E_\varepsilon}{\delta u} \right)^2 + \varepsilon \eta_1^2 u^2, \quad (18)$$

plugging into (17), we have

$$\begin{aligned} F_\varepsilon|_{\Omega_\varepsilon}(u) &\geq \int_{\Omega_\varepsilon} \left\{ \frac{1}{4\varepsilon} \left(\frac{\delta E_\varepsilon}{\delta u} \right)^2 + \frac{\eta_1 \varepsilon}{2} |\nabla u|^2 \right. \\ &\quad \left. + \frac{1}{\varepsilon} \left(\eta_1 W'(u) u - \eta_2 W(u) - \eta_1^2 \varepsilon^2 u^2 \right) \right\} dx. \end{aligned} \quad (19)$$

Since $p \geq 2$, by (6) and (8), we have

$$\eta_1 W'(u) u - \eta_2 W(u) - \eta_1^2 \varepsilon^2 u^2 \geq (C_1(\eta_1 p - \eta_2) - \varepsilon^2 \eta_1^2) |u|^p + (\eta_1 C_4 - \eta_2 C_3).$$

For ε sufficiently small and $\eta_2 < \eta_1 p$ we find $A_1, A_2 > 0$, depending only on $\eta_1, \eta_2, p, C_1, C_3, C_4$ such that

$$\eta_1 W'(u) u - \eta_2 W(u) - \eta_1^2 \varepsilon^2 u^2 \geq A_1 |u|^p - A_2,$$

for all u . From the lower bound (19) we arrive at the estimate (14). $\square$

To establish the existence of a minimizer of F_ε we impose additional restrictions on p .

Theorem 2.2. In addition to the assumptions in Lemma 2.1, assume the upper bound on p described in (9) holds, then there exists $u_\varepsilon \in \mathcal{A}_\varepsilon$ that minimizes $F_\varepsilon|_{\Omega_\varepsilon}$ over $\mathcal{A}_\varepsilon$.

Proof. This theorem can be proved following a standard procedure (see, e.g., [19]). For the convenience of the readers, we briefly describe the procedures for $n \geq 3$. The case $n = 2$ is similar and simpler. Write $2^* := 2n/(n-2)$. Suppose $\{u_k\}$ is a minimizing sequence in $\mathcal{A}_\varepsilon$ for F_ε . By (14), $\{u_k\}$ is bounded in $H^1(\Omega_\varepsilon)$. By the Sobolev embedding theorem, $\{u_k\}$ is bounded in $L^q(\Omega_\varepsilon)$ for any $1 \leq q \leq 2^*$. Furthermore, by the compact embedding theorem, there is a subsequence, not relabeled, and a function $u_\varepsilon \in H^1(\Omega_\varepsilon)$ such that

$$u_k \rightarrow u_\varepsilon \text{ a.e. in } \Omega_\varepsilon \text{ and strongly in } L^q(\Omega_\varepsilon) \text{ for } 1 \leq q < 2^*. \quad (20)$$

If $p < \frac{2n-2}{n-2}$, then $|W'(u_k)| \sim |u_k|^{p-1}$ is bounded in $L^2(\Omega_\varepsilon)$. By (14), $-\varepsilon \Delta u_k + \frac{1}{\varepsilon} W'(u_k) = \frac{\delta E_\varepsilon}{\delta u}(u_k)$ is bounded in $L^2(\Omega_\varepsilon)$. The triangle inequality implies that Δu_k is bounded in $L^2(\Omega_k)$. So actually u_k is bounded in $H^2(\Omega_\varepsilon)$. We can extract a further subsequence, not relabeled, such that

$$u_k \rightharpoonup u_\varepsilon \text{ weakly in } H^2(\Omega_\varepsilon), \quad (21)$$

$$u_k \rightarrow u_\varepsilon \text{ strongly in } H^1(\Omega_\varepsilon), \quad (22)$$

$$u_k \rightarrow u_\varepsilon \text{ a.e. in } \Omega_\varepsilon \text{ and strongly in } L^q(\Omega_\varepsilon) \quad (23)$$

for any $1 \leq q < \infty$ if $n \leq 4$ and $1 \leq q < 2n/(n-4)$ if $n > 4$. Since $\mathcal{A}_\varepsilon$ is a closed convex subset of $H^2(\Omega_\varepsilon)$, we see that $u_\varepsilon \in \mathcal{A}_\varepsilon$.

Since $u_k \rightarrow u_\varepsilon$ a.e. in Ω_ε , by the continuity of W' , we have $W'(u_k) \rightarrow W'(u_\varepsilon)$ a.e. in Ω_ε . By the growth condition (7) of W' , we have $|W'(u_k)| \leq C_1 p |u_k|^{p-1} + C_3$. Since $|u_k|^{p-1} \rightarrow |u_\varepsilon|^{p-1}$ strongly in $L^2(\Omega_\varepsilon)$, using the generalized Dominated Convergence Theorem (see, e.g., [30]), we know that $W'(u_k) \rightarrow W'(u_\varepsilon)$ strongly in $L^2(\Omega_\varepsilon)$. Combined with (21), we have

$$-\varepsilon \Delta u_k + \frac{1}{\varepsilon} W'(u_k) \rightharpoonup -\varepsilon \Delta u_\varepsilon + \frac{1}{\varepsilon} W'(u_\varepsilon) \text{ weakly in } L^2(\Omega_\varepsilon). \quad (24)$$

Hence

$$\int_{\Omega_\varepsilon} \left(-\varepsilon \Delta u_\varepsilon + \frac{1}{\varepsilon} W'(u_\varepsilon) \right)^2 dx \leq \liminf_{k \rightarrow \infty} \int_{\Omega_\varepsilon} \left(-\varepsilon \Delta u_k + \frac{1}{\varepsilon} W'(u_k) \right)^2 dx. \quad (25)$$

By (22), we have

$$\int_{\Omega_\varepsilon} |\nabla u_\varepsilon|^2 dx = \lim_{k \rightarrow \infty} \int_{\Omega_\varepsilon} |\nabla u_k|^2 dx. \quad (26)$$

Since $|W(u)| \sim |u|^p$ as $|u| \rightarrow \infty$ and $2 \leq p < \frac{2n-2}{n-2}$, which is smaller than $2n/(n-4)$ if $n > 4$, by (23) and the generalized Dominated Convergence Theorem, we have

$$\int_{\Omega_\varepsilon} W(u_\varepsilon) dx = \lim_{k \rightarrow \infty} \int_{\Omega_\varepsilon} W(u_k) dx. \quad (27)$$

Combining (25), (26), and (27), we have $F_\varepsilon|_{\Omega_\varepsilon}(u_\varepsilon) \leq \liminf_{k \rightarrow \infty} F_\varepsilon|_{\Omega_\varepsilon}(u_k)$. Since $u_k \in \mathcal{A}_\varepsilon$ is a minimizing sequence for $F_\varepsilon|_{\Omega_\varepsilon}(u_\varepsilon)$ and $u_\varepsilon \in \mathcal{A}_\varepsilon$, we conclude that u_ε is a minimizer for $F_\varepsilon|_{\Omega_\varepsilon}$ in $\mathcal{A}_\varepsilon$. $\square$

Since $F_\varepsilon|_{\Omega_\varepsilon}$ is a non-convex functional, the family of critical points is typically not unique. Since $\mathcal{A}_\varepsilon$ is a closed and convex subset of $H_0^2(\Omega)$, we may resort to techniques of variational inequalities. Let $u_\varepsilon \in \mathcal{A}_\varepsilon$ be any minimizer of $F_\varepsilon|_{\Omega_\varepsilon}$ over $\mathcal{A}_\varepsilon$. Fix any $v \in \mathcal{A}_\varepsilon$, define $j_{\Omega_\varepsilon}(s) := F_\varepsilon|_{\Omega_\varepsilon}(u_\varepsilon + s(v - u_\varepsilon))$ for any $s \in [0, 1]$. Then $j_{\Omega_\varepsilon}(0) \leq j_{\Omega_\varepsilon}(s)$ for any $s \in [0, 1]$. So if $j_{\Omega_\varepsilon}(s)$ is differentiable, then $j'_{\Omega_\varepsilon}(0) \geq 0$, which gives a variational inequality

$$\begin{aligned} & \left\langle \frac{\delta F_\varepsilon|_{\Omega_\varepsilon}}{\delta u}(u_\varepsilon), v - u_\varepsilon \right\rangle \\ &:= \int_{\Omega_\varepsilon} \left\{ \frac{1}{\varepsilon} \left(-\varepsilon \Delta u_\varepsilon + \frac{1}{\varepsilon} W'(u_\varepsilon) \right) \left(-\varepsilon \Delta(v - u_\varepsilon) + \frac{1}{\varepsilon} W''(u_\varepsilon)(v - u_\varepsilon) \right) \right. \\ & \quad \left. - \left(\eta_1 \varepsilon \nabla u_\varepsilon \cdot \nabla(v - u_\varepsilon) + \frac{\eta_2}{\varepsilon} W'(u_\varepsilon)(v - u_\varepsilon) \right) \right\} dx \\ &\geq 0 \quad \text{for all } v \in \mathcal{A}_\varepsilon. \end{aligned} \quad (28)$$

Given a minimizer $u_\varepsilon \in \mathcal{A}_\varepsilon$ for $F_\varepsilon|_{\Omega_\varepsilon}$, we extend u_ε by zero outside of Ω_ε . We denote this extension by $\bar{u}_\varepsilon$. Then

$$\bar{u}_\varepsilon \in \mathcal{A}_{\Omega, \varepsilon} := \left\{ v \in H_0^2(\Omega), \quad v \geq 0 \text{ in } \Omega, \quad \int_{\Omega} v dx = m_\varepsilon \right\}.$$

$\bar{u}_\varepsilon$ may not be a minimizer of F_ε over $\mathcal{A}_{\Omega, \varepsilon}$, but $\bar{u}_\varepsilon$ does have some nice properties. We split F_ε into two parts, $F_\varepsilon|_{\Omega_\varepsilon}$ and $F_\varepsilon|_{\Omega \setminus \bar{\Omega}_\varepsilon}$, where $\bar{\Omega}_\varepsilon$ indicates the closure of Ω_ε . For any $\phi \in H_0^2(\Omega \setminus \bar{\Omega}_\varepsilon)$, a straightforward calculation shows that under the assumption (5), the first order variational derivative of $F_\varepsilon|_{\Omega \setminus \bar{\Omega}_\varepsilon}$ at 0 along ϕ is zero, that is,

$$\left\langle \frac{\delta F_\varepsilon|_{\Omega \setminus \bar{\Omega}_\varepsilon}}{\delta u}(0), \phi \right\rangle := \lim_{s \rightarrow 0} \frac{F_\varepsilon|_{\Omega \setminus \bar{\Omega}_\varepsilon}(s\phi) - F_\varepsilon|_{\Omega \setminus \bar{\Omega}_\varepsilon}(0)}{s} = 0. \quad (29)$$

The combination of (28) and (29) gives that for any $v \in H_0^2(\Omega)$ such that $v|_{\Omega_\varepsilon} \in \mathcal{A}_\varepsilon$, we have

$$\left\langle \frac{\delta F_\varepsilon}{\delta u}(\bar{u}_\varepsilon), v - \bar{u}_\varepsilon \right\rangle \geq 0. \quad (30)$$

Here the variational derivative of F_ε is defined the same way as that of $F_\varepsilon|_{\Omega_\varepsilon}$ in (28), with Ω_ε replaced by Ω . (30) states that $\bar{u}_\varepsilon$ is a critical point of F_ε under perturbations that are away from $\partial\Omega_\varepsilon$, and also preserves the total concentration in Ω_ε . In this sense, we say that $\bar{u}_\varepsilon$ is a geometrically localized minimizer of F_ε . If u is a minimizer of F_ε over $\mathcal{A}_{\Omega, \varepsilon}$, then u satisfies

$$\left\langle \frac{\delta F_\varepsilon}{\delta u}(u), v - u \right\rangle \geq 0 \quad \text{for all } v \in \mathcal{A}_{\Omega, \varepsilon}. \quad (31)$$

In this case, the lipid domain Ω_ε is implicitly defined as $\{x \in \Omega : u(x) > 0\}$. We leave the exploration of (31) for future studies.

3. Codimension one minimizers

We address the issue of convergence of sequences with bounded energy as $\varepsilon \rightarrow 0$ by imposing the additional assumption that Ω_ε is a thin region composed of points $x \in \Omega$ that are $O(\varepsilon)$ from a sufficiently smooth, non-self-intersecting, codimension one hypersurface Γ . In parametric form, we can write $\Gamma = \{\phi(s) : s = (s_1, \dots, s_{n-1}) \in Q \subset \mathbb{R}^{n-1}\}$, where the parameterization is chosen so that s_i is the arc length along the i th coordinate curve and the coordinate curves are lines of curvature. Let $\mathbf{n}$ be the normal of Γ and assume all principal curvatures $\kappa_j(s), j = 1, \dots, n-1$, of Γ are continuously differentiable and bounded. That is, there exists $\kappa_0 > 0$ such that

$$|\kappa_j(s)| \leq \kappa_0, \quad \left| \frac{\partial \kappa_j}{\partial s_i}(s) \right| \leq \kappa_0 \quad \text{for all } s \in Q \text{ and all } i, j = 1, \dots, n-1. \quad (32)$$

The boundedness of $\kappa_j(s)$ guarantees that there exists $\ell > 0$ such that the thin region

$$\Omega_1^\ell := \{\phi(s) + z\mathbf{n}(s) : s \in Q, -\ell < z < \ell\}. \quad (33)$$

does not self-intersect. The change of variables $x \mapsto (s, z)$ for $x \in \Omega_\varepsilon$ given by

$$x = \phi(s) + \varepsilon z \mathbf{n},$$

is well defined and smooth with a smooth inverse $x \mapsto (s, z)$ on Ω_1^ℓ . The inverse $x \mapsto \phi(s(x))$ is the projection of point $x \in \Omega_\varepsilon$ onto Γ , and $z \in (-\ell, \ell)$ is the ε -scaled signed distance of x to Γ .

We define $\Omega_\varepsilon \subset \Omega$ to be the region of distance $2\varepsilon\ell$ to Γ . More specifically

$$\Omega_\varepsilon := \{\phi(s) + z\mathbf{n}(s) : s \in Q, -\varepsilon\ell < z < \varepsilon\ell\}, \quad (34)$$

and it has volume $|\Omega_\varepsilon| = \varepsilon |\Omega_1^\ell|$. Defining $\tilde{u}(s, z) = u(x(s, z))$, then $\tilde{u} \in H^2(\Omega_1^\ell)$, and $\tilde{u}(s, \pm\ell) = 0$ for all $s \in Q$.

We will use a subscript x to indicate operators in the Cartesian coordinates x . Let $\kappa_1, \dots, \kappa_{n-1}$ be the principal curvatures of Γ and $\mathbf{T}_1, \dots, \mathbf{T}_{n-1}$ the corresponding unit tangent vectors. Under the change of variables $x \mapsto (s, z)$, $\nabla_x u(x)$ and $\Delta_x u(x)$ have the following forms in the (s, z) coordinates [13,16]

$$\nabla_x u(x) = \sum_{j=1}^{n-1} \frac{\mathbf{T}_j}{1 + \varepsilon z \kappa_j} \frac{\partial \tilde{u}}{\partial s_j} + \varepsilon^{-1} \mathbf{n} \frac{\partial \tilde{u}}{\partial z} =: \tilde{D}\tilde{u}(s, z), \quad (35)$$

$$\begin{aligned} \Delta_x u(x) &= \sum_{j=1}^{n-1} \frac{1}{(1 + \varepsilon z \kappa_j)^2} \frac{\partial^2 \tilde{u}}{\partial s_j^2} + \varepsilon^{-1} \sum_{j=1}^{n-1} \frac{\kappa_j}{1 + \varepsilon z \kappa_j} \frac{\partial \tilde{u}}{\partial z} + \varepsilon^{-2} \frac{\partial^2 \tilde{u}}{\partial z^2} \\ &\quad - \varepsilon \sum_{j=1}^{n-1} \frac{\partial \kappa_j}{\partial s_j} \frac{1}{(1 + \varepsilon z \kappa_j)^3} \frac{\partial \tilde{u}}{\partial s_j} =: \tilde{\Delta}\tilde{u}(s, z). \end{aligned} \quad (36)$$

By (35) and (36), $F_\varepsilon(u) = \tilde{F}_\varepsilon^\ell(\tilde{u})$ where

$$\tilde{F}_\varepsilon^\ell(\tilde{u}) := \int_{\Omega_1^\ell} \left\{ \frac{1}{2} \left(-\varepsilon \tilde{\Delta}\tilde{u} + \frac{1}{\varepsilon} W'(\tilde{u}) \right)^2 - \left(\frac{\eta_1 \varepsilon^2}{2} |\tilde{D}\tilde{u}|^2 + \eta_2 W(\tilde{u}) \right) \right\} J ds dz. \quad (37)$$

Here the scaled Jacobian can be expressed as

$$J(s, z) = \sum_{j=0}^n \varepsilon^j K_j(s) z^j, \quad (38)$$

in terms of the j th Gaussian curvatures $K_0 = 1$, and

$$K_j := \sum_{1 \leq i_1 < \dots < i_j \leq n-1} \kappa_{i_1} \cdots \kappa_{i_j}.$$

In particular we remark that $K_1 = H_0 := \sum_{j=1}^{n-1} \kappa_j$ is the total curvature of Γ and $J \rightarrow 1$ in all Sobolev norms as $\varepsilon \rightarrow 0$. In the scaled variables the lower bound (14) takes the form,

$$\begin{aligned} \tilde{F}_\varepsilon^\ell(\tilde{u}) &\geq \int_{\Omega_1^\ell} \left\{ \frac{1}{4} \left(-\varepsilon \tilde{\Delta}\tilde{u} + \frac{1}{\varepsilon} W'(\tilde{u}) \right)^2 + \frac{\eta_1 \varepsilon^2}{2} |\tilde{D}\tilde{u}|^2 + A_1 |\tilde{u}|^p \right\} J ds dz \\ &\quad - A_2 |\Omega_1^\ell|. \end{aligned} \quad (39)$$

Taking $m_\varepsilon = m\varepsilon$ in the mass constraint, (12), we rewrite the equivalent condition,

$$\int_{\Omega_1^\ell} \tilde{u} J ds dz = m \quad (40)$$

on the rescaled domain.

Theorem 3.1. Fix a codimension one interface Γ with curvature bound κ_0 as above, and choose $\ell \in (0, 1/(2\kappa_0))$. Then for any codimension-one ℓ -bounded sequence $\{\tilde{u}_k\}_{k=1}^\infty$ from $H^2(\Omega_1^\ell)$ and a sequence $\varepsilon_k \rightarrow 0^+$ such that

$$\limsup_{k \rightarrow \infty} \tilde{F}_{\varepsilon_k}^\ell(\tilde{u}_k) < \infty,$$

there exists $C > 0$ such that the following bounds hold for all $k \in \mathbb{N}_+$,

$$\|\tilde{u}_k\|_{L^p(\Omega_1^\ell)} + \left\| \frac{\partial \tilde{u}_k}{\partial z} \right\|_{L^2(\Omega_1^\ell)} + \varepsilon_k \sum_{j=1}^{n-1} \left\| \frac{\partial \tilde{u}_k}{\partial s_j} \right\|_{L^2(\Omega_1^\ell)} \leq C. \quad (41)$$

If we assume in addition that

$$\sum_{j=1}^{n-1} \left(\left\| \frac{\partial \tilde{u}_k}{\partial s_j} \right\|_{L^2(\Omega_1^\ell)} + \varepsilon_k \left\| \frac{\partial^2 \tilde{u}_k}{\partial s_j^2} \right\|_{L^2(\Omega_1^\ell)} \right) \leq C \quad (42)$$

for all $k \in \mathbb{N}_+$, then we have the following conclusions.

(i) In the limit when $k \rightarrow \infty$, the Cahn–Hilliard energy is equi-partitioned along the normal direction, that is,

$$\lim_{k \rightarrow \infty} \int_{\Omega_1^\ell} \left| \frac{1}{2} \left(\frac{\partial \tilde{u}_k}{\partial z} \right)^2 - W(\tilde{u}_k) \right| J ds dz = 0. \quad (43)$$

(ii) There exists a subsequence $\tilde{u}_{k_i}$ and a $\tilde{u}^* \in H_0^1(\Omega_1^\ell) \cap L^p(\Omega_1^\ell)$, such that $\tilde{u}_{k_i}$ converges weakly to $\tilde{u}^*$. Moreover $\tilde{u}^*$ is a weak solution to the bilayer equation

$$-\frac{\partial^2 \tilde{u}^*}{\partial z^2} + W'(\tilde{u}^*) = 0, \quad (44)$$

over Ω_1^ℓ , in the sense that

$$\int_{\Omega_1^\ell} \left(\frac{\partial \tilde{u}^*}{\partial z} \frac{\partial \phi}{\partial z} + W'(\tilde{u}^*) \phi \right) J ds dz = 0, \quad (45)$$

for all $\phi \in H_0^1(\Omega_1^\ell)$ if $p \leq 2^* = 2n/(n-2)$, and for all $\phi \in H_0^1(\Omega_1^\ell) \cap L^p(\Omega_1^\ell)$ if $p > 2^*$.

Proof. We infer from (39) that there exists $M > 0$ such that

$$\int_{\Omega_1^\ell} \left\{ \frac{1}{4} \left(-\varepsilon_k \tilde{\Delta} \tilde{u}_k + \frac{1}{\varepsilon_k} W'(\tilde{u}_k) \right)^2 + \frac{\eta_1 \varepsilon_k^2}{2} |\tilde{D} \tilde{u}_k|^2 + A_1 |\tilde{u}_k|^p \right\} J ds dz \leq M. \quad (46)$$

Dropping the first two terms on the left-hand side of (46) yields the bound

$$\|\tilde{u}_k\|_{L^p(\Omega_1^\ell)} \leq \left(\frac{M}{A_1} \right)^{1/p}. \quad (47)$$

Recalling (35) and keeping only the second term on the left-hand side of (46) imply the bound

$$\frac{\eta_1}{2} \int_{\Omega_1^\ell} \left\{ \sum_{j=1}^{n-1} \left(\frac{\varepsilon_k}{1 + \varepsilon_k Z \kappa_j} \right)^2 \left| \frac{\partial \tilde{u}_k}{\partial s_j} \right|^2 + \left| \frac{\partial \tilde{u}_k}{\partial z} \right|^2 \right\} J ds dz \leq M. \quad (48)$$

Since $|\kappa_j| \leq \kappa_0$ and $|z| \leq \ell$ on Ω_1^ℓ , we have the uniform estimate

$$\frac{2\varepsilon_k}{3} \leq \frac{\varepsilon_k}{1 + \varepsilon_k Z \kappa_j} \leq 2\varepsilon_k,$$

for all k such that $\varepsilon_k < 1/(2l\kappa_0)$, and hence $\frac{\partial \tilde{u}_k}{\partial z}$ is uniformly bounded while $\frac{\partial \tilde{u}_k}{\partial s_j}$ can grow at most as fast ε_k^{-1} . More specifically we have established that

$$\left\| \frac{\partial \tilde{u}_k}{\partial s_j} \right\|_{L^2(\Omega_1^\ell)} \leq \frac{3\sqrt{M}}{\sqrt{2}\eta_1 \varepsilon_k}, \quad (49)$$

$$\left\| \frac{\partial \tilde{u}_k}{\partial z} \right\|_{L^2(\Omega_1^\ell)} \leq \frac{\sqrt{2M}}{\sqrt{\eta_1}}. \quad (50)$$

Taken together, (47), (49), and (50) imply (41).

To establish the convergence to a weak solution of the bilayer equation, we impose the enhanced constraint and (42) return to the first term on the left-hand side of (46), deducing that

$$\left\| -\varepsilon_k \tilde{\Delta} \tilde{u}_k + \frac{1}{\varepsilon_k} W'(\tilde{u}_k) \right\|_{L^2(\Omega_1^\ell)} \leq 2\sqrt{M}. \quad (51)$$

Using (36) to expand the left-hand side of (51), we group terms by formal powers of ε_k ,

$$\begin{aligned} & -\varepsilon_k \tilde{\Delta} \tilde{u}_k + \frac{1}{\varepsilon_k} W'(\tilde{u}_k) \\ &= -\frac{1}{\varepsilon_k} \frac{\partial^2 \tilde{u}_k}{\partial z^2} + \frac{1}{\varepsilon_k} W'(\tilde{u}_k) - \sum_{j=1}^{n-1} \frac{\kappa_j}{1 + \varepsilon_k Z \kappa_j} \frac{\partial \tilde{u}_k}{\partial z} \\ & \quad - \varepsilon_k \sum_{j=1}^{n-1} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^2} \frac{\partial^2 \tilde{u}_k}{\partial s_j^2} + \varepsilon_k^2 \sum_{j=1}^{n-1} \frac{\partial \kappa_j}{\partial s_j} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^3} \frac{\partial \tilde{u}_k}{\partial s_j}, \end{aligned}$$

and employ the triangle inequality

$$\begin{aligned} & \left\| \frac{1}{\varepsilon_k} \left(-\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right) - \varepsilon_k \sum_{j=1}^{n-1} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^2} \frac{\partial^2 \tilde{u}_k}{\partial s_j^2} \right\|_{L^2(\Omega_1^\ell)} \\ & \leq \left\| -\varepsilon_k \tilde{\Delta} \tilde{u}_k + \frac{1}{\varepsilon_k} W'(\tilde{u}_k) \right\|_{L^2(\Omega_1^\ell)} + \sum_{j=1}^{n-1} \left\| \frac{\kappa_j}{1 + \varepsilon_k Z \kappa_j} \right\|_{L^\infty(\Omega_1^\ell)} \left\| \frac{\partial \tilde{u}_k}{\partial z} \right\|_{L^2(\Omega_1^\ell)} \\ & \quad + \varepsilon_k^2 \sum_{j=1}^{n-1} \left\| \frac{\partial \kappa_j}{\partial s_j} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^3} \right\|_{L^\infty(\Omega_1^\ell)} \left\| \frac{\partial \tilde{u}_k}{\partial s_j} \right\|_{L^2(\Omega_1^\ell)}. \end{aligned} \quad (52)$$

Combining the uniform bounds on ε_k over $k \geq 1$ and on κ_j and $\frac{\partial \kappa_j}{\partial s_j}$ for $j = 1, \dots, n-1$, with the bounds (49), (50), and (51), imply the existence of a constant $M_1 > 0$ such that for all $k \in \mathbb{N}$

$$\left\| \frac{1}{\varepsilon_k} \left(-\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right) - \varepsilon_k \sum_{j=1}^{n-1} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^2} \frac{\partial^2 \tilde{u}_k}{\partial s_j^2} \right\|_{L^2(\Omega_1^\ell)} \leq M_1. \quad (53)$$

The assumption (42) implies that the tangential second derivatives scale as $O(\varepsilon_k^{-1})$ and are lower order. Moving them to the right-hand side we conclude that

$$\begin{aligned} & \left\| \frac{1}{\varepsilon_k} \left(-\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right) \right\|_{L^2(\Omega_1^\ell)} \\ & \leq M_1 + \varepsilon_k \sum_{j=1}^{n-1} \left\| \frac{1}{(1 + \varepsilon_k Z \kappa_j)^2} \right\|_{L^\infty(\Omega_1^\ell)} \left\| \frac{\partial^2 \tilde{u}_k}{\partial s_j^2} \right\|_{L^2(\Omega_1^\ell)} \leq M_2, \end{aligned} \quad (54)$$

for some constant $M_2 > 0$ independent of ε_k , and consequently

$$\left\| -\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right\|_{L^2(\Omega_1^\ell)} \leq M_2 \varepsilon_k \rightarrow 0 \quad (55)$$

as $k \rightarrow \infty$. We use this convergence to establish the equi-partition, (43). Since all terms are zero at $z = \pm \ell$ we have the bound

$$\begin{aligned} & \left| \frac{1}{2} \left(\frac{\partial \tilde{u}_k}{\partial z}(z) \right)^2 - W(\tilde{u}_k(z)) \right| = \left| \int_{-l}^z \left(\frac{\partial^2 \tilde{u}_k}{\partial z^2}(\zeta) - W'(\tilde{u}_k(\zeta)) \right) \frac{\partial \tilde{u}_k}{\partial z}(\zeta) d\zeta \right| \\ & \leq \left(\int_{-l}^l \left(\frac{\partial^2 \tilde{u}_k}{\partial z^2}(\zeta) - W'(\tilde{u}_k(\zeta)) \right)^2 d\zeta \right)^{1/2} \left(\int_{-l}^l \left| \frac{\partial \tilde{u}_k}{\partial z}(\zeta) \right|^2 d\zeta \right)^{1/2}, \end{aligned}$$

from which we deduce the L^1 estimate

$$\begin{aligned} & \int_{\Omega_1^\ell} \left| \frac{1}{2} \left(\frac{\partial \tilde{u}_k}{\partial z}(z) \right)^2 - W(\tilde{u}_k(z)) \right| J ds dz \\ & \leq \left(\int_{\Omega_1^\ell} \int_{-l}^l \left(\frac{\partial^2 \tilde{u}_k}{\partial z^2}(\zeta) - W'(\tilde{u}_k(\zeta)) \right)^2 d\zeta J ds dz \right)^{1/2} \\ & \quad \cdot \left(\int_{\Omega_1^\ell} \int_{-l}^l \left| \frac{\partial \tilde{u}_k}{\partial z}(\zeta) \right|^2 d\zeta J ds dz \right)^{1/2} \\ & \leq 2l \left\| -\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right\|_{L^2(\Omega_1^\ell)} \left\| \frac{\partial \tilde{u}_k}{\partial z} \right\|_{L^2(\Omega_1^\ell)}. \end{aligned}$$

From (41) and (55) we see that the right-hand side tends to zero as $k \rightarrow \infty$ and we deduce (i).

To establish that the limit function $\tilde{u}_*$ is a weak solution of the bilayer equation, (ii)-(44), we recall that assumption (42) implies that the first order tangential derivatives $\frac{\partial \tilde{u}_k}{\partial s_j}$ are uniformly bounded in $L^2(\Omega_1^\ell)$ for $j = 1, \dots, n-1$ and all $k \in \mathbb{N}$. This fact, in conjunction with (47) and (50), implies that $\tilde{u}_k$ is bounded in $H^1(\Omega_1^\ell)$. We deduce that there exist a subsequence $\tilde{u}_{k_i}$ and a function $\tilde{u}^* \in H^1(\Omega_1^\ell)$ such that

$$\tilde{u}_{k_i} \rightharpoonup \tilde{u}^* \quad \text{weakly in } H^1(\Omega_1^\ell). \quad (56)$$

Moreover the Sobolev embedding and compact embedding theorems imply that $\tilde{u}_k$ is bounded in $L^{2^*}(\Omega_1^\ell)$ and $\tilde{u}_{k_i} \rightarrow \tilde{u}^*$ strongly in $L^q(\Omega_1^\ell)$ for any $1 \leq q < 2^* := 2n/(n-2)$. Extracting a further subsequence, not relabeled, we have that $\tilde{u}_{k_i} \rightarrow \tilde{u}^*$ a.e. in Ω_1^ℓ . Since $\tilde{u}_k$ is bounded in $L^p(\Omega_1^\ell)$, we can improve the strong convergence so that

$$\tilde{u}_{k_i} \rightarrow \tilde{u}^* \quad \text{strongly in } L^q(\Omega_1^\ell) \text{ for any } 1 \leq q < q_0 := \max\{p, 2n/(n-2)\}. \quad (57)$$

Proceeding, from the H^1 weak convergence, for any $\phi \in H_0^1(\Omega_1^\ell)$, we have

$$\lim_{i \rightarrow \infty} \int_{\Omega_1^\ell} \frac{\partial \tilde{u}_{k_i}}{\partial z} \frac{\partial \phi}{\partial z} J ds dz = \int_{\Omega_1^\ell} \frac{\partial \tilde{u}^*}{\partial z} \frac{\partial \phi}{\partial z} J ds dz. \quad (58)$$

Since $W'(u)$ is continuous in u , and $|W'(u)| \leq C|u|^{p-1}$ as $|u| \rightarrow \infty$, the strong convergence of $\tilde{u}_{k_i} \rightarrow \tilde{u}^*$ in $L^q(\Omega_1^\ell)$ for any $q \in [p-1, q_0)$ and a.e. convergence in Ω_1^ℓ , together with the Generalized Dominated Convergence Theorem imply that for any $q \in [p-1, q_0)$,

$$W'(\tilde{u}_{k_i}) \rightarrow W'(\tilde{u}^*) \quad \text{strongly in } L^{q/(p-1)}(\Omega_1^\ell) \text{ and a.e. in } \Omega_1^\ell. \quad (59)$$

Since $W'(\tilde{u}_{k_i})$ is bounded in $L^{q_0/(p-1)}(\Omega_1^\ell)$, by extracting a further subsequence if necessary, by (59), we obtain

$$W'(\tilde{u}_{k_i}) \rightharpoonup W'(\tilde{u}^*) \quad \text{weakly in } L^{q_0/(p-1)}(\Omega_1^\ell). \quad (60)$$

Thus

$$\lim_{i \rightarrow \infty} \int_{\Omega_1^\ell} W'(\tilde{u}_{k_i}) \phi J ds dz = \int_{\Omega_1^\ell} W'(\tilde{u}^*) \phi J ds dz, \quad (61)$$

for any $\phi \in L^r(\Omega_1^\ell)$ with $r = q_0/(q_0 - p + 1)$. Combining (58) and (61), we deduce that

$$\begin{aligned} \int_{\Omega_1^\ell} \left(\frac{\partial \tilde{u}^*}{\partial z} \frac{\partial \phi}{\partial z} + W'(\tilde{u}^*) \phi \right) J ds dz &= \lim_{i \rightarrow \infty} \int_{\Omega_1^\ell} \left(\frac{\partial \tilde{u}_{k_i}}{\partial z} \frac{\partial \phi}{\partial z} + W'(\tilde{u}_{k_i}) \phi \right) J ds dz \\ &= \lim_{i \rightarrow \infty} \int_{\Omega_1^\ell} \left(-\frac{\partial^2 \tilde{u}_{k_i}}{\partial z^2} + W'(\tilde{u}_{k_i}) \right) \phi J ds dz \\ &= 0, \end{aligned} \quad (62)$$

for any $\phi \in H_0^1(\Omega_1^\ell) \cap L^r(\Omega_1^\ell)$. We remark that if $p \leq 2^*$, then $q_0 = 2^*$ and $r \leq 2^*$, so that the Sobolev embedding theorem implies that $H_0^1(\Omega_1^\ell) \cap L^r(\Omega_1^\ell) = H_0^1(\Omega_1^\ell)$. On the other hand, if $p > 2^*$, then $q_0 = p$, $r = p$, and $H_0^1(\Omega_1^\ell) \cap L^r(\Omega_1^\ell) = H_0^1(\Omega_1^\ell) \cap L^p(\Omega_1^\ell)$. $\square$

4. Upper and lower bounds on codimension-one sequences

A key goal of our analysis is to identify properties of codimension-one ℓ -bounded energy sequences which characterize the form of their limiting energy. Theorem 3.1 establishes a condition on the tangential derivatives which guarantees that such sequences have subsequences that converge to weak solutions of the bilayer equation. We show that the asymptotic scaling of the tangential derivatives is essential to the form of the limiting energy.

4.1. Codimension-one lower bounds

We establish that a slightly stronger constraint on the tangential derivatives imposes a class of codimension-one lower bounds for the energy of each subsequence that has an H^1 weak limit. More specifically if $\tilde{u}^* \in H^1(\Omega_1^\ell)$ is a weak solution of the bilayer equation in the sense of (45), then we define the associated codimension-one energy

$$G_1(\Gamma, \tilde{u}^*) := \int_{\Gamma} \left(\tilde{a}^* H_0^2 - (\eta_1 + \eta_2) \tilde{b}^* \right) ds, \quad (63)$$

where $H_0 = \sum_{j=1}^{n-1} \kappa_j$ is the total curvature of Γ , and

$$\tilde{a}^*(s) := \frac{1}{2} \int_{-\ell}^{\ell} \left| \frac{\partial \tilde{u}^*}{\partial z} \right|^2 dz, \quad (64)$$

$$\tilde{b}^*(s) := \int_{-\ell}^{\ell} W(\tilde{u}^*) dz. \quad (65)$$

While this result falls short of establishing a unique codimension-one limiting energy it establishes a liminf inequality for a class of codimension one ℓ -bounded sequences.

Theorem 4.1. Suppose $2 \leq p < 2^*$ and let $\{\tilde{u}_k\}_{k=1}^\infty$ be a codimension-one ℓ -bounded sequence satisfying the assumptions of Theorem 3.1; in particular (41) holds. If in addition we strengthen assumption (42) to include a stronger bound on the second tangential derivatives,

$$\sum_{j=1}^{n-1} \left\| \frac{\partial^2 \tilde{u}_k}{\partial s_j^2} \right\|_{L^2(\Omega_1^\ell)} = o(\varepsilon_k^{-1}), \quad (66)$$

then for any subsequence $\tilde{u}_{k_j}$ that converges weakly to a function $\tilde{u}^*$ in $H_0^1(\Omega_1^\ell)$, we have the following codimension-one liminf inequality:

$$\liminf_{j \rightarrow \infty} \tilde{F}_{\varepsilon_{k_j}}^\ell(\tilde{u}_{k_j}) \geq G_1(\Gamma, \tilde{u}^*). \quad (67)$$

Proof. Without loss of generality, we assume $\tilde{u}_k \rightharpoonup \tilde{u}^*$ in $H_0^1(\Omega_1^\ell)$ and $\tilde{u}_k$ satisfies all assumptions in the theorem. We write the energy integral as the difference of the quadratic and functionalization terms,

$$\begin{aligned} \tilde{F}_{\varepsilon_k}^\ell(\tilde{u}_k) &= \int_{\Omega_1^\ell} \frac{1}{2} \left(-\varepsilon_k \tilde{\Delta} \tilde{u}_k + \frac{1}{\varepsilon_k} W'(\tilde{u}_k) \right)^2 J ds dz \\ &\quad - \int_{\Omega_1^\ell} \left(\frac{\eta_1 \varepsilon_k^2}{2} |\tilde{D} \tilde{u}_k|^2 + \eta_2 W(\tilde{u}_k) \right) J ds dz \\ &=: I - II. \end{aligned} \quad (68)$$

Using the Laplacian expansion (36) we rewrite I as

$$\begin{aligned} I &= \int_{\Omega_1^\ell} \frac{1}{2} \left(-\varepsilon_k \tilde{\Delta} \tilde{u}_k + \frac{1}{\varepsilon_k} W'(\tilde{u}_k) \right)^2 J ds dz \\ &= \int_{\Omega_1^\ell} \frac{1}{2} \left\{ -\varepsilon_k \sum_{j=1}^{n-1} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^2} \frac{\partial^2 \tilde{u}_k}{\partial s_j^2} - \sum_{j=1}^{n-1} \frac{\kappa_j}{1 + \varepsilon_k Z \kappa_j} \frac{\partial \tilde{u}_k}{\partial z} \right. \\ &\quad \left. + \varepsilon_k^2 \sum_{j=1}^{n-1} \frac{\partial \kappa_j}{\partial s_j} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^3} \frac{\partial \tilde{u}_k}{\partial s_j} + \frac{1}{\varepsilon_k} \left(-\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right) \right\}^2 J ds dz. \end{aligned} \quad (69)$$

From (42) and (66), it is easy to see that the tangential derivative terms, i.e., the first and third terms in the quadratic expression, tend to zero in $L^2(\Omega_1^\ell)$ as $k \rightarrow \infty$, while from (50) and (55), the through-plane derivative terms, i.e., the second and fourth terms, are uniformly bounded in $L^2(\Omega_1^\ell)$. It follows that the tangential terms may be neglected in the $k \rightarrow \infty$ limit. Moreover

$$\sum_{j=1}^{n-1} \frac{\kappa_j}{1 + \varepsilon_k Z \kappa_j} \rightarrow H_0,$$

in $L^\infty(\Omega_1^\ell)$ as $k \rightarrow \infty$ and we may make this replacement in the limit, observing that

$$\begin{aligned} \lim_{k \rightarrow \infty} I &= \lim_{k \rightarrow \infty} \int_{\Omega_1^\ell} \left\{ \frac{1}{2} H_0^2 \left(\frac{\partial \tilde{u}_k}{\partial z} \right)^2 + \frac{1}{2\varepsilon_k^2} \left(-\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right)^2 \right. \\ &\quad \left. - \frac{1}{\varepsilon_k} H_0 \frac{\partial \tilde{u}_k}{\partial z} \left(-\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right) \right\} J ds dz, \\ &=: \lim_{k \rightarrow \infty} (I_1 + I_2 + I_3). \end{aligned} \quad (70)$$

Addressing these terms one-by-one we find,

$$\begin{aligned} \lim_{k \rightarrow \infty} I_3 &= \lim_{k \rightarrow \infty} -\frac{1}{\varepsilon_k} \int_{\Gamma} H_0 \int_{-\ell}^{\ell} \frac{\partial \tilde{u}_k}{\partial z} \left(-\frac{\partial^2 \tilde{u}_k}{\partial z^2} + W'(\tilde{u}_k) \right) J(s, z) dz ds \\ &= \lim_{k \rightarrow \infty} -\frac{1}{\varepsilon_k} \int_{\Gamma} H_0 \int_{-\ell}^{\ell} \frac{\partial}{\partial z} \left(-\frac{1}{2} \left| \frac{\partial \tilde{u}_k}{\partial z} \right|^2 + W(\tilde{u}_k) \right) J(s, z) dz ds \\ &= \lim_{k \rightarrow \infty} \frac{1}{\varepsilon_k} \int_{\Gamma} H_0 \int_{-\ell}^{\ell} \left(-\frac{1}{2} \left| \frac{\partial \tilde{u}_k}{\partial z} \right|^2 + W(\tilde{u}_k) \right) \partial_z J(s, z) dz ds, \end{aligned} \quad (71)$$

where we used $W(\tilde{u}_k(\pm \ell)) = W(0) = 0$ and $\frac{\partial \tilde{u}_k}{\partial z}(\pm \ell) = 0$ in the integration by parts step. Recalling the form of the Jacobian, (38), and the definitions (64) and (65) we find that

$$\lim_{k \rightarrow \infty} I_3 = \lim_{k \rightarrow \infty} \int_{\Gamma} H_0^2(s) \int_{-\ell}^{\ell} \left(-\frac{1}{2} \left| \frac{\partial \tilde{u}_k}{\partial z} \right|^2 + W(\tilde{u}_k) \right) dz ds = 0, \quad (72)$$

the last conclusion relies on equipartition, (43).

For I_1 , since $\tilde{u}_k \rightharpoonup \tilde{u}^*$ weakly in $H^1(\Omega_1^\ell)$, we have

$$\sum_{j=1}^{n-1} \frac{\kappa_j}{1 + \varepsilon_k Z \kappa_j} \frac{\partial \tilde{u}_k}{\partial z} \rightharpoonup \frac{\partial \tilde{u}^*}{\partial z} \sum_{j=1}^{n-1} \kappa_j = \frac{\partial \tilde{u}^*}{\partial z} H_0 \quad \text{weakly in } H^1(\Omega_1^\ell). \quad (73)$$

By weak lower semicontinuity and the strong convergence of J as $\varepsilon \rightarrow 0$ we deduce that

$$\liminf_{k \rightarrow \infty} I_1 \geq \frac{1}{2} \int_{\Omega_1^\ell} \left(\frac{\partial \tilde{u}^*}{\partial z} H_0 \right)^2 J|_{\varepsilon=0} ds dz = \int_{\Gamma} \tilde{a}^* H_0^2 ds. \quad (74)$$

For I_2 we merely observe that it is positive and bounded below by zero, hence $\liminf_{k \rightarrow \infty} I_2 \geq 0$. For I_1 , we have

$$I_1 = \int_{\Omega_1^\ell} \left\{ \frac{\eta_1}{2} \left| \frac{\partial \tilde{u}_k}{\partial z} \right|^2 + \eta_2 W(\tilde{u}_k) + \frac{\eta_1 \varepsilon_k^2}{2} \sum_{j=1}^{n-1} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^2} \left| \frac{\partial \tilde{u}_k}{\partial s_j} \right|^2 \right\} J ds dz. \quad (75)$$

Since $p < 2^*$, by the compact embedding theorem we have $\tilde{u}_k \rightarrow \tilde{u}^*$ strongly in $L^p(\Omega_1^\ell)$, and hence $W(\tilde{u}_k) \rightarrow W(\tilde{u}^*)$ strongly in $L^1(\Omega_1^\ell)$. From the strong convergence of the tangential derivatives, (42), we have

$$\lim_{k \rightarrow \infty} \int_{\Omega_1^\ell} \frac{\eta_1 \varepsilon_k^2}{2} \sum_{j=1}^{n-1} \frac{1}{(1 + \varepsilon_k Z \kappa_j)^2} \left| \frac{\partial \tilde{u}_k}{\partial s_j} \right|^2 J ds dz = 0.$$

Finally equipartition, (43), allows us to deduce that

$$\begin{aligned} \lim_{k \rightarrow \infty} I_1 &= \lim_{k \rightarrow \infty} \int_{\Omega_1^\ell} \left\{ \frac{\eta_1}{2} \left| \frac{\partial \tilde{u}_k}{\partial z} \right|^2 + \eta_2 W(\tilde{u}_k) \right\} J ds dz, \\ &= (\eta_1 + \eta_2) \lim_{k \rightarrow \infty} \int_{\Omega_1^\ell} W(\tilde{u}_k) J ds dz, \\ &= (\eta_1 + \eta_2) \int_{\Gamma} b^* ds. \end{aligned} \quad (76)$$

Combining (72), (74) and (76) we obtain (67). $\square$

In general $\tilde{a}^*$ and $\tilde{b}^*$ may depend on s . Since we have the limiting equipartition of energy, (43), ideally we would hope to keep the equipartition of energy in the limiting profile $\tilde{u}^*$, i.e., $\tilde{a}^* = \tilde{b}^*$. However, by the weak convergence $\tilde{u}_{k_j} \rightharpoonup \tilde{u}^*$

in $H_0^1(\Omega_1^\ell)$, and the strong convergence $W(\tilde{u}_{k_j}) \rightarrow W(\tilde{u}^*)$ in $L^1(\Omega_1^\ell)$, we can only obtain

$$0 \leq \int_{\Gamma} \tilde{a}^*(s) ds \leq \int_{\Gamma} \tilde{b}^*(s) ds.$$

Indeed we have the following string of inequalities

$$\begin{aligned} \int_{\Gamma} \tilde{a}^*(s) ds &= \int_{\Omega_1^\ell} \left| \frac{\partial \tilde{u}^*}{\partial z} \right|^2 J dz ds \leq \liminf_{j \rightarrow \infty} \int_{\Omega_1^\ell} \left| \frac{\partial \tilde{u}_{k_j}}{\partial z} \right|^2 J dz ds \\ &= \liminf_{j \rightarrow \infty} \int_{\Omega_1^\ell} W(\tilde{u}_{k_j}) J dz ds = \int_{\Omega_1^\ell} W(\tilde{u}^*) J dz ds = \int_{\Gamma} \tilde{b}^*(s) ds. \end{aligned}$$

It is an interesting question to explore the possible loss of energy in the weak convergence. This is left for future studies.

We define $\mathcal{S}(\Gamma, \ell)$ to consist of the set of $\tilde{u} \in H^1(\Omega_1^\ell)$ that are weak solutions of the bilayer equation, and introduce the set $\overline{\{\tilde{u}_k\}}^{H^1}$ of functions $\tilde{u} \in H^1(\Omega_1^\ell)$ that are H^1 weak limits of a subsequence of $\{\tilde{u}_k\}$. With this notation we reformulate Theorem 4.1.

Corollary 4.2. Fix a codimension-one interface Γ satisfying (32). Every codimension-one ℓ -bounded sequence $\{\tilde{u}_k\}_{k=1}^\infty$ that satisfies (42) and (66) has the lower bound

$$\liminf_{k \rightarrow \infty} \tilde{F}_{\varepsilon_k}^\ell(\tilde{u}_k) \geq \sup \left\{ G_1(\Gamma, \tilde{u}^*) \mid \tilde{u}^* \in \mathcal{S}(\Gamma, \ell) \cap \overline{\{\tilde{u}_k\}}^{H^1} \right\}. \quad (77)$$

Proof. By Theorem 3.1 the set $\mathcal{S}(\Gamma, \ell) \cap \overline{\{\tilde{u}_k\}}^{H^1}$ is not empty and by Theorem 4.1 for each $\tilde{u}_*$ in this set, the value $G_1(\Gamma, \tilde{u}_*)$ is a lower bound for $\liminf_{\varepsilon_k} \tilde{F}_{\varepsilon_k}^\ell(\tilde{u}_k)$. $\square$

4.2. Codimension-one upper bounds

For a given codimension one interface, Γ , upper bounds on the limiting energy of codimension-one ℓ -bounded sequences can be obtained for specific examples. We present a sequence that satisfies the enhanced bounds (42) and (66), and whose codimension one energy provides a sharp lower bound. We also present a codimension-one ℓ -bounded sequence that does not satisfy the enhanced bounds, has no subsequences that are weakly convergent in H^1 , yet nonetheless has a limiting energy that may be higher or lower than the codimension-one energy, particularly if the curvatures of Γ are sufficiently large.

4.2.1. Sharp codimension-one energy

In light of Corollary 4.2, to construct sharp bounds it seems meritorious to reduce the size of the set $\mathcal{S}(\Gamma, \ell)$. If the H^1 weak closure of the sequence is also a H^2 weak closure, then the limiting bilayer equation solution will reside in $H_0^2(\Omega_1^\ell)$. The additional regularity implies that $\tilde{u}^*$ is a strong solution of the bilayer equation and hence is comprised of N , s -dependent curves of translates of the bilayer profile, $U_*^1 \in H^2(\mathbb{R})$, defined as the unique single-pulse solution of (79) that is symmetric about $z = 0$. The profile U_*^1 has compact support, denoted by $[-L, L]$, and remark that N must satisfy $NL \leq \ell$.

Indeed, for $\tilde{u}^* \in \mathcal{S}(\Gamma, \ell) \cap H_0^2(\Omega_1^\ell)$, then the extension

$$\tilde{u}_{\text{ext}}^* := \begin{cases} \tilde{u}^* & \text{if } x \in \Omega_1^\ell, \\ 0 & \text{otherwise} \end{cases} \quad (78)$$

belongs to $H^2(\mathbb{R}^n)$ and $\tilde{u}^*$ is a strong solution of the bilayer equation

$$-\frac{\partial^2 \tilde{u}^*}{\partial z^2} + W'(\tilde{u}^*) = 0, \quad \tilde{u}^*(\pm\ell) = 0, \quad \frac{\partial \tilde{u}^*}{\partial z}(\pm\ell) = 0. \quad (79)$$

This equation has a unique solution on each whisker $W(s) := \{x \in \Omega_1^\ell \mid \phi(x) = s\}$. By standard dynamical systems techniques we find that $\tilde{u}^*$ is a superposition of at most N compactly supported single-pulse bilayer solutions

$$\tilde{u}_* = \sum_{k=1}^N U_*^1(z - p_k(s)), \quad (80)$$

where the translates $p_k : \Gamma \mapsto \mathbb{R}$ are sufficiently far apart that their supports are disjoint and avoid the boundary. More specifically this is achieved if require that $p_k < p_{k+1} + 2L$, $p_1 > -\ell + L$, $p_N < \ell - L$, uniformly over $s \in \Gamma$. Since $u_* \in H^2$ we deduce that each $p_k \in H^2(\Gamma)$. The precise value of N depends upon the choice of ℓ and the value of the mass constraint.

Pulling $\tilde{u}_*$ back to its unscaled version u_* , we see that total mass can only take discrete values at leading order

$$\int_{\Omega} u_* dx = \varepsilon \int_{\Omega_1^\ell} \tilde{u}_* J ds dz = \varepsilon |\Gamma| N \int_{-L}^L U_*^1(z) dz + O(\varepsilon^2). \quad (81)$$

Due to the rescaling, the translates have no impact on the mass in the limit as $\varepsilon \rightarrow 0$.

For fixed Γ and ℓ sufficiently large we may tune value of the total mass, so that $N = 1$. The H^2 solution set then reduces to the translates of the single pulse, which we denote by $\tilde{u}^1$, and for any sequence $\{\varepsilon_k\}$ we construct the corresponding sequence $\{\tilde{u}_k\}$ which agrees trivially with $\tilde{u}^1$ for each k , and their un-scaled forms $\{u_k\}$. This is a codimension-one ℓ -bounded sequence that satisfies (42) and (66). To evaluate its energy we rewrite (37) as

$$\begin{aligned} \tilde{F}_{\varepsilon_k}^\ell(\tilde{u}_k) := & \int_{\Omega_1^\ell} \left[\frac{1}{2} (\varepsilon_k^{-1} (-\partial_z^2 \tilde{u}^1 + W'(\tilde{u}^1)) - H \partial_z \tilde{u}^1 - \varepsilon_k \Delta_s \tilde{u}^1)^2 \right. \\ & \left. - \frac{\eta_1}{2} (\varepsilon_k^2 |\nabla_s \tilde{u}^1|^2 + |\partial_z \tilde{u}^1|^2) - \eta_2 W(\tilde{u}^1) \right] J ds dz. \end{aligned} \quad (82)$$

A simple calculation shows that

$$\lim_{k \rightarrow \infty} \tilde{F}_{\varepsilon_k}^\ell(\tilde{u}_k) = \int_{\Gamma} (a_*^1 H_0^2(s) - (\eta_1 + \eta_2) b_*^1) ds = G_1(\Gamma, U_*^1), \quad (83)$$

where $a_*^1 = b_*^1 > 0$ are the corresponding constants

$$a_*^1 = \frac{1}{2} \int_{-L}^L \left| \frac{\partial U_*^1}{\partial z} \right|^2 dz, \quad b_*^1 = \int_{-L}^L W(U_*^1) dz. \quad (84)$$

4.2.2. Codimension-one sequence without codimension one energy

Pearling is a bifurcation characterized by rapid tangential oscillations in bilayer thickness. The existence of pearled solutions as critical points of the FCH free energy has been established in a weakly nonlinear setting for a smooth well W , [31]. However this construction requires analysis of the linearization about the underlying bilayer solution and does not immediately extend to the case of a non-smooth well considered here. However in the strongly nonlinear setting pearled solutions may reduce to disconnected micelles, that is, codimension n balls. These are radial solutions whose profile U_*^n solves

$$\partial_R^2 U_*^n + \frac{n-1}{R} \partial_R U_*^n = W'(U_*^n), \quad (85)$$

where R is the ε scaled distance to a center point. The codimension n profile U_*^n satisfies $\partial_R U_*^n(0) = 0$ and has support contained within $R \in [0, R_0]$. For a fixed codimension one interface Γ , we form a codimension-one ℓ bounded sequence with $\ell > R_0$. Taking $\{\varepsilon_j\}$ tending to zero as $j \rightarrow \infty$ and for each j identify N_j points $\{x_{j,k}\}_{k=1}^{N_j}$ on Γ whose separation is greater than $\varepsilon_j R_0$. Since Γ is far from self intersection there exists $\alpha_0 > 0$ sufficiently small such that for each $\alpha \in (0, \alpha_0)$ we may choose the points so that $N_j \sim \alpha \varepsilon_j^{1-n}$. We form the sequence $\{w_j\}$ according to the formula

$$w_j(x) = \sum_{k=1}^{N_j} U_*^n \left(\frac{|x - x_{j,k}|}{\varepsilon_j} \right). \quad (86)$$

To evaluate the energy we first consider, U_*^n . Multiplying (85) by $\partial_R U_*^n$, integrating from $s = R$ to $s = \infty$, and using $W(U_*^n(\infty)) = W(0) = 0$, we obtain

$$\frac{1}{2} |\partial_R U_*^n|^2 - (n-1) \int_R^\infty \frac{1}{s} |\partial_R U_*^n(s)|^2 ds = W(U_*^n). \quad (87)$$

Multiplying this expression by R^{n-1} and integrating over the region $R = 0$ to $R = \infty$ yields

$$\int_0^\infty W(U_*^n) R^{n-1} dR = \int_0^\infty \left[\frac{R^{n-1}}{2} |\partial_R U_*^n|^2 - \frac{n-1}{n} \partial_R (R^n) \int_R^\infty \frac{1}{s} |\partial_R U_*^n(s)|^2 ds \right] dR. \quad (88)$$

The integral over s is identically zero for R beyond the support of U_*^n , while it is bounded as $R \rightarrow 0$. We may integrate by parts on the second term on the right hand side, obtaining

$$\int_0^\infty W(U_*^n) R^{n-1} dR = \frac{2-n}{2n} \int_0^\infty |\partial_R U_*^n|^2 R^{n-1} dR = \frac{2-n}{2n} \sigma_n, \quad (89)$$

where we have introduced the codimension- n surface tension

$$\sigma_n := \int_0^\infty |\partial_R U_*^n|^2 R^{n-1} dR. \quad (90)$$

With these results it is easy to see that

$$F_\varepsilon(U_*^n) = -\varepsilon^{n-1} \left(\frac{\eta_1}{2} + \frac{2-n}{2n} \eta_2 \right) \sigma_n, \quad (91)$$

and hence

$$\lim_{j \rightarrow \infty} \tilde{F}_\varepsilon^\ell(w_j) = -\alpha \left(\frac{\eta_1}{2} + \frac{2-n}{2n} \eta_2 \right) \sigma_n. \quad (92)$$

Moreover there exists a constant $c > 0$ such that

$$\begin{aligned} \|w_j\|_{L^2(\Omega_1^\ell)} &\geq c, \\ \|\nabla_s w_j\|_{L^2(\Omega_1^\ell)} &\geq c\varepsilon_j^{-1}, \\ \|\Delta_s w_j\|_{L^2(\Omega_1^\ell)} &\geq c\varepsilon_j^{-2}, \end{aligned} \quad (93)$$

for all $j \geq 1$. The codimension-one ℓ -bounded sequence satisfies (41) but neither satisfies the enhanced bounds (42) nor (66). In particular it is straightforward to choose the points $\{x_{j,k}\}$ so that no subsequence of $\{w_j\}_{j=1}^\infty$ converges strongly in $L^2(\Omega_1^\ell)$.

5. Discussion

We have shown that sequences of FCH-energy bounded functions whose support converges to the same codimension one interface, Γ , may have fundamentally different structure and that their limiting energy can target different features of the underlying interface. Consequently, the relative size of the corresponding limiting energy can be exchanged under subtle changes in the parameters in the FCH energy. Specifically, the bilayer sequence $\{\tilde{u}_k\}$ constructed in Section 4.2.1 and the micelle sequence $\{\tilde{w}_k\}$ constructed in Section 4.2.2 are both codimension-one ℓ -bounded for any codimension-one interface Γ satisfying the curvature bounds (32). If $\eta_2 = -\eta_1 < 0$, then the energy of the bilayer sequence converges to a positive number. Indeed from Corollary 4.2, any codimension-one ℓ -bounded sequence that satisfies the enhanced tangential derivative bounds (42) or (66) has its energy bounded below by a positive lower bound, since $G_1(\Gamma, \tilde{u}^*) > 0$ for all $\tilde{u} \in \mathcal{S}(\Gamma, \ell)$ when $\eta_2 < -\eta_1$. The energy of the micelle based sequence $\{\tilde{w}_k\}$ has a negative limit, $-\alpha(1 - \frac{1}{n})\eta_1\sigma_n$ in space dimension $n \geq 2$. Conversely, if $\eta_2 > \frac{n}{n-2}\eta_1 > 0$, then the micelle sequence has a positive energy limit while the bilayer sequence has a negative energy limit if the curvatures of Γ are sufficiently small.

The attempt to obtain well defined lower bounds to free energy by restricting the support of u to lie in a thin codimension-one domain is frustrated by the fact that the FCH free energy supports higher codimensional structures that can be naturally embedded within a codimension one domain. However, we have shown that for sequences whose tangential variation is sufficiently tame and whose H^1 weak limits lie in $H^2(\Omega_1^\ell)$, then the possible limit set corresponds to N translates of a bilayer, with a corresponding limiting energy. It is natural to extend this analysis to restrict the support of u to lie in a thin neighborhood of a codimension- m domain, including codimension two filamentous pores in $\mathbb{R}^3$. It is also important to characterize defect structures such as triple junctions, and open edges.

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