

On the sharp interface limit of a phase field model for near spherical two phase biomembranes

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Abstract. We consider sharp interface asymptotics for a phase field model motivated by lipid raft formation on near spherical biomembranes involving a coupling between the local mean curvature and the local composition. A reduced diffuse interface energy depending only on the membrane composition is introduced and a Γ -limit is derived. It is shown that the Euler–Lagrange equations for the limiting functional and the sharp interface energy coincide. Finally, we consider a system of gradient flow equations with conserved Allen–Cahn dynamics for the phase field model. Performing a formal asymptotic analysis, we obtain a system of gradient flow equations for the sharp interface energy coupling geodesic curvature flow for the phase interface to a fourth order PDE free boundary problem for the surface deformation.

1. Introduction

Biological membranes are lipid bilayers which separate a cell’s interior from its exterior and often contain embedded molecules such as proteins. Biomembranes also exhibit fluid-like properties which enables the lateral transport of these molecules and can lead to the formation of intramembrane domains [6]. In this paper, we consider a mathematical model in which domains are one phase of a two phase biomembrane. Since the length scales of a biomembrane are much larger than its width, biomembranes are typically modelled by hypersurfaces and the introduction of surface energy functionals.

In [16] the first and second authors considered surfaces Γ_ρ of the form

$$\Gamma_\rho = \{x + \rho u(x)v(x) : x \in \Gamma\},$$

where Γ is a sphere of radius R . A surface of this type is a graph over the base surface Γ with unit normal v and described by a height function $u : \Gamma \rightarrow \mathbb{R}$ with small positive constant ρ . Domains on Γ_ρ are distinguished by the values ± 1 of an order parameter ϕ . Using the smallness assumption on ρ , the following perturbation of a Canham–Helfrich energy was derived in [16]:

$$\mathcal{E}_{DI}(u, \phi) = \int_{\Gamma} (e_m(\phi, u, \Delta_{\Gamma} u) + e_{DI}(\phi, \nabla_{\Gamma} \phi)) \, d\Gamma, \quad (1.1)$$

where an approximate membrane elastic energy, $e_m(\phi, u, \Delta_\Gamma u)$, and a diffuse interface energy, $e_{DI}(\phi, \nabla_\Gamma \phi)$, are given by

$$e_m(\phi, u, \Delta_\Gamma u) := \frac{\kappa}{2} \left(\left(\Delta_\Gamma u + \frac{2u}{R^2} + \Lambda \phi \right)^2 - \frac{u}{R^2} \left(\Delta_\Gamma u + \frac{2u}{R^2} \right) \right) + \frac{\sigma}{2} u \left(\Delta_\Gamma u + \frac{2u}{R^2} \right)$$

$$e_{DI}(\phi, \nabla_\Gamma \phi) := b \left(\frac{\varepsilon}{2} |\nabla_\Gamma \phi|^2 + \frac{1}{\varepsilon} W(\phi) \right).$$

Here, $W(\cdot)$ is a double well potential defined by $W(\phi) := \frac{1}{4}(\phi^2 - 1)^2$. The constant $\Lambda > 0$ couples the composition to the curvature. The constant $b > 0$ is a diffuse interface energy coefficient associated with the phase boundary separating the domains and $\varepsilon > 0$ is a small parameter commensurate with the width of a diffuse interface separating the two phases. As $\varepsilon \rightarrow 0$ then ϕ is forced to the roots of $W(\cdot)$ given by $\phi = \pm 1$ with these values corresponding to the two phases. The boundary between the domains is then the level set $\phi = 0$ on Γ .

In this paper, we wish to relate the diffuse interface energy (1.1) as $\varepsilon \rightarrow 0$ to the sharp interface energy

$$\mathcal{E}_{SI}(u, \gamma) = \int_\Gamma e_m(\chi_\gamma, u, \Delta_\Gamma u) \, d\Gamma + \int_\gamma \hat{b} \, d\gamma, \tag{1.2}$$

where the sphere Γ is decomposed into subsets $\Gamma^{(1)}$ and $\Gamma^{(2)}$ both with common boundary γ and

$$\chi_\gamma := \begin{cases} -1 & \text{on } \Gamma^{(1)}, \\ +1 & \text{on } \Gamma^{(2)}. \end{cases} \tag{1.3}$$

The line energy coefficient \hat{b} is scaled with the diffuse interface energy coefficient b and double well potential W so $\hat{b} = c_W b$, where

$$c_W := \int_{-1}^1 \sqrt{2W(s)} \, ds = \frac{2\sqrt{2}}{3}.$$

We relate the diffuse interface approach to the sharp interface approach in two ways.

(1) First, by calculating the Euler–Lagrange equations we express the height function u in terms of the functions ϕ and χ_γ for the diffuse and sharp interface energies respectively. By substituting these into our energies we eliminate u and obtain a reduced diffuse interface energy $\tilde{\mathcal{E}}_{DI}(\phi)$, and a reduced sharp interface energy $\tilde{\mathcal{E}}_{SI}(\gamma)$ in terms of only ϕ and χ_γ . We prove that a suitable minimisation problem of the energy (1.1) coincides with the associated minimisation problem of the reduced diffuse energy $\tilde{\mathcal{E}}_{DI}(\phi)$. A similar result is shown for the sharp interface energies. Returning to the reduced diffuse interface energy $\tilde{\mathcal{E}}_{DI}(\phi)$, we calculate its Γ -limit by showing it can be written as the Modica–Mortola functional plus a continuous perturbation. Finally, we show that if minimisers of the Γ -limit are regular enough, then they coincide with minimisers of the reduced sharp interface energy $\tilde{\mathcal{E}}_{SI}(\gamma)$.

(2) Secondly, since gradient flow methods are often used to numerically investigate critical points, we consider a gradient flow of (1.1) with conserved Allen–Cahn dynamics which was considered in [16]. Again, we apply a reduction method which enables us to write the fourth order equation for the height function as a second order equation, but at the cost that the reduced order equation contains a non-local operator. A formal asymptotic analysis of the limit $\varepsilon \rightarrow 0$ for more general surfaces was performed in [19], but only for the equilibrium equations. Here we perform it for the time-dependent problem and show how the non-local term which arises from this reduction method can be dealt with. We show that the resulting free boundary problem coincides with a corresponding conserved L^2 -gradient flow for the sharp interface energy (1.2).

1.1. Background

By applying a perturbation method introduced in [15] (see also [17]), it was shown that (1.1) approximates the following energy functional of Canham–Helfrich type [11,30]:

$$\mathcal{F}_{DI}(\Gamma, \phi) := \int_{\Gamma_\rho} \left(\frac{1}{2} \kappa (H - H_s(\phi))^2 + \sigma \right) d\Gamma_\rho + b \int_{\Gamma_\rho} \left(\frac{\varepsilon}{2} |\nabla_\Gamma \phi|^2 + \frac{1}{\varepsilon} W(\phi) \right) d\Gamma_\rho. \tag{1.4}$$

The first term in (1.4) is a Canham–Helfrich surface energy. Here H is the mean curvature of Γ_ρ . The parameter $\kappa > 0$ is a bending rigidity and $\sigma \geq 0$ is the surface tension. The membrane composition is given by the order parameter $\phi : \Gamma \rightarrow \mathbb{R}$. The function $H_s(\phi) \equiv \Lambda \phi$ is a composition-dependent spontaneous curvature in which the coefficient $\Lambda > 0$ couples the local order parameter, ϕ , to the local membrane curvature. Note that in the surface energy we have omitted $\kappa_G K$, where K is the Gauss curvature and κ_G is a bending rigidity constant. This is valid when considering hypersurfaces of constant genus. The energy functional (1.4) is a phase field approximation of the sharp interface elastic energy first introduced by Jülicher and Lipowsky [34,35], given by

$$\mathcal{F}_{SI}(\Gamma, \gamma) := \int_{\Gamma^{(1)} \cup \Gamma^{(2)}} \left(\frac{1}{2} \kappa (H - H_s^i)^2 + \sigma \right) d\Gamma + \int_\gamma \hat{b} \, d\gamma \tag{1.5}$$

for hypersurfaces $\Gamma = \Gamma^{(1)} \cup \gamma \cup \Gamma^{(2)}$. For the axisymmetric case, a minimisation problem has been addressed [12] and numerical simulations explored [25]. In the non-axisymmetric case, very little has been rigorously proven, although Brazda et al. have recently dealt with the minimisation problem in the weaker setting of oriented curvature varifolds [10] and computations for a gradient flow dynamics are presented in [5]. Analogous to the diffuse interface approach, the same perturbation method could be applied to (1.5) to obtain (1.2).

The coupling of the elastic energy to a composition field was first considered by Leibler in [36]. More recently, it has been considered using computational and formal asymptotic perspectives [18–20], applying a bifurcation analysis [29], addressing non-equilibrium properties such as dissipation effects [46], and calculating the Γ -limit in the axisymmetric case [31–33]. Note that this last example differs from our work since the

biomembranes are only assumed to be C^0 , which allows for kinks across the interface between domains.

Our work here extends that of Ren and Wei in [40], who determine the Γ -limit in the approximately planar case, although they limit themselves to only considering a one-dimensional problem. This differs from our work which is for two-dimensional approximately spherical surfaces. Our work also differs from that of Fonseca et al. in [22], who focus on surface tension effects and consider Γ -convergence of an approximately planar surface but for a different parameter regime.

Remark 1.1. Examples of phase domains are lipid rafts. These are small (10–200nm), heterogeneous domains which compartmentalise cellular processes and are enriched with various molecules such as cholesterol and sphingolipids, and which can form larger platforms through protein-protein and protein-lipid interactions [38]. They were first introduced by Simons in [45], and have since received large academic interest. For example, see [13, 27, 42, 43] and their references. For technical reasons, direct microscopic detection of lipid rafts has not been possible. However, domain formation has been observed on large artificial membranes for which the curvature of the membrane plays an important role [7, 39]. Numerical simulations [16] of the model considered in this paper display domain formation similar to those occurring in experiments [7].

1.2. Outline

The outline for the rest of this paper is as follows: In Section 2 we briefly cover some notation and preliminaries needed for this paper. In Section 3 we derive the reduced diffuse interface energy $\tilde{\mathcal{E}}_{DI}(\phi)$ and calculate its Γ -limit. We then state regularity results for minimisers of the Γ -limit. In Section 4 we calculate the Euler–Lagrange equations for the sharp interface energy, and use these to obtain the reduced sharp interface energy $\tilde{\mathcal{E}}_{SI}(\gamma)$ which coincides with the Γ -limit obtained in Section 3 for suitably regular solutions. In Section 5 we perform the formal asymptotic analysis for the diffuse interface gradient flow equations and show the resulting free boundary problems coincides with the corresponding sharp interface gradient flow equations. Finally, in Section 6 we finish with some concluding remarks.

2. Notation and preliminaries

Here, we outline some important calculus results for stationary and evolving surfaces. For a thorough treatment of the material covered here we refer the reader to [14].

Although throughout the paper Γ is the sphere with radius R , in this section, we present some notation for general oriented two-dimensional hypersurfaces Γ that are smooth with smooth boundary (unless stated otherwise). Suppose $x \in \Gamma$ and U is an open subset containing x . Then given a function $u \in C^1(U)$, we define the surface gradient

$\nabla_\Gamma u(x)$ of u at x by

$$\nabla_\Gamma u(x) = \nabla u(x) - (\nabla u(x) \cdot \nu(x))\nu(x),$$

where ν is a smooth unit normal field to Γ . Note that this derivative depends only on the values of u on Γ . Denoting its components by

$$\nabla_\Gamma u = (\underline{D}_1 u, \underline{D}_2 u, \underline{D}_3 u),$$

we can also define the Laplace–Beltrami operator of u at x by

$$\Delta_\Gamma u(x) = \sum_{i=1}^3 \underline{D}_i \underline{D}_i u(x),$$

provided that $u \in C^2(U)$. We define the Lebesgue space $L^p(\Gamma)$ for $p \in [1, \infty)$ to be the space of functions which are measurable with respect to the surface measure $d\Gamma$ and have finite norm

$$\|u\|_{L^p(\Gamma)} = \left(\int_\Gamma |u|^p d\Gamma \right)^{\frac{1}{p}}.$$

We say a function $u \in L^1(\Gamma)$ has the weak derivative $v_i = \underline{D}_i u$ if for every function $\phi \in C_0^1(\Gamma)$ we have the relation

$$\int_\Gamma u \underline{D}_i \phi d\Gamma = - \int_\Gamma \phi v_i d\Gamma + \int_\Gamma u \phi H \nu_i d\Gamma,$$

where H is the mean curvature of Γ .

We define the Sobolev space $W^{1,p}(\Gamma)$ and Hilbert spaces $H^1(\Gamma)$ and $H^2(\Gamma)$ by

$$W^{1,p}(\Gamma) := \{f \in L^p(\Gamma) : f \text{ has weak derivatives } \underline{D}_i f \in L^p(\Gamma), i \in \{1, 2, 3\}\},$$

$$H^1(\Gamma) := \{f \in L^2(\Gamma) : f \text{ has weak derivatives } \underline{D}_i f \in L^2(\Gamma), i \in \{1, 2, 3\}\},$$

$$H^2(\Gamma) := \{f \in H^1(\Gamma) : f \text{ has weak derivatives } \underline{D}_i \underline{D}_j f \in L^2(\Gamma), i, j \in \{1, 2, 3\}\}.$$

In addition, we say a function $f \in L^1(\Gamma)$ has bounded variation and write $f \in BV(\Gamma)$ if

$$|Df|(\Gamma) := \sup_{\eta \in C_c^1(\Gamma; \mathbb{R}^3)} \left\{ \int_\Gamma f \nabla_\Gamma \cdot \eta d\Gamma : |\eta| \leq 1 \right\} < \infty.$$

Here, $|Df|(\Gamma)$ is known as the total variation of f . We will denote by $BV(\Gamma; \{-1, 1\})$ functions of bounded variation on Γ which only takes values ± 1 .

Integration by parts on bounded C^2 -hypersurfaces reads as

$$\begin{aligned} \int_\Gamma \nabla_\Gamma \cdot f d\Gamma &= \int_\Gamma f \cdot H \nu d\Gamma + \int_{\partial\Gamma} f \cdot \nu_{\partial\Gamma} d(\partial\Gamma), \\ \int_\Gamma \nabla_\Gamma \eta \cdot \nabla_\Gamma v d\Gamma &= - \int_\Gamma \eta \Delta_\Gamma v d\Gamma + \int_{\partial\Gamma} \eta \nabla_\Gamma v \cdot \nu_{\partial\Gamma} d(\partial\Gamma) \end{aligned}$$

for $f \in W^{1,1}(\Gamma, \mathbb{R}^3)$, $\eta \in H^1(\Gamma)$, $v \in H^2(\Gamma)$ and where $\nu_{\partial\Gamma}$ denotes the conormal to γ ; see [14, Theorems 2.10 and 2.14].

3. Diffuse interface energy minimisation

3.1. Diffuse interface minimisers

Recall that Γ is the sphere of radius R and consider the diffuse interface energy $\mathcal{E}_{DI}(u, \phi)$ as given in (1.1) for $u \in H^2(\Gamma)$, $\phi \in H^1(\Gamma)$ and equal to $+\infty$ if $u \in L^2(\Gamma) \setminus H^2(\Gamma)$ or $\phi \in L^1(\Gamma) \setminus H^1(\Gamma)$.

For $(u, \phi) \in H^2(\Gamma) \times H^1(\Gamma)$, consider the constraints $(f_\Gamma := \frac{1}{|\Gamma|} \int_\Gamma$

$$\int_\Gamma \phi \, d\Gamma = \alpha, \quad \int_\Gamma u \, d\Gamma = 0, \quad \int_\Gamma v_i u \, d\Gamma = 0 \quad \text{for } i \in \{1, 2, 3\}. \quad (3.1)$$

Here, $\alpha \in [-1, 1]$ and v_i for $i \in \{1, 2, 3\}$ are the three components of the normal $\nu(x) = x/|x|$ at $x \in \Gamma$. We define the space \mathcal{K}_{DI} as

$$\mathcal{K}_{DI} := \{(u, \phi) \in H^2(\Gamma) \times H^1(\Gamma) : (u, \phi) \text{ satisfy (3.1)}\}.$$

The diffuse interface minimisation problem is

Problem 3.1. Find $(u^*, \phi^*) \in \mathcal{K}_{DI}$ such that

$$\mathcal{E}_{DI}(u^*, \phi^*) = \inf_{(u, \phi) \in \mathcal{K}_{DI}} \mathcal{E}_{DI}(u, \phi).$$

The first condition of (3.1) corresponds to a conservation of mass constraint on the order parameter ϕ , the second condition is a volume constraint and relates to impermeability of the membrane, and the third condition is a nullspace constraint related to a translation invariance property of the membrane energy. The functional is coercive over this set, see [16], so there exist minimisers. Proceeding as in [16], we may calculate the first variation of (1.1) to be

$$\begin{aligned} \langle \mathcal{E}'_{DI}(u, \phi), (\zeta, \eta) \rangle &= \int_\Gamma \left(\kappa \Delta_\Gamma u \Delta_\Gamma \zeta + \left(\sigma - \frac{2\kappa}{R^2} \right) \nabla_\Gamma u \cdot \nabla_\Gamma \zeta - \frac{2\sigma}{R^2} u \zeta + \kappa \Lambda \phi \Delta_\Gamma \zeta \right. \\ &\quad + \frac{2\kappa \Lambda}{R^2} \phi \zeta \kappa \Lambda \Delta_\Gamma u \eta + \frac{2\kappa \Lambda}{R^2} u \eta + \kappa \Lambda^2 \phi \eta + b \varepsilon \nabla_\Gamma \phi \cdot \nabla_\Gamma \eta \\ &\quad \left. + \frac{b}{\varepsilon} W'(\phi) \eta \right) d\Gamma \end{aligned}$$

for all $\zeta \in H^2(\Gamma)$ and for all $\eta \in H^1(\Gamma)$ such that the variations of the constraints (3.1) vanish, so we have

$$\int_\Gamma \eta \, d\Gamma = 0, \quad \int_\Gamma \zeta \, d\Gamma = 0, \quad \int_\Gamma v_i \zeta \, d\Gamma = 0 \quad \text{for } i \in \{1, 2, 3\}.$$

For further details see [16, Section 4.1]. The Lagrange multipliers corresponding to the constraints for the constrained optimisation problem, Problem 3.1, may be determined

easily and we obtain the following form of Euler–Lagrange equations:

$$\frac{\widehat{b}}{\varepsilon} \left(W'(\phi^*) - \int_{\Gamma} W'(\phi^*) \, d\Gamma \right) - \widehat{b} \varepsilon \Delta_{\Gamma} \phi^* + \kappa \Lambda \Delta_{\Gamma} u^* + \frac{2\kappa \Lambda}{R^2} u^* + \kappa \Lambda^2 (\phi^* - \alpha) = 0, \tag{3.2}$$

$$\left(\Delta_{\Gamma} + \frac{2}{R^2} \right) (\kappa \Delta_{\Gamma} u^* - \sigma u^* + \kappa \Lambda (\phi^* - \alpha)) = 0. \tag{3.3}$$

3.2. Reduced diffuse interface energy

The Euler–Lagrange equation (3.3) motivates seeking a reduced order PDE. We begin by noting that if

$$-\Delta_{\Gamma} z - \frac{2}{R^2} z = 0,$$

then z is an eigenfunction of $-\Delta_{\Gamma}$ with eigenvalue $\frac{2}{R^2}$. Such eigenfunctions z belong to the space $\text{span}\{v_1, v_2, v_3\}$ (see [15]). It is convenient to work with the $L^2(\Gamma)$ -orthogonal complement of $\text{span}\{1, v_1, v_2, v_3\}$ and we set

$$S := \text{span}\{1, v_1, v_2, v_3\}^{\perp}.$$

Note that if $\eta \in S \cap H^2(\Gamma)$, then, since v_i are eigenfunctions of $-\Delta_{\Gamma}$, a short calculation shows that $\Delta_{\Gamma} \eta \in S$. Also, it is convenient to define an operator $\mathcal{G} : S \rightarrow H^2(\Gamma) \cap S$ where for each $\eta \in S$, $\mathcal{G}(\eta)$ is the unique function in $H^2(\Gamma) \cap S$ satisfying

$$(\sigma - \kappa \Delta_{\Gamma}) \mathcal{G}(\eta) = \kappa \Lambda \eta. \tag{3.4}$$

Let (u^*, ϕ^*) be a diffuse interface energy minimiser. It follows from (3.3) that

$$-\kappa \Delta_{\Gamma} u^* + \sigma u^* - \kappa \Lambda (\phi^* - \alpha) \in \text{span}\{v_1, v_2, v_3\},$$

so we may write

$$-\kappa \Delta_{\Gamma} u^* + \sigma u^* = \kappa \Lambda ((\phi^* - \alpha) - \beta_{DI}) \quad \text{on } \Gamma, \tag{3.5}$$

where $\beta_{DI} \in \text{span}\{v_1, v_2, v_3\}$. Denoting by $\mathbf{P} : L^2(\Gamma) \rightarrow S$ the orthogonal projection onto S , we find after applying it to (3.5)

$$(\sigma - \kappa \Delta_{\Gamma}) u^* = \kappa \Lambda \mathbf{P}(\phi^*), \tag{3.6}$$

so

$$u^* = \mathcal{G}(\mathbf{P}(\phi^*)). \tag{3.7}$$

This motivates defining the *reduced diffuse interface energy*, $\widetilde{\mathcal{E}}_{DI}(\phi)$,

$$\begin{aligned} \widetilde{\mathcal{E}}_{DI}(\phi) &:= \mathcal{E}_{DI}(\mathcal{G}(\mathbf{P}(\phi)), \phi) \\ &= \int_{\Gamma} \left(\frac{\kappa}{2} \left(\Delta_{\Gamma} \mathcal{G}(\mathbf{P}(\phi)) + \frac{2\mathcal{G}(\mathbf{P}(\phi))}{R^2} + \Lambda \phi \right)^2 \right. \\ &\quad \left. - \left(\frac{\kappa}{R^2} + \frac{\sigma}{2} \right) \mathcal{G}(\mathbf{P}(\phi)) \left(\Delta_{\Gamma} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\phi)) + \frac{b\varepsilon}{2} |\nabla_{\Gamma} \phi|^2 + \frac{b}{\varepsilon} W(\phi) \right) \, d\Gamma \end{aligned}$$

$$\begin{aligned}
 &= \int_{\Gamma} \left(\frac{\kappa}{2} \left(\Delta_{\Gamma} - \frac{\sigma}{\kappa} \right) \mathcal{G}(\mathbf{P}(\phi)) \left(\Delta_{\Gamma} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\phi)) + \frac{\kappa \Lambda^2 \phi^2}{2} \right. \\
 &\quad \left. + \kappa \Lambda \phi \left(\Delta_{\Gamma} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\phi)) + \frac{b\varepsilon}{2} |\nabla_{\Gamma} \phi|^2 + \frac{b}{\varepsilon} W(\phi) \right) d\Gamma, \tag{3.8}
 \end{aligned}$$

and the admissible set

$$\tilde{\mathcal{K}}_{DI} := \left\{ \phi \in H^1(\Gamma) : \int_{\Gamma} \phi \, d\Gamma = \alpha \right\}.$$

Using (3.6) and that $(\Delta_{\Gamma} + \frac{2}{R^2})\mathcal{G}(\mathbf{P}(\phi)) \in S$, we can simplify (3.8) to obtain that

$$\tilde{\mathcal{E}}_{DI}(\phi) = \int_{\Gamma} \left(\frac{\kappa \Lambda}{2} \mathbf{P}(\phi) \left(\Delta_{\Gamma} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\phi)) + \frac{b\varepsilon}{2} |\nabla_{\Gamma} \phi|^2 + \frac{b}{\varepsilon} W(\phi) + \frac{\kappa \Lambda^2 \phi^2}{2} \right) d\Gamma. \tag{3.9}$$

We write the constrained minimisation problem for the reduced energy below.

Problem 3.2. Find $\tilde{\phi}^* \in \tilde{\mathcal{K}}_{DI}$ such that

$$\tilde{\mathcal{E}}_{DI}(\tilde{\phi}^*) = \inf_{\phi \in \tilde{\mathcal{K}}_{DI}} \tilde{\mathcal{E}}_{DI}(\phi).$$

Finding a minimiser of Problem 3.2 is equivalent to finding a minimiser of Problem 3.1, since

$$\begin{aligned}
 \mathcal{E}_{DI}(u^*, \phi^*) &\leq \mathcal{E}_{DI}(\mathcal{G}(\mathbf{P}(\tilde{\phi}^*)), \tilde{\phi}^*) = \tilde{\mathcal{E}}_{DI}(\tilde{\phi}^*) \leq \tilde{\mathcal{E}}_{DI}(\phi^*) \\
 &= \mathcal{E}_{DI}(\mathcal{G}(\mathbf{P}(\phi^*)), \phi^*) = \mathcal{E}_{DI}(u^*, \phi^*). \tag{3.10}
 \end{aligned}$$

3.3. Γ -convergence

We will now calculate the Γ -limit of Problem 3.2 as $\varepsilon \rightarrow 0$. First we decompose the energy (3.9) and write

$$\tilde{\mathcal{E}}_{DI}(\phi) = \mathcal{J}_{\varepsilon}(\phi) + \mathcal{K}(\phi),$$

where $\mathcal{J}_{\varepsilon}(\phi)$ contains the local, ε -dependent part of the energy and $\mathcal{K}(\phi)$ is a non-local, ε -independent perturbation, given by

$$\begin{aligned}
 \mathcal{J}_{\varepsilon}(\phi) &:= \begin{cases} \int_{\Gamma} \frac{b\varepsilon}{2} |\nabla_{\Gamma} \phi|^2 + \frac{b}{\varepsilon} W(\phi) \, d\Gamma & \text{for } \phi \in H^1(\Gamma), \\ +\infty & \text{for } \phi \in L^1(\Gamma) \setminus H^1(\Gamma) \end{cases} \\
 \mathcal{K}(\phi) &:= \begin{cases} \int_{\Gamma} \frac{\kappa \Lambda}{2} \mathbf{P}(\phi) \left(\Delta_{\Gamma} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\phi)) + \frac{\kappa \Lambda^2 \phi^2}{2} \, d\Gamma & \text{for } \phi \in L^2(\Gamma), \\ +\infty & \text{for } \phi \in L^1(\Gamma) \setminus L^2(\Gamma). \end{cases} \tag{3.11}
 \end{aligned}$$

To calculate the Γ -limit we reformulate (3.11). Since

$$\begin{aligned}
 \left(\Delta_{\Gamma} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\phi)) &= \left(\left(\frac{\sigma}{\kappa} + \frac{2}{R^2} \right) - \left(-\Delta_{\Gamma} + \frac{\sigma}{\kappa} \right) \right) \mathcal{G}(\mathbf{P}(\phi)) \\
 &= \left(\frac{\sigma}{\kappa} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\phi)) - \Lambda \mathbf{P}(\phi),
 \end{aligned}$$

it follows that

$$\mathcal{K}(\phi) = \begin{cases} \int_{\Gamma} \frac{\kappa\Lambda}{2} \mathbf{P}(\phi) \left(\frac{\sigma}{\kappa} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\phi)) \\ \quad + \frac{\kappa\Lambda^2}{2} (\phi^2 - (\mathbf{P}(\phi))^2) \, d\Gamma & \text{for } \phi \in L^2(\Gamma), \\ +\infty & \text{for } \phi \in L^1(\Gamma) \setminus L^2(\Gamma). \end{cases} \tag{3.12}$$

It is straightforward to show the following proposition giving the Γ -limit:

Proposition 3.3. *The Γ -limit of $\tilde{\mathcal{E}}_{DI}(\phi) = \mathcal{J}_\varepsilon(\phi) + \mathcal{K}(\phi)$ is given by*

$$\tilde{\mathcal{E}}_0(\phi) := \mathcal{J}_0(\phi) + \mathcal{K}(\phi) \tag{3.13}$$

where

$$\mathcal{J}_0(\phi) = \begin{cases} \frac{\hat{b}}{2} |D\phi|(\Gamma) & \text{for } \phi \in BV(\Gamma; \{-1, 1\}), \\ +\infty & \text{for } \phi \in L^1(\Gamma) \setminus BV(\Gamma; \{-1, 1\}), \end{cases}$$

with $\hat{b} = bc_W$ and $c_W = \int_{-1}^1 \sqrt{2W(s)} \, ds = \frac{2\sqrt{2}}{3}$.

Proof. It is known (for example, see [3, 23, 37]) that $\mathcal{J}_\varepsilon(\phi)$ Γ -converges to the functional $\mathcal{J}_0(\phi)$. Furthermore, by considering (3.12) and using elliptic regularity, it follows that \mathcal{K} is a continuous functional. Γ -convergence is stable under continuous perturbations [9, Remark 1.7]. Therefore $\mathcal{J}_\varepsilon + \mathcal{K}$ Γ -converges to $\mathcal{J}_0 + \mathcal{K}$ as $\varepsilon \rightarrow 0$. ■

The Γ -limit problem is:

Problem 3.4. Find $\phi^* \in \mathcal{D} := \{\eta \in BV(\Gamma; \{-1, 1\}) : \int_{\Gamma} \eta \, d\Gamma = \alpha\}$ such that

$$\tilde{\mathcal{E}}_0(\phi^*) = \inf_{\phi \in \mathcal{D}} \tilde{\mathcal{E}}_0(\phi).$$

Remark 3.5. Suppose that the solution ϕ^* of Problem 3.4 is such that the sets $\Gamma^{(1)} := \{\phi^* = -1\}$ and $\Gamma^{(2)} := \{\phi^* = +1\}$ have a smooth common boundary. Denoting this boundary by γ^* and using the definition (1.3), we thus have that $\phi^* = \chi_{\gamma^*}$. It is well known that

$$\mathcal{J}_0(\phi^*) = \mathcal{J}_0(\chi_{\gamma^*}) = \int_{\gamma^*} \hat{b} \, d\gamma^*,$$

so that

$$\tilde{\mathcal{E}}_0(\phi^*) = \mathcal{K}(\chi_{\gamma^*}) + \int_{\gamma^*} \hat{b} \, d\gamma^*. \tag{3.14}$$

4. Sharp interface optimisation problem

The objective of this section is to derive the Euler–Lagrange equations of the sharp interface energy functional $\mathcal{E}_{SI}(u, \gamma)$ defined in (1.2). Using these to eliminate the membrane height, a reduced energy functional is derived. This is then shown to coincide with the Γ -limit of the reduced diffuse interface energy derived in the previous section.

4.1. Minimisation problem

We define \mathcal{K}_{SI} to be the set of all pairs (u, γ) satisfying

- $u : \Gamma \rightarrow \mathbb{R}$ is a height function such that $u \in H^2(\Gamma)$,
- Γ is decomposed as $\Gamma = \Gamma^{(1)} \cup \gamma \cup \Gamma^{(2)}$, where γ consists of finitely many, C^1 closed curves and is the common boundary of hypersurfaces $\Gamma^{(1)}$ and $\Gamma^{(2)}$,

and such that (γ, u) satisfy the constraints,

$$C_1(\gamma) := |\Gamma^{(1)}| - |\Gamma^{(2)}| + \alpha|\Gamma| = 0, \tag{4.1}$$

$$C_2(u) := \int_{\Gamma} u = 0, \tag{4.2}$$

$$\mathcal{N}_i(u) := \int_{\Gamma} u v_i = 0, \quad \text{for } i \in \{1, 2, 3\}. \tag{4.3}$$

These constraints correspond to (3.1) for the diffuse interface approach.

We will use the notation of an upper index of the form $(\cdot)^{(1)}$ or $(\cdot)^{(2)}$ to indicate the limit of quantities on γ approached from either $\Gamma^{(1)}$ or $\Gamma^{(2)}$, and use the notation $[\cdot]_{(1)}^{(2)} = (\cdot)^{(2)} - (\cdot)^{(1)}$ for the jump of a quantity across γ . We define $\nu_{\Gamma^{(i)}}$ to be the unit conormal, tangential to $\Gamma^{(i)}$, normal to γ and pointing out of $\Gamma^{(i)}$. Since Γ is C^1 , we may introduce μ so that

$$\mu := \nu_{\Gamma^{(1)}} = -\nu_{\Gamma^{(2)}}.$$

Furthermore, using that $H^2(\Gamma) \hookrightarrow C^0(\Gamma)$, we have that

$$[u]_{(1)}^{(2)} = 0 \quad \text{on } \gamma.$$

In addition, since $u \in H^2(\Gamma)$, trace values of the first weak derivatives exist on γ for the domains $\Gamma^{(1)}$ and $\Gamma^{(2)}$, and these trace values coincide (see [2, Lemma A8.9]). Therefore, we also have that

$$[\nabla_{\Gamma} u \cdot \mu]_{(1)}^{(2)} = 0 \quad \text{a.e. on } \gamma.$$

Problem 4.1 (Sharp interface minimisation problem). Find $(u^*, \gamma^*) \in \mathcal{K}_{SI}$ such that

$$\mathcal{E}_{SI}(u^*, \gamma^*) = \inf_{(u, \gamma) \in \mathcal{K}_{SI}} \mathcal{E}_{SI}(u, \gamma).$$

Minimisers in \mathcal{K}_{SI} of \mathcal{E}_{SI} are critical points of the following Lagrangian \mathcal{L}_{SI} :

Definition 4.2. We define the sharp interface Lagrangian by

$$\mathcal{L}_{SI}(u, \gamma, \lambda) := \mathcal{E}_{SI}(u, \gamma) + \lambda_1 C_1(\gamma) + \lambda_2 C_2(u) + \sum_{i=1}^3 \lambda_{i+2} \mathcal{N}_i(u)$$

for $\gamma \in C^1$ an embedded curve on Γ , $u \in H^2(\Gamma)$, and $\lambda \in \mathbb{R}^5$.

In Sections 4.2 and 4.3 which follow, we will define and calculate the first variation of the sharp interface energy and the constraint functionals. Using the function χ_γ defined in (1.3), and the geodesic curvature H_γ defined by $H_\gamma = h \cdot \mu$ for curvature vector h , we derive the following result:

Proposition 4.3. *A pair $(u^*, \gamma^*) \in \mathcal{K}_{SI}$ which minimises the sharp interface energy subject to the constraints (4.1)–(4.3), and is sufficiently regular so that all the following terms are well defined, solves the free boundary problem*

$$\left(\Delta_\Gamma + \frac{2}{R^2}\right)(\kappa \Delta_\Gamma u^* - \sigma u^* + \kappa \Lambda (\chi_{\gamma^*} - \alpha)) = 0 \quad \text{on } \Gamma^{(1)} \cup \Gamma^{(2)}, \quad (4.4)$$

$$\begin{aligned} & \widehat{b} H_{\gamma^*} - \kappa \Lambda \left[\chi_{\gamma^*} \left(\Delta_\Gamma u^* + \frac{2}{R^2} u^* \right) \right]_{(1)}^{(2)} \\ & = + \int_{\gamma^*} \left(\widehat{b} H_{\gamma^*} - \kappa \Lambda \left[\chi_{\gamma^*} \left(\Delta_\Gamma u^* + \frac{2}{R^2} u^* \right) \right]_{(1)}^{(2)} \right) d\gamma^* \quad \text{on } \gamma^*, \end{aligned} \quad (4.5)$$

with jump conditions

$$[\nabla_\Gamma \Delta_\Gamma u^* \cdot \mu]_{(1)}^{(2)} = 0, \quad [\Delta_\Gamma u^*]_{(1)}^{(2)} = -2\Lambda \quad \text{on } \gamma^*. \quad (4.6)$$

Remark 4.4. We note that equations (4.4) and (4.6) are order $\mathcal{O}(\rho)$ approximations and (4.5) is an order $\mathcal{O}(\rho^2)$ approximation of the sharp interface equilibrium equations given in [19, Problem 3.10]. In this case, the Lagrange multiplier λ_A for the area constraint is interpreted as the surface tension σ .

4.2. Variation of the membrane height

As a first step to prove Proposition 4.3, we consider the variation with respect to u in the direction $\zeta \in H^2(\Gamma)$ whilst keeping γ fixed. It is defined in the usual sense and is fairly straightforward to compute. For the constraints (4.2) and (4.3), we obtain that

$$\begin{aligned} \langle C'_2(u), (\zeta) \rangle &= \int_\Gamma \zeta d\Gamma, \\ \langle \mathcal{N}'_i(u), (\zeta) \rangle &= \int_\Gamma \zeta v_i d\Gamma, \quad \text{for } i \in \{1, 2, 3\}, \end{aligned}$$

whilst for the sharp interface energy we have

$$\begin{aligned} \langle \mathcal{E}'_{SI}(u, \gamma), (\zeta, 0) \rangle &= \int_\Gamma \left(\kappa \Delta_\Gamma u \Delta_\Gamma \zeta + \left(\sigma - \frac{2\kappa}{R^2} \right) \nabla_\Gamma u \cdot \nabla_\Gamma \zeta \right. \\ & \quad \left. - \frac{2\sigma}{R^2} u \zeta + \kappa \Lambda \chi_\gamma \Delta_\Gamma \zeta + \frac{2\kappa \Lambda}{R^2} \chi_\gamma \zeta \right) d\Gamma. \end{aligned}$$

Let $(u^*, \gamma^*, \lambda^*)$ be a critical point of the Lagrangian \mathcal{L}_{SI} which is sufficiently smooth and such that all terms are well defined for the remainder of this subsection. The vanishing

of the first variation of the Lagrangian yields the variational equation

$$\int_{\Gamma} \left(\kappa \Delta_{\Gamma} u^* \Delta_{\Gamma} \zeta + \left(\sigma - \frac{2\kappa}{R^2} \right) \nabla_{\Gamma} u^* \cdot \nabla_{\Gamma} \zeta - \frac{2\sigma}{R^2} u^* \zeta + \kappa \Lambda \chi_{\gamma^*} \Delta_{\Gamma} \zeta + \frac{2\kappa \Lambda}{R^2} \chi_{\gamma^*} \zeta \right) d\Gamma + \int_{\Gamma} \left(\lambda_2^* \zeta + \sum_{i=1}^3 \lambda_{i+2}^* v_i \zeta \right) d\Gamma = 0, \quad \forall \zeta \in H^2(\Gamma). \tag{4.7}$$

By testing with $\zeta = 1$ and using that (u^*, γ^*) satisfies (4.2), we obtain that

$$\lambda_2^* = \frac{2\kappa \Lambda}{R^2} \frac{|\Gamma^{(1)}| - |\Gamma^{(2)}|}{|\Gamma|} = -\frac{2\kappa \Lambda \alpha}{R^2}.$$

By testing with $\zeta = v_i$ and using that (u^*, γ^*) satisfies (4.3), we find that

$$\lambda_3^* = \lambda_4^* = \lambda_5^* = 0,$$

where we have used that $-\Delta_{\Gamma} v_i = \frac{2}{R^2} v_i$ (see [15]). Integrating (4.7) by parts we calculate that

$$\begin{aligned} 0 &= \int_{\Gamma^{(1)}} \left(\left(\Delta_{\Gamma} + \frac{2}{R^2} \right) (\kappa \Delta_{\Gamma} u^* - \sigma u^* + \kappa \Lambda (-1 - \alpha)) \right) \zeta d\Gamma^{(1)} \\ &\quad + \int_{\Gamma^{(2)}} \left(\left(\Delta_{\Gamma} + \frac{2}{R^2} \right) (\kappa \Delta_{\Gamma} u^* - \sigma u^* + \kappa \Lambda (1 - \alpha)) \right) \zeta d\Gamma^{(2)} \\ &\quad - \int_{\gamma} \kappa (\Delta_{\Gamma} u^{*(2)} - \Delta_{\Gamma} u^{*(1)} + 2\Lambda) \nabla_{\Gamma} \zeta \cdot \mu \\ &\quad - (\nabla_{\Gamma} \Delta_{\Gamma} u^{*(2)} - \nabla_{\Gamma} \Delta_{\Gamma} u^{*(1)}) \cdot \mu \zeta d\gamma, \end{aligned}$$

for all $\zeta \in H^2(\Gamma)$. This proves (4.4) and (4.6) from Proposition 4.3.

4.3. Variation of the interface

The second step to prove Proposition 4.3 is to calculate the first variation of the Lagrangian \mathcal{L}_{SI} with respect to γ . This variation is defined by the instantaneous change of the energy due to the deformation of the interface between rafts and non-rafts regions.

Given any smooth tangential vector field $v : \Gamma \rightarrow \mathbb{R}^3$, let $x(\tau)$ be the solution to $x'(\tau) = v(x(\tau))$ and let

$$\begin{aligned} \Gamma^{(i)}(\tau) &= \{x(\tau) \mid x(0) \in \Gamma^{(i)}\}, \quad i = 1, 2, \\ \gamma(\tau) &= \{x(\tau) \mid x(0) \in \gamma\}. \end{aligned}$$

Thanks to the smoothness of v , for all τ close to 0 an admissible two phase surface $\Gamma = \Gamma^{(1)}(\tau) \cup \gamma(\tau) \cup \Gamma^{(2)}(\tau)$ is obtained in the sense that $(u, \gamma(\tau)) \in \mathcal{K}_{SI}$. The variation of the Lagrangian is defined as

$$\langle \mathcal{L}'_{SI}(u, \gamma, \lambda), (0, v, 0) \rangle = \left. \frac{d}{d\tau} \mathcal{L}_{SI}(u, \gamma(\tau), \lambda) \right|_{\tau=0}.$$

Regarding derivatives of τ -dependent domains, we note the following identities that are, for instance, proved in [14, Theorem 5.1]: For any smooth function $f : \Gamma \rightarrow \mathbb{R}$,

$$\frac{d}{d\tau} \int_{\Gamma^{(i)}(\tau)} f \, d\Gamma^{(i)}(\tau) = \int_{\gamma(\tau)} f v \cdot v^{(i)} \, d\gamma(\tau), \quad i = 1, 2,$$

and moreover,

$$\frac{d}{d\tau} \int_{\gamma(\tau)} 1 \, d\gamma(\tau) = \int_{\gamma(\tau)} H_\gamma v \cdot \mu \, d\gamma(\tau).$$

Using these identities the variation of the sharp interface energy can be calculated, which yields

$$\langle \mathcal{E}'_{SI}(u, \gamma), (0, v) \rangle = \int_\gamma \left[\widehat{b} H_\gamma - \kappa \Lambda \left(\Delta_\Gamma u^{(2)} + \Delta_\Gamma u^{(1)} + \frac{4u}{R^2} \right) \right] v \cdot \mu \, d\gamma.$$

For the constraint functional (4.1) we obtain that

$$\langle C'_1(\gamma), v \rangle = 2 \int_\gamma v \cdot \mu \, d\gamma.$$

If $(u^*, \gamma^*, \lambda^*)$ is a critical point of the Lagrangian \mathcal{L}_{SI} , then

$$0 = \langle \mathcal{L}'_{SI}(u^*, \gamma^*, \lambda^*), (0, v, 0) \rangle = \langle \mathcal{E}'_{SI}(u^*, \gamma^*), (0, v) \rangle + \lambda_1^* \langle C'_1(\gamma^*), v \rangle$$

for all smooth tangential vector fields v on Γ . We find that

$$2\lambda_1^* = \int_{\gamma^*} \left(\left(\widehat{b} H_{\gamma^*} - \frac{4\kappa \Lambda u^*}{R^2} - \kappa \Lambda \right) \Delta_\Gamma u^{*(1)} + \Delta_\Gamma u^{*(2)} \right) d\gamma^*,$$

and hence obtain (4.5). This completes the proof of Proposition 4.3.

4.4. Reduced sharp interface energy

Analogously to Section 3.2, we introduce a reduced sharp interface energy. By using the Euler–Lagrange equation (4.4), that $BV(\Gamma) \hookrightarrow L^2(\Gamma)$ ([4, Corollary 3.49]), and repeating the argument of Section 3.2 we find that

$$u^* = \mathcal{G}(\mathbf{P}(\chi_{\gamma^*})). \tag{4.8}$$

Here, \mathcal{G} is the Green’s function defined in (3.4) and \mathbf{P} is the L^2 -projection onto $\text{span}\{1, v_1, v_2, v_3\}^\perp$.

By elliptic regularity, we obtain that $\mathcal{G}(\mathbf{P}(\chi_{\gamma^*})) \in H^2(\Gamma)$, and hence obtain that $(\gamma^*, \mathcal{G}(\mathbf{P}(\chi_{\gamma^*}))) \in \mathcal{K}_{SI}$.

Using (4.8) we define the *reduced sharp interface energy*,

$$\tilde{\mathcal{E}}_{SI}(\gamma^*) := \mathcal{E}_{SI}(\mathcal{G}(\mathbf{P}(\chi_{\gamma^*})), \gamma^*). \tag{4.9}$$

Using the same method as Section 3.3, we simplify the reduced sharp interface energy to

$$\tilde{\mathcal{E}}_{SI}(\gamma^*) = \begin{cases} \mathcal{K}(\chi_{\gamma^*}) + \int_{\gamma^*} \widehat{b} \, d\gamma^* & \text{for } \gamma^* \in \tilde{\mathcal{K}}_{SI}, \\ +\infty & \text{otherwise,} \end{cases} \tag{4.10}$$

where

$$\mathcal{K}(\chi_{\gamma^*}) = \int_{\Gamma} \frac{\kappa\Lambda}{2} \mathbf{P}(\chi_{\gamma^*}) \left(\frac{\sigma}{\kappa} + \frac{2}{R^2} \right) \mathcal{G}(\mathbf{P}(\chi_{\gamma^*})) + \frac{\kappa\Lambda^2}{2} (\chi_{\gamma^*}^2 - (\mathbf{P}(\chi_{\gamma^*}))^2) \, d\Gamma$$

as defined in (3.12), where and $\widehat{b} = c_W b$ (see Proposition 3.3), and where

$$\tilde{\mathcal{K}}_{SI} := \{ \gamma^* \in C^1(\Gamma) : |\Gamma^{(1)}| - |\Gamma^{(2)}| + \alpha|\Gamma| = 0 \}.$$

We write the constrained minimisation problem for the reduced sharp interface energy below.

Problem 4.5. Find $\tilde{\gamma}^* \in \tilde{\mathcal{K}}_{SI}$ such that

$$\tilde{\mathcal{E}}_{SI}(\tilde{\gamma}^*) = \inf_{\gamma \in \tilde{\mathcal{K}}_{SI}} \tilde{\mathcal{E}}_{SI}(\gamma).$$

Finally, we note that finding a minimiser of Problem 4.5 is equivalent to finding a minimiser to Problem 4.1, since

$$\begin{aligned} \mathcal{E}_{SI}(\gamma^*, u^*) &\leq \mathcal{E}_{SI}(\tilde{\gamma}^*, \mathcal{G}(\mathbf{P}(\chi_{\tilde{\gamma}^*}))) = \tilde{\mathcal{E}}_{SI}(\tilde{\gamma}^*) \\ &\leq \tilde{\mathcal{E}}_{SI}(\gamma^*) = \mathcal{E}_{SI}(\gamma^*, \mathcal{G}(\mathbf{P}(\chi_{\gamma^*}))) = \mathcal{E}_{SI}(\gamma^*, u^*). \end{aligned} \tag{4.11}$$

To summarise the previous two sections, we have related the diffuse interface energy given in (1.1) to the sharp interface energy (1.2) as follows:

- (1) Minimisers of the diffuse interface energy $\mathcal{E}_{DI}(u, \phi)$ defined in (1.1) coincide with minimisers of the reduced diffuse interface energy $\tilde{\mathcal{E}}_{DI}(\phi)$ defined in (3.8), see (3.10).
- (2) The reduced diffuse interface energy $\tilde{\mathcal{E}}_{DI}(\phi)$ Γ -converges to $\tilde{\mathcal{E}}_0(\phi)$ defined in (3.13), see Proposition 3.3. Subject to sufficient regularity of its minimisers, this limit coincides with the reduced sharp interface energy $\tilde{\mathcal{E}}_{SI}(\gamma^*)$ defined in (4.9), see Remark 3.5 and compare (3.14) with (4.10).
- (3) Minimisers of the reduced sharp interface energy $\tilde{\mathcal{E}}_{SI}(\gamma^*)$ coincide with minimisers of the sharp interface energy $\mathcal{E}_{SI}(u, \gamma)$ defined in (1.2), see (4.11).

5. Formal asymptotics for a phase field gradient flow

We now consider the following time evolution problem,

$$0 = \left(\Delta_\Gamma + \frac{2}{R^2}\right)(\kappa\Delta_\Gamma u - \sigma u + \kappa\Lambda(\phi - \alpha)) \quad \text{on } \Gamma, \tag{5.1}$$

$$\beta\varepsilon\phi_t = b\varepsilon\Delta_\Gamma\phi - \frac{b}{\varepsilon}W'(\phi) - \kappa\Lambda\Delta_\Gamma u - \frac{2\kappa\Lambda u}{R^2} - \kappa\Lambda^2\phi + \lambda \quad \text{on } \Gamma, \tag{5.2}$$

with initial conditions $\phi(0) = \phi_0$ and $u(0) = u_0$ and satisfying constraints (3.1). Here, λ is the Lagrange multiplier associated with the constraint $\int_\Gamma \phi = \alpha$ and $\beta > 0$ is a kinetic coefficient. These equations were introduced in [16] as a conserved L^2 -gradient flow of the diffuse interface energy (1.1) and were used to numerically compute local equilibria of (1.1), which are solutions to the Euler–Lagrange equations (3.2) and (3.3).

Similarly, turning to consider the sharp interface energy (1.2), the following evolution problem can be obtained as a conserved L^2 -gradient flow for two phase surfaces $(u(t), \gamma(t)) \in \mathcal{K}_{SI}$ [28],

$$0 = \left(\Delta_\Gamma + \frac{2}{R^2}\right)(\kappa\Delta_\Gamma u - \sigma u + \kappa\Lambda(-1 - \alpha)) \quad \text{on } \Gamma^{(1)}(t), \tag{5.3}$$

$$0 = \left(\Delta_\Gamma + \frac{2}{R^2}\right)(\kappa\Delta_\Gamma u - \sigma u + \kappa\Lambda(1 - \alpha)) \quad \text{on } \Gamma^{(2)}(t), \tag{5.4}$$

$$\begin{aligned} \widehat{\beta}\mathcal{V} = & -\widehat{b}H_\gamma + \widehat{b}\int_\gamma H_\gamma \, d\gamma + \frac{4\kappa\Lambda}{R^2}\left(u - \int_\gamma u \, d\gamma\right) \\ & + \kappa\Lambda\left(\Delta_\Gamma u^{(1)} + \Delta_\Gamma u^{(2)} - \int_\gamma (\Delta_\Gamma u^{(1)} + \Delta_\Gamma u^{(2)}) \, d\gamma\right) \quad \text{on } \gamma(t), \end{aligned} \tag{5.5}$$

with initial conditions $u(0) = u_0$ and $\gamma(0) = \gamma_0$ satisfying constraints (4.1)–(4.3), and with the following jump conditions across $\gamma(t)$:

$$[u]_{(1)}^{(2)} = 0, \quad [\nabla_\Gamma u \cdot \mu]_{(1)}^{(2)} = 0, \tag{5.6}$$

$$[\Delta_\Gamma u]_{(1)}^{(2)} = -2\Lambda, \quad [\nabla_\Gamma \Delta_\Gamma u \cdot \mu]_{(1)}^{(2)} = 0. \tag{5.7}$$

Here, $\mathcal{V}(t)$ is the velocity of $\gamma(t)$ in the direction of the conormal μ and $\widehat{\beta} = c_W\beta$. Note that stationary solutions of the gradient flow equations (5.3)–(5.7) are the Euler–Lagrange equations (4.4)–(4.6).

Our objective in this section is to show that the limiting problem of (5.1)–(5.2) as $\varepsilon \rightarrow 0$ is (5.3)–(5.7). For this purpose we note that since (5.1) coincides with (3.3), the calculation given in Section 3.2 can be repeated here and (5.1) can be reduced to (3.7). This has the benefit of only considering a second order equation instead of a fourth order equation for the height function, but has the added cost of involving the non-local projection operator \mathbf{P} . To deal with the non-local term, it will prove helpful to write $p := \mathbf{P}(\phi)$.

Hence, the system (5.1)–(5.2) can be reduced to

$$p = -\Delta_\Gamma u + \frac{\sigma}{\kappa} u \quad \text{on } \Gamma, \tag{5.8}$$

$$p = \mathbf{P}(\phi) \quad \text{on } \Gamma, \tag{5.9}$$

$$\beta \varepsilon \phi_t = b \varepsilon \Delta_\Gamma \phi - \frac{b}{\varepsilon} W'(\phi) - \kappa \Lambda \Delta_\Gamma u - \frac{2\kappa \Lambda u}{R^2} - \kappa \Lambda^2 \phi + \lambda \quad \text{on } \Gamma. \tag{5.10}$$

On (5.8)–(5.10) we perform a formal asymptotic analysis based on matching asymptotic ε expansions in the diffuse interfaces and in the bulk phases away from the interfaces. The technique is well established for phase field models; for instance, see [21] for details of the procedure. We denote by $(\phi_\varepsilon, u_\varepsilon, \lambda_\varepsilon, p_\varepsilon)$ a family of solutions to (5.8)–(5.10) that converges formally to some limit denoted by (ϕ, u, λ, p) . We assume that $\phi = \chi_\gamma$ for some smooth curve γ that separates the regions $\Gamma^{(1)} = \{(x, t) \in \Gamma \times [0, T] : \phi(x, t) = -1\}$ and $\Gamma^{(2)} = \{(x, t) \in \Gamma \times [0, T] : \phi(x, t) = +1\}$, see (1.3). Using that \mathbf{P} is the L^2 -projection onto $\text{span}\{1, \nu_1, \nu_2, \nu_3\}^\perp$, we calculate that

$$\mathbf{P}(\phi) = \begin{cases} -1 - \frac{1}{|\Gamma|} (|\Gamma^{(2)}| - |\Gamma^{(1)}|) - \frac{1}{3|\Gamma|} \sum_{i=1}^3 \nu_i (\int_{\Gamma^{(2)}} \nu_i - \int_{\Gamma^{(1)}} \nu_i) & \text{on } \Gamma^{(1)}, \\ +1 - \frac{1}{|\Gamma|} (|\Gamma^{(2)}| - |\Gamma^{(1)}|) - \frac{1}{3|\Gamma|} \sum_{i=1}^3 \nu_i (\int_{\Gamma^{(2)}} \nu_i - \int_{\Gamma^{(1)}} \nu_i) & \text{on } \Gamma^{(2)}. \end{cases} \tag{5.11}$$

We will show that the limit solution (ϕ, u, λ, p) satisfies the following free boundary value problem on Γ :

$$\phi = \begin{cases} -1 & \text{on } \Gamma^{(1)}, \\ +1 & \text{on } \Gamma^{(2)}, \end{cases} \tag{5.12}$$

$$-\Delta_\Gamma u + \frac{\sigma}{\kappa} u = \Lambda p \quad \text{on } \Gamma^{(1)} \cup \Gamma^{(2)}, \tag{5.13}$$

$$p = \mathbf{P}(\phi) \quad \text{on } \Gamma^{(1)} \cup \Gamma^{(2)}, \tag{5.14}$$

$$[u]_{(1)}^{(2)} = 0 \quad \text{on } \gamma, \tag{5.15}$$

$$[\nabla_\Gamma u]_{(1)}^{(2)} \cdot \mu = 0 \quad \text{on } \gamma, \tag{5.16}$$

$$\begin{aligned} \widehat{\beta} \mathcal{V} = & -\widehat{b} H_\gamma + \widehat{b} \int_\gamma H_\gamma \, d\gamma + \left(\frac{4\kappa \Lambda}{R^2} + 2\sigma \Lambda \right) \left(u - \int_\gamma u \, d\gamma \right) \\ & - \kappa \Lambda^2 \left(\mathbf{P}(\phi)^{(1)} + \mathbf{P}(\phi)^{(2)} - \int_\gamma \mathbf{P}(\phi)^{(1)} + \mathbf{P}(\phi)^{(2)} \, d\gamma \right) \quad \text{on } \gamma. \end{aligned} \tag{5.17}$$

We comment that (5.3)–(5.7) can be obtained from (5.12)–(5.17). Firstly, by combining (5.13) and (5.14), applying the operator $(\Delta_\Gamma + \frac{2}{R^2})$, and using that the components of the normal ν_i are in the null space of $(\Delta_\Gamma + \frac{2}{R^2})$, we obtain (5.3) and (5.4). Secondly, again combining (5.13) and (5.14), and substituting this into (5.17) to eliminate $\mathbf{P}(\phi)^{(i)}$, we obtain (5.5). Finally, using (5.11) we calculate that

$$[\mathbf{P}(\phi)]_{(1)}^{(2)} = 2, \quad [\nabla_\Gamma \mathbf{P}(\phi)]_{(1)}^{(2)} \cdot \mu = 0.$$

Hence, we obtain (5.6) and (5.7) from (5.13), (5.15) and (5.16). Altogether, we see that equations (5.12)–(5.17) do indeed yield the sharp-interface gradient flow equations (5.3)–(5.5). Therefore, it only remains to show (5.12)–(5.17).

Remark 5.1. Let us mention that approaches such as in [44] may be useful in establishing rigorous results of Γ -convergence for the gradient flow.

5.1. Matching conditions

As is standard for these problems, we will consider outer expansions (solutions that are only valid away from the interface γ) and inner expansions (solutions that are only valid near to the interface). We consider inner expansions in addition to the outer expansions since near the interface γ it is possible that there could be very steep transition layers. Therefore, the derivatives could contribute non-zero order $\mathcal{O}(\varepsilon)$ terms which need to be accounted for. On the region where both inner and outer expansions are valid, matching conditions relate the outer expansions to the inner expansions.

We will assume that the outer expansions have the form

$$f_\varepsilon(x, t) = \sum_{k=0}^{\infty} \varepsilon^k f_k(x, t),$$

where $f_\varepsilon = \phi_\varepsilon, u_\varepsilon, \lambda_\varepsilon$ or p_ε . To write down the inner expansions we consider a parameterisation $\Theta(s, r, t)$ such that $s \mapsto \Theta(s, 0, t)$ gives a parameterisation of $\gamma(t)$ and r denotes the signed geodesic distance of a point $x = \Theta(s, r, t) \in \Gamma$ to the interface $\gamma(t)$. Further details of a suitable parameterisation for the sphere can be found in [24]. Since the length scale of the transition layers is ε , we introduce the parameter z given by

$$z = \frac{r}{\varepsilon}.$$

We then assume that the inner expansions are of the form

$$f_\varepsilon(x, t) = F(s, z, t; \varepsilon) = \sum_{k=0}^{\infty} \varepsilon^k F_k(s, z, t),$$

where again $f_\varepsilon = \phi_\varepsilon, u_\varepsilon, \lambda_\varepsilon$ or p_ε with $F_k = \Phi_k, U_k, L_k$ or P_k , respectively. On the region where both outer and inner expansions are valid we prescribe the following matching conditions to ensure consistency:

$$F_0(s, \pm\infty, t) \sim f_0^\pm(x, t), \tag{5.18}$$

$$\partial_z F_0(s, \pm\infty, t) \sim 0, \tag{5.19}$$

$$\partial_z F_1(s, \pm\infty, t) \sim \nabla_\Gamma f_0^\pm(x, t) \cdot \mu(x, t), \tag{5.20}$$

where $f_0^\pm(x, t) = \lim_{\delta \rightarrow 0} f(\Theta(s, \pm\delta, t), t)$. A derivation of these matching conditions can be found in [26].

5.2. Outer expansions

We begin by matching orders of ε for the outer expansions first. In [41], Rubinstein and Sternberg considered a formal asymptotic analysis for the conserved Allen–Cahn equation and demonstrated that for faster timescales it is sufficient to suppose the lowest order term of the Lagrange multiplier is of order $\mathcal{O}(\varepsilon^0)$. Their analysis can equally be applied to our system of equations and so we make the assumption that the lowest order term of the Lagrange multiplier λ is of order $\mathcal{O}(\varepsilon^0)$. Hence, considering terms of order $\mathcal{O}(\varepsilon^{-1})$ in (5.10), we obtain that

$$W'(\phi_0) = 0,$$

and hence, the only stable solutions are

$$\phi_0 = \pm 1. \tag{5.21}$$

Therefore, we deduce that $\phi_\varepsilon \rightarrow \pm 1$, which justifies (5.12). Furthermore, by considering terms of order $\mathcal{O}(\varepsilon^0)$ in (5.8) and (5.9) we readily obtain (5.13) and (5.14).

5.3. Inner expansions

Before considering the inner expansions we first have to write the Laplace–Beltrami operator and the time derivative in local coordinates near to the interface. Calculations in [24] show that the following expressions are obtained for a function $f(s, z, t)$ defined on a neighbourhood around the interface γ :

$$\Delta_\Gamma f = \frac{1}{\varepsilon^2} \partial_{zz} f + \frac{H_\gamma}{\varepsilon} \partial_z f + \Delta_\gamma f + \mathcal{O}(\varepsilon),$$

and

$$\frac{d}{dt} f = -\frac{1}{\varepsilon} \mathcal{V} \partial_z f + \partial_t f + \mathcal{O}(\varepsilon), \tag{5.22}$$

where Δ_γ is the Laplace–Beltrami operator along the curve γ .

Since we have assumed that the limit as $\varepsilon \rightarrow 0$ exists, it follows that the terms of leading order in ε cancel out. We denote the inner expansions of $\phi_\varepsilon, u_\varepsilon, \lambda_\varepsilon$ by Φ, U and L , respectively. We begin by considering terms of order $\mathcal{O}(\varepsilon^{-2})$ and $\mathcal{O}(\varepsilon^{-1})$ in (5.8) to obtain that

$$\partial_{zz} U_0 = 0, \tag{5.23}$$

$$H_\gamma \partial_z U_0 + \partial_{zz} U_1 = 0. \tag{5.24}$$

Integrating (5.23) from $-\infty$ to z and using the matching condition (5.19), we obtain that

$$\partial_z U_0 = 0. \tag{5.25}$$

Hence, we have

$$U_0(z = +\infty) = U_0(z = -\infty),$$

from which we obtain (5.15) with the matching condition (5.18).

Similarly, integrating (5.24) from $-\infty$ to ∞ and using the matching condition (5.20), we obtain (5.16).

The terms of order $\mathcal{O}(\varepsilon^{-1})$ in (5.10) are

$$0 = b\partial_{zz}\Phi_0 - bW'(\Phi_0) - \kappa\Lambda(H_\gamma\partial_z U_0 + \partial_{zz}U_1),$$

which, using (5.24), simplify to

$$0 = b\partial_{zz}\Phi_0 - bW'(\Phi_0).$$

Hence, using the outer expansion (5.21) and matching condition (5.18), we have that $\Phi_0(z, s, t)$ is a solution of

$$\begin{cases} \partial_{zz}\Phi_0 = W'(\Phi_0), \\ \Phi_0(\pm\infty) = \pm 1. \end{cases} \quad (5.26)$$

We find that $\Phi_0(z, s, t)$ is independent of s and t and given by

$$\Phi_0(z) = \tanh\left(\frac{z}{\sqrt{2}}\right). \quad (5.27)$$

Finally, we consider terms of order $\mathcal{O}(\varepsilon^0)$ in (5.10) to obtain

$$\begin{aligned} -\beta\partial_z\Phi_0\mathcal{V} &= bH_\gamma\partial_z\Phi_0 - bW''(\Phi_0)\Phi_1 + L_0 + b\partial_{zz}\Phi_1 - \kappa\Lambda^2\Phi_0 \\ &\quad - \kappa\Lambda(\Delta_\gamma U_0 + H_\gamma\partial_z U_1 + \partial_{zz}U_2) - \frac{2\kappa\Lambda U_0}{R^2}. \end{aligned} \quad (5.28)$$

Considering the terms of order $\mathcal{O}(\varepsilon^0)$ in (5.8) we obtain

$$-(\Delta_\gamma U_0 + H_\gamma\partial_z U_1 + \partial_{zz}U_2) = \Lambda P_0 - \frac{\sigma}{\kappa}U_0. \quad (5.29)$$

Using (5.29) to simplify (5.28), we have

$$\begin{aligned} -\beta\partial_z\Phi_0\mathcal{V} &= bH_\gamma\partial_z\Phi_0 - bW''(\Phi_0)\Phi_1 + L_0 + b\partial_{zz}\Phi_1 \\ &\quad - \kappa\Lambda^2\Phi_0 + \kappa\Lambda\left(\Lambda P_0 - \left(\frac{\sigma}{\kappa} + \frac{2}{R^2}\right)U_0\right). \end{aligned}$$

It is straightforward to show that the function $\partial_z\Phi_0$ is in the kernel of the operator $-\partial_{zz} + W''(\Phi_0)$. To ensure solvability of the equation for Φ_1 , the source term has to be orthogonal to $\partial_z\Phi_0$ with respect to the L^2 inner product. We refer to [1, Lemma 2.2]

for the details (see also [24, Lemma 4.1]). This condition reads as

$$0 = \int_{-\infty}^{+\infty} -\beta(\partial_z \Phi_0)^2 \mathcal{V} - bH_\gamma(\partial_z \Phi_0)^2 - L_0 \partial_z \Phi_0 - \kappa\Lambda \left(\Lambda P_0 - \left(\frac{\sigma}{\kappa} + \frac{2}{R^2} \right) U_0 \right) \partial_z \Phi_0 + \frac{\kappa\Lambda^2}{2} \partial_z (\Phi_0^2) dz.$$

Applying (5.26), we see that the last term vanishes. Using (5.27) we calculate that

$$\int_{-\infty}^{\infty} (\partial_z \Phi_0)^2 dz = \frac{2\sqrt{2}}{3},$$

and using that $\widehat{b} = \frac{2\sqrt{2}b}{3}$ and $\widehat{\beta} = \frac{2\sqrt{2}\beta}{3}$, it follows that

$$\widehat{\beta}\mathcal{V} = -\widehat{b}H_\gamma - 2L_0 - \kappa\Lambda \int_{-\infty}^{+\infty} \left(\Lambda P_0 - \left(\frac{\sigma}{\kappa} + \frac{2}{R^2} \right) U_0 \right) \partial_z \Phi_0 dz,$$

where above we have used that $\Phi_0(\pm\infty) = \pm 1$.

We recall from Section 3.2 that \mathbf{P} is the L^2 -projection onto $\text{span}\{1, \nu_1, \nu_2, \nu_3\}^\perp$. Then, since $\int_\Gamma \phi d\Gamma = \alpha$ and the components of the normal, ν_i , are in the kernel of the operator $(\Delta_\Gamma + \frac{2}{R^2})$, it follows that

$$\left(\Delta_\Gamma + \frac{2}{R^2} \right) (\phi - \alpha) = \left(\Delta_\Gamma + \frac{2}{R^2} \right) \mathbf{P}(\phi). \tag{5.30}$$

Considering terms of $\mathcal{O}(\varepsilon^{-2})$ in (5.30), we obtain that

$$\partial_{zz} \Phi_0 = \partial_{zz} P_0.$$

So, by integrating this and using the matching condition (5.19), it follows that

$$\partial_z \Phi_0 = \partial_z P_0. \tag{5.31}$$

Using (5.25) (that is, the fact that U_0 is independent of z) and (5.31), we obtain that

$$\widehat{\beta}\mathcal{V} = -\widehat{b}H_\gamma - 2L_0 - \frac{\kappa\Lambda^2}{2} \int_{-\infty}^{\infty} \partial_z ((P_0)^2) dz + \kappa\Lambda \left(\frac{\sigma}{\kappa} + \frac{2}{R^2} \right) U_0 \int_{-\infty}^{\infty} \partial_z \Phi_0 dz,$$

which using (5.26) simplifies to give

$$\widehat{\beta}\mathcal{V} = -\widehat{b}H_\gamma - 2L_0 + 2\kappa\Lambda \left(\frac{\sigma}{\kappa} + \frac{2}{R^2} \right) U_0 - \frac{\kappa\Lambda^2}{2} ((P_0(+\infty))^2 - (P_0(-\infty))^2).$$

By integrating (5.31) and using the matching condition (5.18), we obtain that

$$P_0(+\infty) - P_0(-\infty) = \Phi_0(+\infty) - \Phi_0(-\infty) = 2. \tag{5.32}$$

Therefore, using (5.32) gives that

$$\widehat{\beta}\mathcal{V} = -\widehat{b}H_\gamma - 2L_0 + \left(\frac{4\kappa\Lambda}{R^2} + 2\sigma\Lambda \right) U_0 - \kappa\Lambda^2 (P_0(-\infty) + P_0(+\infty)). \tag{5.33}$$

It remains to determine L_0 , for which we use the constraint $\int_{\Gamma} \phi_\varepsilon = \alpha$ (a similar example can be found in [8]). Hence, it follows using (5.22) and considering terms of order $\mathcal{O}(\varepsilon^{-1})$ that

$$0 = \int_{\gamma} \mathcal{V} \partial_z \Phi_0 \, d\gamma,$$

and hence, using that $\partial_z \Phi_0$ is independent of s we obtain that

$$\int_{\gamma} \mathcal{V} \, d\gamma = 0.$$

Integrating (5.33) and using the above result, we obtain that

$$2L_0 = \int_{\gamma} -\widehat{b} H_{\gamma} + \left(\frac{4\kappa\Lambda}{R^2} + 2\sigma\Lambda \right) U_0 - \kappa\Lambda^2 (P_0(-\infty) + P_0(+\infty)) \, d\gamma.$$

Finally, applying the matching condition (5.18) and using (5.14) gives (5.17).

6. Conclusion

We have analysed and related sharp and diffuse interface energies obtained by applying a perturbation approach for two phase approximately spherical biomembranes. We simplified the diffuse interface energy by using the Euler–Lagrange equations to eliminate the height function in order to obtain what we have referred to as the reduced diffuse interface energy. In particular, we showed that the minimisation problem for the original energy is equivalent to the minimisation problem for the reduced energy. Furthermore, we calculated the Γ -limit of the reduced diffuse interface energy and considered the minimisation problem. This is important since results relating to Γ -convergence can be used to show that minimisers of (1.1) converge to a minimiser of (1.2).

We then performed a formal asymptotic analysis for a system of gradient flow equations of the diffuse interface energy that had previously been considered in [16]. The free boundary problem attained from this analysis coincided with the corresponding gradient flow equations for the sharp interface energy. Here, we again showed how using this reduced energy could simplify this calculation.

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