#### ORIGINAL PAPER



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# Sharp interface analysis of a diffuse interface model for cell blebbing with linker dynamics

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We investigate the convergence of solutions of a recently proposed diffuse interface/phase field model for cell blebbing by means of matched asymptotic expansions. It is a biological phenomenon that increasingly attracts attention by both experimental and theoretical communities. Key to understanding the process of cell blebbing mechanically are proteins that link the cell cortex and the cell membrane. Another important model component is the bending energy of the cell membrane and cell cortex which accounts for differential equations up to sixth order. Both aspects pose interesting mathematical challenges that will be addressed in this work like showing non-singularity formation for the pressure at boundary layers, deriving equations for asymptotic series coefficients of uncommonly high order, and dealing with a highly coupled system of equations.

#### INTRODUCTION

The phenomenon of cell blebbing is connected with various biological processes such as locomotion of primordial germ or cancer cells, the programmed cell death (apoptosis) or cell division. Its importance has been recognised and emphasized in the last decade [1-3], and attracts more and more interest. Cell blebbing results from chemical reactions that cause the selection of sites on the cell cortex, which lies underneath the cell membrane, where it contracts. This contraction causes the fluid inside the cell (the cytosol) to be pushed towards the cell membrane, which is then stretched out and moved away from the cell cortex. The cell membrane is pinned to the cell cortex via linker proteins. Only if a sufficient amount of protein bonds can be broken, the membrane can freely develop a protrusion that is called a bleb.

Besides experimental studies [4], there are also many endeavours to understand cell blebbing from a theoretical perspective, compare Refs. [5-12]. While all these modelling approaches concentrate on selected aspects of the whole process, a full 3D model that brings together the linker proteins, their surface diffusion and the fluid-structure interaction has only recently been proposed in Werner et al. [13]: the authors derive a phase field model in which cell cortex and cell membrane are defined by two coupled phase fields, with phase field parameter  $\varepsilon$ , that interact with the cytosol. The coupling of the phase fields reflects the linker proteins connecting both surfaces and brings in new interesting mathematical challenges such as well-posedness of equations on evolving 'diffuse manifolds' (the linker protein densities on the cell cortex undergo

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changes due to surface diffusion and bond breaking), developing numerical schemes for solving non-linear, sixth-order phase field equations and answering the question what model is reached in the limit  $\varepsilon \to 0$ .

This article is aimed at investigating the last problem and showing that the phase field model of Werner et al. [13] formally approximates a sharp interface model that has also been derived by physical first principles [14]. For that, we will use the method of formal asymptotic analysis. The techniques we employ are similar to those applied for the asymptotic analysis of related phase field models like Caginalp and Fife [15], the Stokes-Allen-Cahn system in Abels and Liu [16] or the Willmore  $L^2$ -flow [17]. Another related asymptotic analysis is that of Wang [18] for minimisers of the Canham-Helfrich energy.

We start by briefly recalling the phase field model from Werner et al. [13] and show the sharp interface system that is expected in the limit. After we have introduced the notation and gained some understanding of the system of partial differential equations, we introduce foundations of the technique we use to pass to the limit  $\varepsilon \to 0$ . Here, the parameter  $\varepsilon$  is proportional to the interfacial thickness of the diffuse interfacial layer in the phase field model. The major part of this paper follows, which is to plug in series expansions of the solutions of the phase field model in powers of  $\varepsilon$ . Via separation of scales, we are able to derive equations for the leading order summands of the series. Using these findings, we can finally pass to the limit in the equations of the phase field model and find the sharp interface system of equations that we initially reviewed.

#### 1.1 | Preliminaries

We denote the *n*-dimensional Lebesgue measure by  $\mathcal{L}^n$  and the Hausdorff measure of Hausdorff dimension m by  $\mathcal{H}^m$ . Recall that for a two-dimensional submanifold  $\Gamma \subset \mathbb{R}^3$  with a smooth global chart  $\varphi : \Gamma \to \mathbb{R}^2$ , and for a summable function  $f : \Gamma \to \mathbb{R}$ , it holds by definition

$$\int_{\Gamma} f \, \mathrm{d}\mathcal{H}^2 = \int_{\varphi(\Gamma)} f \circ \varphi^{-1} J\left[\varphi^{-1}\right] \, \mathrm{d}\mathcal{L}^2,$$

where  $J[u] = \sqrt{\det(\nabla u^T \nabla u)}$  is the Jacobian of  $u = \varphi^{-1}$ .

Let  $\Gamma \subseteq \mathbb{R}^3$  be a sufficiently smooth submanifold. We denote by  $N_\delta(\Gamma) = \{x \in \mathbb{R}^3 \mid \operatorname{dist}_\Gamma(x) < \delta\}$  the tubular neighbourhood around  $\Gamma$ , where  $\operatorname{dist}_\Gamma(x)$  is the distance of x to  $\Gamma$  defined via the orthogonal projection; by  $d_\Gamma(x)$ , we denote the signed distance. If we partition  $N_\delta(\Gamma) = \bigcup_{r \in (-\delta, \delta)} \Gamma_r$ , where  $\Gamma_r = \{x \in N_\delta(\Gamma) \mid d_\Gamma(x) = r\}$ , we may define extensions of quantities defined on  $\Gamma$  into  $N_\delta(\Gamma)$  (cf. [19, Sec. 14.6]). The extended principal curvatures are defined as

$$\bar{\kappa}_i : N_{\delta}(\Gamma) \to \mathbb{R},$$

$$x \mapsto \kappa_{\Gamma_{d_{\Gamma}(x)},i}(x),$$

where  $\kappa_{S,i}(x)$  is the *i*th principal curvature of the surface S. Accordingly, the mean curvature is

$$\bar{H}: N_{\delta}(\Gamma) \to \mathbb{R},$$

$$x \mapsto H_{\Gamma_{d_{\Gamma}(x)}}(x),$$

Another extension method we will encounter is the *normal extension* of a quantity  $f: \Gamma \to V$ , for a set V, meaning that the quantity is extended constantly in normal direction. We denote those extensions by  $\bar{f}^{\nu}$ .

The surface gradient,  $\nabla_{\Gamma} f|_{p}$ , of a function  $f: \Gamma \to \mathbb{R}$  in a point  $p \in \Gamma$  is the vector

$$\nabla_{\Gamma} f|_{p} = \mathbb{P}_{\Gamma}(p) \nabla \bar{f}^{\nu}|_{p},$$

where  $\mathbb{P}_{\Gamma}(p) = I - \nu_{\Gamma}(p) \otimes \nu_{\Gamma}(p)$  is the tangential projection onto  $\Gamma$ . Other surface differential operators such as the divergence or the Jacobi matrix can be derived analogously.

For a differentiable functional  $S: X \to [0, \infty)$  on a Banach space X, the element  $\nabla^Y S(u)$ ,  $u \in X$ , of a subspace  $Y \subseteq X$  that fulfills

$$\left(\nabla^Y S(u), v\right)_Y = S'(u)v \quad \forall v \in Y,$$

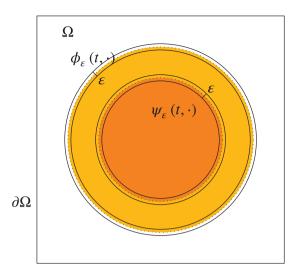


FIGURE 1 Illustration of the relationship of the two diffuse layers. The dotted lines indicate the centres of the transition layers of  $\phi$  and  $\psi$ . In the white region, both  $\phi_{\varepsilon}$  and  $\psi_{\varepsilon}$  take values close to 1. In the light orange region,  $\psi_{\varepsilon}$  takes values close to 1, but  $\phi_{\varepsilon}$  has values close to -1. In the dark orange region, both  $\phi_{\varepsilon}$  and  $\psi_{\varepsilon}$  have values close to -1.

where S'(u) is the Gateaux derivative of S in u, is called the Y-gradient of S. Consider, for example, the functional  $S(u) = \int_{B_1(0)} |\nabla u(x)|^2 d\mathcal{L}^3(x)$ ; its  $L^2$ -gradient is  $\nabla^{L^2} S(u) = -\Delta u$ , whereas the  $H_0^1$ -gradient takes the form  $\nabla^{H_0^1} S(u) = u$ , and the  $H^{-1}$ -gradient is  $\nabla^{H^{-1}}S(u) = \Delta^2 u$ .

#### MODELLING

Besides the numerical advantage of making topological changes such as pinch-offs (like when vesicles form out of the membrane) easy to handle, a phase field approach for modelling cell blebbing is also apt for bio-physical reasons: cell membranes are bilayers of lipid molecules which can be subject to undulations, and so the membrane is not strictly demarcated to the surrounding fluid. Depending on the scale, we look at these membranes, the diameter of the lipid molecules involved, and the spacing between them, it may be desirable to model uncertainty in the lipid molecules' position and thus take them to be diffuse layers of some thickness  $\varepsilon$ . Another peculiarity when considering cell blebbing is experimental evidence [4] that at sites where blebbing occurs, the cell membrane is folded multiple times providing for enough material to be unfolded, and is thus thicker than a typical biological membrane.

Let us assume that we observe the process of cell blebbing for a certain time  $T \in (0, \infty)$  in a domain  $\Omega \subseteq \mathbb{R}^3$ . We consider two evolving diffuse interfaces – the cell membrane and the cell cortex – that can be defined as those subsets of  $\Omega$ , on which phase fields  $\phi_{\varepsilon}$  (modelling the membrane) and  $\psi_{\varepsilon}$  (modelling the cell cortex) are close to zero, respectively. Additionally, there is a surrounding fluid with density  $\rho$ , velocity  $v_{\varepsilon}$  and pressure  $p_{\varepsilon}$ . Also in the domain, but concentrated on the cell cortex, are linker proteins with mass volume density  $\rho_{a.\epsilon}$ . They connect the cell membrane and the cell cortex. The linker proteins behave like springs, but may break if overstretched, so we introduce another density  $\rho_{i,\varepsilon}$  which gives the mass of linkers per volume that are broken. This is important because 'repairing mechanisms' of the cell take care of reconnecting those broken linkers back to the cell membrane. A scheme in which the aforementioned quantities are all depicted together is given in Figure 1.

For deriving the phase field model, Onsager's variational principle [20, 21] is combined with a reaction-diffusion-like surface evolution equation for the active and inactive linker proteins. To establish a basic understanding of how a PDE system for cell blebbing can be obtained, let us mention the principle steps in the derivation.

- 1. Definition of an energy functional  $U[v_{\varepsilon}, p_{\varepsilon}, \phi_{\varepsilon}, \psi_{\varepsilon}]$  that is the sum of all kinds of energy of the cell: the ingredients are the kinetic energy of the fluid, the surface and bending energy of the cell cortex and cell membrane, and a potential energy that accounts for the coupling of both membrane and cortex via the linker proteins.
- 2. Definition of appropriate boundary conditions (see below).

- 3. Variation of *U* plus a dissipation functional. With regard to the linker proteins, our process is assumed to be quasi-static, that is, we assume the linker proteins to be given parameters of *U* although their evolution is given by a reaction—diffusion-like surface equation.
- 4. Extending the stationarity condition derived by the previous variation step, the aforementioned surface evolution equations for the linker proteins are added.

#### 2.1 | Phase field model

Several computations and formulae are the same for the phase field representing the cell membrane  $\phi_{\varepsilon}$  and that representing the cell cortex  $\psi_{\varepsilon}$ . For those, we always use the symbols  $\varphi \in \{\phi, \psi\}$  and  $\Phi \in \{\Gamma, \Sigma\}$  to avoid copious repetition.

In the phase field approach, we approximate two important geometrical quantities known from the sharp interface perspective, namely the normal

$$u_{\Phi} = \nu_{\varphi_{\varepsilon}} + O(\varepsilon), \quad \nu_{\varphi_{\varepsilon}} = \frac{\nabla \varphi_{\varepsilon}}{|\nabla \varphi_{\varepsilon}|}$$

(everywhere where  $\varphi_{\varepsilon} \neq 0$ ), and the mean curvature

$$H_{\Phi} = H_{\varphi_{\varepsilon}} + O(\varepsilon), \quad H_{\varphi_{\varepsilon}} = |\nabla \varphi_{\varepsilon}| \left( -\varepsilon \Delta \varphi_{\varepsilon} + \varepsilon^{-1} W'(\varphi_{\varepsilon}) \right)$$

with  $W(\varphi_{\varepsilon}) = \frac{1}{4} (\varphi_{\varepsilon}^2 - 1)^2$ . Having the velocity v and density  $\rho$  of the fluid, we may express the kinetic energy as

$$\frac{1}{2} \int_{\Omega} \rho |v|^2 d\mathcal{L}^3.$$

Let us consider the following energies at a particular point in time  $t \in [0, T]$ , so we can ignore the time-dependency for now. The surface energy of the diffuse cell membrane with a surface tension proportional to  $\gamma_{\Gamma}$  is given by the Ginzburg–Landau energy

$$\mathcal{G}_{\varepsilon,\Gamma}[\phi] = \gamma_{\Gamma} \int_{\Omega} \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} W(\phi) \, \mathrm{d}\mathcal{L}^3 = \gamma_{\Gamma} \int_{\Omega} g_{\varepsilon}[\phi] \, \mathrm{d}\mathcal{L}^3$$

with  $g_{\varepsilon}[\phi] = \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} W(\phi)$ . A well-established [22–24] model for the bending energy of a cell membrane with bending rigidity  $\beta_{\Gamma}$  and spontaneous mean curvature  $C_0^{\Gamma}$  is the phase field version of the Canham–Helfrich energy

$$\mathcal{W}_{arepsilon,\Gamma}[\phi] = rac{eta_{\Gamma}}{2arepsilon} \int_{\Omega} \left( -arepsilon \Delta \phi + \left(rac{1}{arepsilon}\phi + C_{0}^{\Gamma}
ight) \left(\phi^{2} - 1
ight)
ight)^{2} \,\mathrm{d}\mathcal{L}^{3}.$$

The additional term in the energy introduced by that, however, does not introduce new theoretical challenges compared to using a Willmore functional, which is why we will omit it for the sake of a straightforward presentation, that is,  $C_0^{\Gamma} = 0$ . In this configuration,  $\mathcal{W}_{\varepsilon,\Gamma}[\phi]$  is the phase field version of the Willmore energy. We simplify the situation for the cell cortex in that we assume it to be just a stiffer membrane thus employing the same types of energies just with different surface tension and bending rigidity. Both energies associated to membrane and cortex are summarised in the energy functionals

$$S^\varepsilon_\Phi[\varphi] = \mathcal{W}_{\varepsilon,\Phi}[\varphi] + \mathcal{G}_{\varepsilon,\Phi}[\varphi].$$

For the coupling of cell membrane and cell cortex, we account with a generalised Hookean spring energy.

$$C_{\varepsilon}\left[\phi_{\varepsilon},\psi_{\varepsilon},\rho_{a,\varepsilon}\right] = \int_{\Omega} g_{\varepsilon}[\phi](y) \frac{\xi}{2} \int_{\Omega} g_{\varepsilon}[\psi](x) |x-y|^{2} \rho_{a,\varepsilon}(t,x) \omega\left(x,y,\nu_{\psi_{\varepsilon}}\right) d\mathcal{L}^{3}(x) d\mathcal{L}^{3}(y),$$

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where  $\xi$  is a spring constant, and  $\omega(x, y, \nu_{\psi_{\varepsilon}})$  assigns to points  $x, y \in \Omega$  the particle-per-volume density of protein linkers connecting in direction x - y. A possible choice is

$$\omega\left(x,y,\nu_{\psi_{\varepsilon}}\right) = \tilde{\omega}\left(\frac{(x-y)\cdot\nu_{\psi_{\varepsilon}}(x)}{|x-y|}\right), \quad \tilde{\omega}(r) = \hat{\omega}\exp\left(\frac{(r-1)^2}{s^2}\right)$$

with *s* being a suitable standard deviation and  $\hat{\omega}$  an appropriate scaling factor. To outline the idea for this modelling choice, we first point out that  $g_{\varepsilon} [\phi_{\varepsilon}]$  can be pictured as a 'smooth Dirac delta function' if  $\phi_{\varepsilon}$  is the so-called optimal profile

$$x \mapsto \tanh\left(\frac{d_{\Gamma}(x)}{\varepsilon\sqrt{2}}\right).$$

The same holds for  $g_{\varepsilon}[\psi_{\varepsilon}]$ , so that

$$\int_{\Omega} g_{\epsilon}[\phi] \cdot d\mathcal{L}^{3} \approx \frac{2\sqrt{2}}{3} \int_{\Gamma(t)} \cdot d\mathcal{H}^{2}$$

and

$$\int_{\Omega} g_{\epsilon}[\phi] \cdot d\mathcal{L}^{3} \approx \frac{2\sqrt{2}}{3} \int_{\Sigma(t)} \cdot d\mathcal{H}^{2}$$

approximate surface integrals for small  $\varepsilon$ . Thus,

$$\begin{split} \mathcal{C}_{\varepsilon}\left[\phi_{\varepsilon},\psi_{\varepsilon},\rho_{a,\varepsilon}\right] &= \int_{\Omega} g_{\varepsilon}[\phi](y) \frac{\xi}{2} \int_{\Omega} g_{\varepsilon}[\psi](x) |x-y|^{2} \rho_{a,\varepsilon}(t,x) \omega\left(x,y,\nu_{\psi_{\varepsilon}}\right) \, \mathrm{d}\mathcal{L}^{3}(x) \, \mathrm{d}\mathcal{L}^{3}(y) \\ &\approx \int_{\Gamma(t)} \frac{\xi}{2} \int_{\Sigma(t)} |x-y|^{2} \rho_{a,\varepsilon}(t,x) \omega\left(x,y,\nu_{\Sigma(t)}\right) \, \mathrm{d}\mathcal{H}^{2}(x) \, \mathrm{d}\mathcal{H}^{2}(y). \end{split}$$

Looking at the sharp interface equivalent of the coupling energy, we can identify

- 1.  $\frac{\xi}{2}|x-y|^2$  as a Hookean energy density, which is integrated over the membrane and cortex, and weighted additionally by
- 2.  $\omega\left(x,y,\nu_{\Sigma(t)}\right)$  to incorporate the likeliness of the two spatial points  $x\in\Sigma,y\in\Gamma$  being connected, and
- 3. the volume–density of linker particles  $\rho_{a,\varepsilon}(t,x)$  actually linking.

The Hookean energy ansatz accounts for the earlier mentioned assumption that the linker proteins behave like springs. Additionally, since linkers might not be distributed homogeneously, we should scale the coupling force by their actual amount, which explains 3. The necessity to consider a weight  $\omega$  might not be so obvious: it has not yet been agreed upon in the biological literature how to identify the pairs of points  $(x,y) \in \Sigma \times \Gamma$  that are connected by protein linkers. That is why we allow the weight  $\omega$  to model a certain probability for this state. An easy way to describe such a probability is in terms of the angle between y-x and a gauge direction. As this gauge direction, we chose the cortex normal, which enters as the third argument of  $\omega$ .

Remark 2.1. It shall be remarked that there are other choices for 'smooth Dirac delta functions' like  $\frac{1}{\varepsilon}W(\varphi)$ , which is smoother and easier to handle analytically and numerically. It turns out, however, that for passing to the limit  $\varepsilon \to 0$ , the latter two choices are not appropriate. The reason for that becomes clear when we compare the right hand side K of the momentum balance for the different choices of the integral weight: only for  $g_{\varepsilon}[\varphi]$ , we have phase field counterparts in K for every term we expect in the sharp interface system as derived from physical first principles (cf. Werner et al. [13]).

Summing all potential energies, we obtain the Helmoltz free energy of the cell as

$$\mathcal{F}_{\varepsilon}\left[\phi_{\varepsilon},\psi_{\varepsilon},\rho_{a,\varepsilon}\right] = \mathcal{S}^{\varepsilon}_{\Gamma}\left[\phi_{\varepsilon}\right] + \mathcal{S}^{\varepsilon}_{\Sigma}\left[\psi_{\varepsilon}\right] + \mathcal{C}_{\varepsilon}\left[\phi_{\varepsilon},\psi_{\varepsilon},\rho_{a,\varepsilon}\right],$$

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and the inner energy as

$$U\left[v_{\varepsilon},\phi_{\varepsilon},\psi_{\varepsilon},\rho_{a,\varepsilon}\right] = \frac{1}{2} \int_{\Omega} \rho \left|v_{\varepsilon}\right|^{2} d\mathcal{L}^{3} + \mathcal{F}_{\varepsilon}\left[\phi_{\varepsilon},\psi_{\varepsilon},\rho_{a,\varepsilon}\right].$$

Via Onsager's variational principle (cf. Werner et al. [13]), the following system of partial differential equations is then found as stationarity conditions

$$\rho\left(\partial_{t}v_{\varepsilon} + (v_{\varepsilon} \cdot \nabla)v_{\varepsilon}\right) - \nabla \cdot \left(\eta\left(\nabla v_{\varepsilon} + \nabla v_{\varepsilon}^{T}\right) - p_{\varepsilon}\right) = K,\tag{1a}$$

$$\nabla \cdot v_{\varepsilon} = 0 \tag{1b}$$

$$\partial_{t}\phi_{\varepsilon} + \upsilon_{\varepsilon} \cdot \nabla\phi_{\varepsilon} = \nabla \cdot \left( m\left(\phi_{\varepsilon}\right) \left( \nabla \left( \nabla_{\phi}^{L^{2}} \mathcal{S}_{\Gamma}^{\varepsilon} \left[\phi_{\varepsilon}\right] \right) + \nabla \left( \nabla_{\phi_{\varepsilon}}^{L^{2}} \mathcal{C}_{\varepsilon} \left[\phi_{\varepsilon}, \psi_{\varepsilon}, \rho_{a, \varepsilon}\right] \right) \right) \right), \tag{1c}$$

$$\partial_{t}\psi_{\varepsilon} + \upsilon_{\varepsilon} \cdot \nabla\psi_{\varepsilon} = \nabla \cdot \left( m(\psi_{\varepsilon}) \left( \nabla \left( \nabla_{\psi}^{L^{2}} S_{\Sigma}^{\varepsilon} [\psi_{\varepsilon}] \right) + \nabla \left( \nabla_{\psi_{\varepsilon}}^{L^{2}} C_{\varepsilon} [\phi_{\varepsilon}, \psi_{\varepsilon}, \rho_{a, \varepsilon}] \right) \right) \right), \tag{1d}$$

where

$$\begin{split} K &= \nabla^{L^{2}} S_{\Gamma}^{\varepsilon} \left[ \phi_{\varepsilon} \right] \nabla \phi_{\varepsilon} + \nabla^{L^{2}} S_{\Sigma}^{\varepsilon} \left[ \psi_{\varepsilon} \right] \nabla \psi_{\varepsilon} \\ &+ \nabla_{\phi}^{L^{2}} C_{\varepsilon} \left[ \phi_{\varepsilon}, \psi_{\varepsilon}, \rho_{a, \varepsilon} \right] \nabla \phi + \nabla_{\psi}^{L^{2}} C_{\varepsilon} \left[ \phi_{\varepsilon}, \psi_{\varepsilon}, \rho_{a, \varepsilon} \right] \nabla \psi \\ &- \int_{\Omega} g_{\varepsilon} \left[ \phi_{\varepsilon} \right] (y) \partial_{\rho_{a, \varepsilon}} c \left( \cdot, y, \rho_{a, \varepsilon}, \nu_{\psi} \right) H_{\psi_{\varepsilon}} \rho_{a, \varepsilon} \nu_{\psi} \, \mathrm{d} \mathcal{L}^{3}(y) \\ &- \int_{\Omega} g_{\varepsilon} \left[ \phi_{\varepsilon} \right] (y) \mathbb{P}_{\nu_{\psi}} \nabla \left( \partial_{\rho_{a, \varepsilon}} c \left( \cdot, y, \rho_{a, \varepsilon}, \nu_{\psi} \right) \right) g_{\varepsilon} [\psi] \rho_{a, \varepsilon} \, \mathrm{d} \mathcal{L}^{3}(y). \end{split}$$

The imposed boundary conditions are

$$v_{\varepsilon}|_{\partial\Omega} = 0,$$
 (1e)

$$\partial_{\nu}\phi_{\varepsilon}|_{\partial\Omega} = \partial_{\nu}\psi_{\varepsilon}|_{\partial\Omega} = 0,\tag{1f}$$

$$J_{\phi_{\alpha}}|_{\partial\Omega} \cdot \nu = J_{\psi_{\alpha}}|_{\partial\Omega} \cdot \nu = 0, \tag{1g}$$

$$\rho_{a,\varepsilon}|_{\partial\Omega} = \rho_{i,\varepsilon}|_{\partial\Omega} = 0,\tag{1h}$$

where

$$J_{\phi_{\varepsilon}} = \nabla \left( \nabla_{\phi}^{L^{2}} \mathcal{S}_{\Gamma}^{\varepsilon}[\phi] + \nabla_{\phi_{\varepsilon}}^{L^{2}} \mathcal{C}_{\varepsilon} \left[ \phi, \psi, \rho_{a, \varepsilon} \right] \right),$$

and

$$J_{\psi_{\varepsilon}} = \nabla \left( \nabla_{\psi}^{L^2} \mathcal{S}_{\Sigma}^{\varepsilon}[\psi] + \nabla_{\psi_{\varepsilon}}^{L^2} C_{\varepsilon} \left[ \phi, \psi, \rho_{a, \varepsilon} \right] \right).$$

In addition, we consider evolution equations for the active and inactive linkers on the diffuse surface of the cell cortex:

$$g_{\varepsilon} [\psi_{\varepsilon}] \partial_{t} \rho_{a,\varepsilon} - v_{\nu_{\psi_{\varepsilon}}} H_{\psi_{\varepsilon}} \rho_{a,\varepsilon} - \nabla \cdot (g_{\varepsilon} [\psi_{\varepsilon}] \eta_{a} \nabla \rho_{a}) + \nabla \cdot (g_{\varepsilon} [\psi_{\varepsilon}] v_{\varepsilon\tau} \rho_{a}) =$$

$$g_{\varepsilon} [\psi_{\varepsilon}] \mathcal{R} [\rho_{a}, \rho_{i}, \phi_{\varepsilon}, \nu_{ib}], \qquad (1i)$$

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$$g_{\varepsilon} [\psi_{\varepsilon}] \partial_{t} \rho_{i,\varepsilon} - v_{\nu_{\psi_{\varepsilon}}} H_{\psi_{\varepsilon}} \rho_{i,\varepsilon} - \nabla \cdot (g_{\varepsilon} [\psi_{\varepsilon}] \eta_{i} \nabla \rho_{i}) + \nabla \cdot (g_{\varepsilon} [\psi_{\varepsilon}] v_{\varepsilon\tau} \rho_{i}) = -g_{\varepsilon} [\psi_{\varepsilon}] \mathcal{R} [\rho_{\alpha}, \rho_{i}, \phi_{\varepsilon}, \nu_{\psi}],$$

$$(1j)$$

where

$$\mathcal{R}\left[\rho_{a,\varepsilon},\rho_{i,\varepsilon},\phi_{\varepsilon},\nu_{\psi}\right] = k\rho_{i,\varepsilon} - \rho_{a,\varepsilon}r\left[\phi_{\varepsilon},\nu_{\psi}\right].$$

The term  $k\rho_{i,\varepsilon}$  is the effective reconnection rate,  $k \ge 0$ , of the inactive linkers, and

$$\rho_{a,\varepsilon}r\left[\phi_{\varepsilon},\nu_{\psi}\right]$$

is the effective disconnection rate of the active linkers in relation to the membrane position in space and the orientation of the cortex given by its normal.

For a thorough discussion and further references, the reader may please refer to Werner [14]. In the following section, we describe steps one, two and four, but leave out the lengthy calculations involved for step three. For the following discussion, however, we need the concrete expression for all the  $L^2$ -gradients of the energies, so we give them here without doing the calculations. Note that these calculations depend on the boundary conditions (1e), (1f), (1g) and (1h):

$$\nabla_{\varphi}^{L^{2}} S_{\Phi}^{\varepsilon} = \nabla_{\varphi}^{L^{2}} \mathcal{W}_{\varepsilon} + \nabla_{\varphi}^{L^{2}} \mathcal{G}_{\varepsilon}$$
 (2a)

$$\nabla_{\varphi}^{L^{2}} \mathcal{G}_{\varepsilon} = -\varepsilon \Delta \varphi_{\varepsilon} + \frac{1}{\varepsilon} W'(\varphi_{\varepsilon}) = : \mu \left[ \varphi_{\varepsilon} \right], \tag{2b}$$

$$\nabla_{\varphi}^{L^{2}} \mathcal{W}_{\varepsilon} = -\Delta \left( \mu_{\varepsilon}[] \varphi_{\varepsilon} \right) + \mu \left[ \varphi_{\varepsilon} \right] \frac{1}{\varepsilon^{2}} W^{\prime \prime} \left( \varphi_{\varepsilon} \right)$$
 (2c)

For easier expression of the coupling energy gradients, we introduce

$$C_{\psi}(t,y) = \int_{\Omega} g_{\varepsilon} \left[ \psi_{\varepsilon} \right](x) c\left( x, y, \rho_{a}(t,x), \nu_{\psi_{\varepsilon}(t)}(x) \right) d\mathcal{L}^{3}(x),$$

$$C_{\phi}(t,x) = \int_{\Omega} g_{\varepsilon} \left[\phi_{\varepsilon}\right](y) c\left(x,y,\rho_{a}(t,x),\nu_{\psi_{\varepsilon}(t)}(x)\right) d\mathcal{L}^{3}(y).$$

Then,

$$\nabla^{L^{2}}_{\phi_{\varepsilon}}C_{\varepsilon} = \mu_{0}\left[\phi_{\varepsilon}\right](y)C_{\psi}(y) - \int_{\Omega}\varepsilon g_{\varepsilon}\left[\psi_{\varepsilon}\right](x)\nabla_{y}\phi_{\varepsilon} \cdot \nabla_{y}\left(c\left(x,y,\rho_{a,\varepsilon},\nu_{\psi}\right)\right) d\mathcal{L}^{3}(x), \tag{2d}$$

$$\nabla_{\psi_{\varepsilon}}^{L^{2}} C_{\varepsilon} = \mu_{0} \left[ \psi_{\varepsilon} \right] (x) C_{\phi}(x) - \int_{\Omega} \varepsilon g_{\varepsilon} \left[ \phi_{\varepsilon} \right] (y) \nabla_{x} \left( c \left( x, y, \rho_{a, \varepsilon}, \nu_{\psi} \right) \right) \cdot \nabla_{x} \psi_{\varepsilon} \, d\mathcal{L}^{3}(y)$$

$$- \int_{\Omega} g_{\varepsilon} \left[ \phi_{\varepsilon} \right] (y) \nabla_{x} \cdot \left( g_{\varepsilon} \left[ \psi_{\varepsilon} \right] (x) \nabla_{\nu} c \left( x, y, \rho_{a, \varepsilon}, \nu_{\psi} \right)^{T} \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}} \right) d\mathcal{L}^{3}(y). \tag{2e}$$

Solutions of Equation (1) fulfil an energy inequality, compare Werner et al. [13]. This energy inequality reads

$$\begin{split} \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F}_{\varepsilon} \left[ \phi_{\varepsilon}, \psi_{\varepsilon}, \rho_{a, \varepsilon} \right] &\leq - \left\| \nabla v_{\varepsilon} \right\|_{\left[ L^{2}(\Omega) \right]^{(3, 3)}}^{2} \\ &- m \left( \phi_{\varepsilon} \right) \left\| \nabla \left( \nabla_{\phi_{\varepsilon}}^{L^{2}} \mathcal{S}_{\Gamma}^{\varepsilon} \left[ \phi_{\varepsilon} \right] + \nabla_{\phi_{\varepsilon}}^{L^{2}} \mathcal{C}_{\varepsilon} \left[ \phi_{\varepsilon}, \psi_{\varepsilon}, \rho_{a, \varepsilon} \right] \right) \right\|_{L^{2}(\Omega)}^{2} \end{split}$$

(4g)

### Sharp interface model

We introduce two evolving, two-dimensional manifolds  $\Gamma_T = (\Gamma(t))_{t \in [0,T]}$  for the cell membrane, and  $\Sigma_T = (\Sigma(t))_{t \in [0,T]}$ for the cell cortex. These evolving manifolds can also be described as the level sets  $\Gamma(t) = \phi^{-1}(t,0)$  and  $\Sigma(t) = \psi^{-1}(t,0)$  of functions  $\phi: \Omega \times [0,T] \to \mathbb{R}$  and  $\psi: \Omega \times [0,T] \to \mathbb{R}$ . The cell we consider is swimming in a fluid with pressure p and velocity v. Additionally, we have the density  $\rho_a: \Sigma_T \to \mathbb{R}$  of linker proteins connecting cell membrane and cell cortex, which we call active linkers. Another density  $\rho_i: \Sigma_T \to \mathbb{R}$  is introduced to model the density of the disconnected or broken proteins, called inactive linkers; these no longer couple cell membrane and cell cortex, but may be reconnected due to healing mechanisms inside the cell.  $\Omega = \Omega \setminus (\Gamma(t) \cup \Sigma(t))$ 

$$\rho \left(\partial_{t} v + (v \cdot \nabla)v\right) - \nabla \cdot \mathbb{T} = 0 \qquad \text{in } \stackrel{\circ}{\Omega} \qquad (4a)$$

$$\nabla \cdot v = 0 \qquad \text{in } \stackrel{\circ}{\Omega} \qquad (4b)$$

$$v(t, \cdot) = 0 \qquad \text{on } \partial\Omega, \qquad (4c)$$

$$\|v\|_{\Gamma(t)} = 0 \qquad \text{on } \Gamma(t), \qquad (4d)$$

$$\|v\|_{\Sigma(t)} = 0 \qquad \text{on } \Sigma(t), \qquad (4e)$$

$$-\|\mathbb{T}v\| = \nabla_{\phi}^{L^{2}} S_{\Gamma} \nabla \phi - \left(\nabla_{y} C_{\Sigma}^{0} \cdot \nu_{\Gamma}\right) \nu_{\Gamma} + H_{\Gamma} C_{\Sigma}^{0} \nu_{\Gamma} \qquad \text{on } \Gamma(t), \qquad (4f)$$

$$-\|\mathbb{T}v\| = \nabla_{\psi}^{L^{2}} S_{\Sigma} \nabla \psi - \left(\nabla_{x} C_{\Gamma}^{0} \cdot \nu_{\Sigma}\right) \nu_{\Sigma} + H_{\Sigma} C_{\Gamma}^{0} \nu_{\Sigma}$$

$$- \partial_{\rho_{a}} C_{\Gamma}^{0} H_{\Sigma} \rho_{a} \nu_{\Sigma} - \nabla_{\Sigma} \left(\partial_{\rho_{a}} C_{\Gamma}^{0}\right) \rho_{a} - \nabla_{\Sigma} \cdot \left(\nabla_{\nu} C_{\Gamma}^{0}\right) \nu_{\Sigma}$$

$$- H_{\Sigma} \left(\nabla_{\nu} C_{\Gamma}^{0} \cdot \nu_{\Sigma}\right) \nu_{\Sigma} \qquad \text{on } \Sigma(t), \qquad (4g)$$

$$\partial_t \phi + \upsilon \cdot \nabla \phi = 0 \qquad \text{in } \Omega, \qquad (4h)$$

$$\partial_t \psi + \upsilon \cdot \nabla \psi = 0 \qquad \text{in } \Omega, \tag{4i}$$

$$\partial_t \rho_a - H \mathbf{v}_{\nu_0} \rho_a - \nabla_{\Sigma(t)} \cdot (\eta_a \nabla \rho_a) + \nabla_{\Sigma(t)} \cdot (\rho_a \nu_\tau) = \mathcal{R} \left[ \rho_a, \rho_i, \phi \nu_\Sigma \right]$$
 on  $\Sigma(t)$ , (4j)

$$\partial_{t}\rho_{i} - Hv_{\nu_{v}}\rho_{i} - \nabla_{\Sigma(t)} \cdot (\eta_{i}\nabla\rho_{i}) + \nabla_{\Sigma(t)} \cdot (\rho_{i}v_{\tau}) = S\left[\rho_{a}, \rho_{i}, \phi, \nu_{\Sigma}\right]$$
on  $\Sigma(t)$ . (4k)

The equations have to be solved with appropriate initial and boundary conditions. The initial data need to be related to the initial data of the phase field field model as specified in item 1. of Section 3.2.

#### 3 FORMAL ASYMPTOTIC ANALYSIS

Having outlined the physical principles, we are going to analyse the sharp interface limit of the phase field model. Let us now turn to the main result of this paper: we will demonstrate, using the method of formal asymptotic expansions,

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that classical solutions of the system (1) converge, for  $\varepsilon \to 0$ , to solutions of Equation (4). For a thorough theoretical introduction into the subject of formal asymptotic expansions, we refer to Eckhaus [25], whereas a more applicationoriented perspective is taken in Holmes [26].

#### 3.1 Interfacial coordinates

For the following analysis, we will need a coordinate transformation typical for asymptotic analysis of phase field equations for which boundary layers are expected in the regions where the phase fields are close to zero.

Let us denote a tubular neighbourhood of a smooth, orientable hypersurface  $S \subseteq \mathbb{R}^3$  by  $N_{\delta}(S)$ . We require that  $\delta \in (0, \infty)$  is small enough such that  $N_{\delta}(\Gamma(t)) \cap N_{\delta}(\Sigma(t)) = \emptyset$  for all  $t \in [0, T]$ . The local boundary layer coordinates, or interfacial coordinates (as they are most often termed in this context), with respect to S are defined by the map

$$\iota_{S,\varepsilon}: N_{\delta}(S) \to S \times \mathbb{R},$$

$$x \mapsto \left(\pi_{S}(x), \frac{d_{S}(x)}{\varepsilon}\right).$$

For two evolving manifolds  $\Gamma_T$ ,  $\Sigma_T$ , we extent this definition to

$$\iota_{\varepsilon}: \bigcup_{t \in [0,T]} \{t\} \times (N_{\delta}(\Gamma(t)) \cup N_{\delta}(\Sigma(t))) \to \bigcup_{t \in [0,T]} \{t\} \times (\Gamma(t) \cup \Sigma(t)) \times \mathbb{R},$$

$$\int (t \iota_{\Gamma(t),\sigma}(x)) \quad x \in N_{\varepsilon}(\Gamma(t))$$

$$(t,x) \mapsto \begin{cases} \left(t,\iota_{\Gamma(t),\varepsilon}(x)\right) & x \in N_{\delta}(\Gamma(t)) \\ \left(t,\iota_{\Sigma(t),\varepsilon}(x)\right) & x \in N_{\delta}(\Sigma(t)) \end{cases},$$

and then set

$$\iota_{S_T,\varepsilon} = \iota_{\varepsilon} \mid \bigcup_{t \in [0,T]} {\{t\} \times S(t)}$$

for  $S(t) \in \{\Gamma(t), \Sigma(t)\}$ . We always consider  $\delta$  small enough such that the interfacial coordinate transformations are welldefined. Generally, for a function f on  $\bigcup_{t\in[0,T]}\{t\}\times(N_{\delta}(\Gamma(t))\cup N_{\delta}(\Sigma(t)))$ , we define

$$\hat{f} \circ \iota_{\varepsilon}(t, x) = f(t, x).$$

The function  $\hat{f}$  depends on three arguments: The first is time, the second a point on one of the manifolds  $\Gamma(t)$  or  $\Sigma(t)$  and the third a real number from  $\left(-\frac{\delta}{\varepsilon}, \frac{\delta}{\varepsilon}\right)$ . The latter is occasionally referred to as 'fast variable' and derivatives with respect to this variable are denoted by  $(\cdot)'$ ; derivatives with respect to the first variable are denoted by  $\partial_s(\cdot)$ .

The following (standard) formulae will be important later.

**Lemma 3.1** cf. Gilbarg and Trudinger [19, Sec. 14.6]. Let  $S \subseteq \mathbb{R}^3$  be a real, orientable and sufficiently smooth submanifold and  $N_{\delta}(S)$ ,  $\delta \in \mathbb{R} > 0$ , a tubular neighbourhood on which all the following extended functions are defined. For all  $x \in N_{\delta}(S)$ , it holds

$$\bar{H}(x) = \sum_{i=1}^{2} \frac{\bar{\kappa}_{S,i}^{\nu}(x)}{1 - d_{S}(x)\bar{\kappa}_{S,i}^{\nu}(x)}$$

$$= \sum_{i=1}^{2} \bar{\kappa}_{S,i}^{\nu}(x) + d_{S}(x)\bar{\kappa}_{S,i}^{\nu}(x)^{2} + O\left(d_{S}(x)^{2}\right)$$

$$= \sum_{i=1}^{2} \left(\hat{\kappa}_{S,i} + \varepsilon z \hat{\kappa}_{S,i}^{2} + O\left(\varepsilon^{2}\right)\right) \circ \iota_{S,\varepsilon}\left(\pi_{S}(x)\right),$$
(5a)

$$\nabla(\bar{H})|_{x} \cdot \bar{\nu}(x) = \bar{H}(x)^{2} - 2\bar{K}(x). \tag{5c}$$

$$\nabla^2(\bar{H})|_{x} : \bar{\nu}(x) \otimes \bar{\nu}(x) = 2\bar{H}(x) \left(\bar{H}(x)^2 - 3\bar{K}(x)\right). \tag{5d}$$

#### 3.2 | Assumptions on the solution

Typically, formal asymptotic theories rely on non-trivial properties on the solution of the system under investigation, (1) in our case. A rigorous justification requires treatment of its own and is not in the scope of this work. We shall restrict ourselves to clearly formulating the properties we need in form of assumptions, and rather focus on the relation of the quantities of a solution of Equation (1) that assure a sensible behaviour in the limit. These assumptions can serve as a hint what needs to be investigated when a mathematical proof is to be given.

1. For every  $\varepsilon > 0$  the system (1) with boundary conditions (1e), (1f), (1g), (1h) and initial data  $\phi_{\varepsilon}(0,\cdot), \psi_{\varepsilon}(0,\cdot), \rho_{a,\varepsilon}(0,\cdot)$ , which converge in  $L^2(\Omega) \times L^2(\Omega) \times H^1(\Omega)$  for  $\varepsilon \searrow 0$  and form a recovery sequence of  $\mathcal{F}$ , has a classical solution

$$(v_{\varepsilon}, p_{\varepsilon}, \phi_{\varepsilon}, \psi_{\varepsilon}, \rho_{a,\varepsilon}, \rho_{i,\varepsilon})$$

on  $\Omega_T = [0, T] \times \Omega$  for some time T > 0 being independent of  $\varepsilon$ . Throughout this work, we choose the mobilities of the phase field to be a power of  $\varepsilon$ :  $m(\phi) = m(\psi) = \varepsilon^{\alpha}$  for  $\alpha \in \mathbb{R}_{>0}$ .

2. Additionally, there shall be two-dimensional, orientable, smoothly evolving manifolds

$$\Gamma(t) = \{ x \in \Omega \mid \phi_{\varepsilon}(t, x) = 0 \}, \quad \Sigma(t) = \{ x \in \Omega \mid \psi_{\varepsilon}(t, x) = 0 \},$$

which both enclose open sets  $\Omega_{\Gamma(t)}^-$  and  $\Omega_{\Sigma(t)}^-$ . The corresponding outer domains are defined such that  $\Omega_{\Gamma(t)}^+ = \Omega \setminus \Omega_{\Gamma(t)}^- \setminus \Gamma(t)$  and  $\Omega_{\Sigma(t)}^+ = \Omega \setminus \Omega_{\Sigma(t)}^- \setminus \Sigma(t)$ . It shall hold,  $\lim_{\epsilon \searrow 0} \phi_{\epsilon}(0, \cdot) = -1$  pointwise on  $\Omega_{\Gamma}^-$ , and  $\lim_{\epsilon \searrow 0} \phi_{\epsilon}(0, \cdot) = 1$  pointwise on  $\Omega_{\Gamma}^+$ , and analogously for  $\psi$  and  $\Sigma$ .

- 3. For sufficiently small T, it shall hold  $\Gamma(t) \cap \Sigma(t) = \emptyset$  for all  $t \in [0, T]$ .
- 4. The components of every classical solution to (1) shall have a regular asymptotic expansion in every compact subset U of  $\Omega_0 = \Omega \setminus \Gamma(t) \setminus \Sigma(t)$ , that is, for every  $q \in \{\phi_{\varepsilon}, \psi_{\varepsilon}, v_{\varepsilon}, p_{\varepsilon}, \rho_{a,\varepsilon}, \rho_{i,\varepsilon}\}$ , it holds

$$q|_{U}(t,x) = \sum_{i=0}^{n} q_{i}^{o}(t,x)\varepsilon^{i} + o(\varepsilon^{n}), \qquad (6)$$

for some  $n \in \mathbb{N}_0$ . All  $q_i^o$  shall be as smooth as q. We call these series *outer expansions of* q. This implies that a boundary layer is to be expected at most at  $\Gamma(t) \cup \Sigma(t)$ .

5. If  $q = \phi$ , Equation (6) shall even hold for all  $U \in \Omega_0 \cup \Sigma$  and if  $q = \psi$  for all  $U \in \Omega_0 \cup \Gamma$ . Thus, every phase field is expected to have only one boundary layer.

- 6. The species densities' evolution is irrelevant outside the diffuse layers around  $\Gamma_T$ ,  $\Sigma_T$ . We thus consider them to be asymptotically constant in time away from the diffuse layers: For every  $U \in \Omega_0$ , it holds  $\partial_t \left( \rho_{a,\varepsilon} |_U \right) \in O\left(\varepsilon^2\right)$ , which is equivalent to claiming  $\partial_t \rho_{a,\varepsilon_0}^o = 0 = \partial_t \rho_{a,\varepsilon_1}^o$ .
- 7. The components of every classical solution to Equation (1) shall have a regular asymptotic expansion in  $N_{\delta}(S)$ ,  $S \in \{\Gamma(t), \Sigma(t)\}$ , after transformation into local coordinates: For all  $q \in \{\phi_{\varepsilon}, \psi_{\varepsilon}, v_{\varepsilon}, p_{\varepsilon}, \rho_{a,\varepsilon}, \rho_{i,\varepsilon}\}$ , it holds  $q|_{\Gamma(t) \cup \Sigma(t)} = \hat{q} \circ \iota_{\varepsilon}$  such that

$$\hat{q}(t, s, z) = \sum_{k=-N}^{n} \varepsilon^{k} \hat{q}_{k}^{i}(t, s, z) + o(\varepsilon^{n})$$

for  $N, n \in \mathbb{N}_0$ , where all  $\hat{q}_k^i$  shall be integrable in z and as smooth as q. We call these series *inner expansions of* q.

- 8. Physically, the phase fields model the volume fraction of phases. Thus, they should always take values between -1 and 1, independent of how small  $\varepsilon$  may be. Hence, for  $q \in \{\phi, \psi\}$ , we assume  $\hat{q}^i_{\ell} = 0$  for all  $\ell \in \{-N, ..., -1\}$ .
- 9. For the species density  $\rho_{a,\varepsilon}$ , we additionally require that blow-ups are of order at most -1, that is,  $\hat{\rho}^i_{a,\varepsilon_\ell} = 0$  for all  $\ell \in \{-N, ..., -2\}$ . The reason why we cannot naturally expect boundedness here is that  $\rho_{a,\varepsilon}$  does not give the volume fraction, but the number of particles per volume of the active linkers.

We will often have to compute differential operators of functions that are expressed in interfacial coordinates:

Remark 3.2. For a sufficiently smooth function  $q: S_T \times \mathbb{R} \to \mathbb{R}$  on an evolving manifold  $S_T = \bigcup_{t \in [0,T]} \{t\} \times S_t$ , and  $t^* \in [0,T], x^* \in \Omega$ , it holds

$$\nabla_{x} \left( q \circ \iota_{S_{T}, \varepsilon} \right) (t^{*}, x^{*}) = \varepsilon^{-1} q' \left( \iota_{S_{T}, \varepsilon} (t^{*}, x^{*}) \right) \bar{v} \left( t^{*}, x^{*} \right) + \nabla_{S(t^{*})_{d(x^{*})}} q \left( \iota_{S_{T}, \varepsilon} (t^{*}, x^{*}) \right), \tag{7}$$

$$\Delta_{x}\left(q \circ \iota_{S_{T},\varepsilon}\right)(t^{*}, x^{*}) = \varepsilon^{-2}q''\left(\iota_{S_{T},\varepsilon}\left(t^{*}, x^{*}\right)\right) - \varepsilon^{-1}q'\left(\iota_{S_{T},\varepsilon}\left(t^{*}, x^{*}\right)\right)\bar{H}\left(t^{*}, x^{*}\right) + \Delta_{S\left(t^{*}\right)_{d_{(x^{*})}}}\vec{q}\left(\iota_{S_{T},\varepsilon}\left(t^{*}, x^{*}\right)\right),$$

$$(8)$$

$$\partial_{t} \left( q \circ \iota_{S_{T}, \varepsilon} \right) (t^{*}, x^{*}) = -\varepsilon^{-1} V_{\nu}^{S} \left( t^{*}, x^{*} \right) q' \left( \iota_{S_{T}, \varepsilon} \left( t^{*}, x^{*} \right) \right) + \partial_{t} q \left( \iota_{S_{T}, \varepsilon} \left( t^{*}, x^{*} \right) \right). \tag{9}$$

For  $\vec{q}: S_T \times \mathbb{R} \to \mathbb{R}^n$ , it holds

$$\nabla_{x} \cdot \left( \vec{q} \circ \iota_{S_{T}, \varepsilon} \right) (t^{*}, x^{*}) = \varepsilon^{-1} \vec{q}' \left( \iota_{S_{T}, \varepsilon} \left( t^{*}, x^{*} \right) \right) \cdot \bar{\nu} \left( t^{*}, x^{*} \right) + \nabla_{S(t^{*})_{d(x^{*})}} \cdot \vec{q} \left( \iota_{S_{T}, \varepsilon} \left( t^{*}, x^{*} \right) \right), \tag{10}$$

$$\nabla_{x} \left( \vec{q} \circ \iota_{S_{T}, \varepsilon} \right) (t^{*}, x^{*}) = \varepsilon^{-1} \vec{q}' \left( \iota_{S_{T}, \varepsilon} \left( t^{*}, x^{*} \right) \right) \otimes \bar{\nu} \left( t^{*}, x^{*} \right) + \nabla_{S(t^{*})_{d(x^{*})}} \vec{q} \left( \iota_{S_{T}, \varepsilon} \left( t^{*}, x^{*} \right) \right), \tag{11}$$

$$\Delta_{x}\left(\vec{q} \circ \iota_{S_{T},\varepsilon}\right)(t^{*}, x^{*}) = \varepsilon^{-2}\vec{q}^{\prime\prime}\left(\iota_{S_{T},\varepsilon}\left(t^{*}, x^{*}\right)\right) - \varepsilon^{-1}(\vec{q})^{\prime} \circ \iota_{S_{T},\varepsilon}\left(t^{*}, x^{*}\right)\bar{H}\left(t^{*}, x^{*}\right) + \Delta_{S(t^{*})_{d(x^{*})}}\vec{q}\left(\iota_{S_{T},\varepsilon}\left(t^{*}, x^{*}\right)\right). \tag{12}$$

For  $Q: S_T \times \mathbb{R} \to \mathbb{R}^{(n,n)}$ , it holds

$$\nabla_{x} \cdot \left( Q \circ \iota_{S_{T}, \varepsilon} \right) (t^{*}, x^{*}) = \varepsilon^{-1} Q' \left( \iota_{S_{T}, \varepsilon} \left( t^{*}, x^{*} \right) \right) \bar{\nu} \left( t^{*}, x^{*} \right) + \nabla_{S \left( t^{*} \right)_{d(x^{*})}} \cdot Q \left( \iota_{S_{T}, \varepsilon} \left( t^{*}, x^{*} \right) \right)$$

$$\tag{13}$$

Let us further exercise some smaller expansions.

**Lemma 3.3.** For  $\varphi \in \{\psi, \phi\}$ , the following expansions hold:

$$|\nabla \varphi| = \nu \cdot \nabla \varphi = \left(\varepsilon^{-1} \hat{\varphi}_0' + \hat{\varphi}_1' + \varepsilon \hat{\varphi}_2'\right) \circ \iota_{\varepsilon} + O\left(\varepsilon^2\right),\tag{14}$$

$$W(\varphi) = W(\varphi_0) + \varepsilon W'(\varphi_0) \varphi_1 + \varepsilon^2 \left( W'(\varphi_0) \varphi_2 + W''(\varphi_0) \varphi_1^2 \right) + O(\varepsilon^3), \tag{15}$$

$$g_{\varepsilon}[\varphi] = \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\varphi}_{0}^{\prime} \right)^{2} \circ \iota_{\varepsilon} + W \left( \varphi_{0} \right) \right) + 2 \left( \hat{\varphi}_{0}^{\prime} \hat{\varphi}_{1}^{\prime} \right) \circ \iota_{\varepsilon} + W^{\prime} \left( \varphi_{0} \right) \varphi_{1} + O(\varepsilon), \tag{16}$$

$$|\nabla \varphi|^{-1} = \varepsilon \left(\hat{\varphi}_0'\right)^{-1} \circ \iota_{\varepsilon} + \varepsilon^2 \frac{\hat{\varphi}_1' \circ \iota_{\varepsilon}}{\left(\hat{\varphi}_0'\right)^2 \circ \iota_{\varepsilon}} + O\left(\varepsilon^3\right). \tag{17}$$

If  $\varphi$  is the optimal profile at leading order, that is,  $\hat{\varphi}_{0}'' \circ \iota_{\varepsilon} - W'(\varphi_{0}) = 0$  we further have

$$H_{\varphi} = \varepsilon^{-1} \hat{\varphi}_{0}^{\prime} \circ \iota_{\varepsilon} \left( \hat{\varphi}_{0}^{\prime} \circ \iota_{\varepsilon} \bar{H} + \hat{\varphi}_{1}^{\prime\prime} \circ \iota_{\varepsilon} + W^{\prime\prime} \left( \varphi_{0} \right) \varphi_{1} \right) + O(1). \tag{18}$$

Proof. Ad (16): We use Equation (14) to compute

$$g_{\varepsilon}[\rho] = \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\rho}_{0}^{\prime} \right)^{2} \circ \iota_{\varepsilon} + W \left( \rho_{0} \right) \right) + 2 \left( \hat{\rho}_{0}^{\prime} \hat{\rho}_{1}^{\prime} \right) \circ \iota + W^{\prime} \left( \rho_{0} \right) \rho_{1} + O(\varepsilon).$$

Ad (17): Observe,

$$\left|\nabla\left(\rho_{0} + \varepsilon r_{1}\right)\right|^{-1} = \left|\nabla\rho_{0}\right|^{-1} - \varepsilon \frac{\nabla\rho_{0} \cdot \nabla r_{1}}{\left|\nabla\rho_{0}\right|^{3}} + O\left(\varepsilon^{3}\right). \tag{19}$$

Note further that  $|\nabla \rho_0|^{-1} = (\nabla \rho_0 \cdot \nu)^{-1} = (\varepsilon^{-1} \hat{\rho}_0' \circ \iota_{\varepsilon})^{-1} = \varepsilon (\hat{\rho}_0' \circ \iota_{\varepsilon})^{-1}$  and  $\nabla r_1 = \varepsilon^{-1} \hat{\rho}_1' \circ \iota_{\varepsilon} \nu + O(1)$  so that

$$\varepsilon \frac{\nabla \rho_{0} \cdot \nabla r_{1}}{\left|\nabla \rho_{0}\right|^{3}} = \frac{\varepsilon^{-1} \hat{\rho}_{0}' \circ \iota_{\varepsilon} \hat{\rho}_{1}' \circ \iota_{\varepsilon} + O(1)}{\left|\nabla \rho_{0}\right|^{3}} \in O\left(\varepsilon^{2}\right).$$

Ad (18): Expand

$$\begin{split} H_{\rho} &= |\nabla \rho| \left( -\varepsilon \Delta \rho + \varepsilon^{-1} W'(\rho) \right) \\ &\stackrel{(1)}{=} \left( \varepsilon^{-1} \hat{\rho}_{0}' \circ \iota_{\varepsilon} + \hat{\rho}_{1}' \circ \iota_{\varepsilon} + O(\varepsilon) \right) \left( -\varepsilon^{-1} \hat{\rho}_{0}'' \circ \iota_{\varepsilon} + \hat{\rho}_{0}' \circ \iota_{\varepsilon} \bar{H} + \hat{\rho}_{1}'' \circ \iota_{\varepsilon} + \varepsilon^{-1} W'(\rho_{0}) + W''(\hat{\rho}_{0}) \rho_{1} + O(\varepsilon) \right) \\ &\stackrel{(2)}{=} \varepsilon^{-1} \hat{\rho}_{0}' \circ \iota_{\varepsilon} \left( \hat{\rho}_{0}' \circ \iota_{\varepsilon} \bar{H} + \hat{\rho}_{1}'' \circ \iota_{\varepsilon} + W''(\rho_{0}) \rho_{1} \right) + O(1), \end{split}$$

where for Equation (1), we employ Equation (8), and for Equation (2), the optimal profile equation.

A common principle, which we will make use of in the following multiple times, is summarised in the following:

**Lemma 3.4.** Let  $\Gamma \subseteq \Omega$  be a smooth hypersurface. Let  $p \in L^1(\mathbb{R})$  with

$$\sup_{|t|>s} |p(t)t| \le \frac{C}{s^m}$$

for some  $C \in [0, \infty)$  and  $m \in (0, \infty)$ ,  $f_{\varepsilon} \in C(\Omega)$ , and for all sequences  $x_{\varepsilon} \xrightarrow{\varepsilon \to 0} x$ , it holds  $f_{\varepsilon}(x_{\varepsilon}) \xrightarrow{\varepsilon \to 0} f(x)$  with  $||f_{\varepsilon}||_{L^{\infty}(\Omega)} < M$  for some  $M \in (0, \infty)$  being independent of  $\varepsilon$ . Then,

$$\varepsilon^{-1} \int_{\Omega} p\left(\frac{d_{\Gamma}(x)}{\varepsilon}\right) f_{\varepsilon}(x) d\mathcal{L}^{3}(x) \xrightarrow{\varepsilon \to 0} \int_{-\infty}^{\infty} p(s) d\mathcal{L}^{1}(s) \int_{\Gamma} f(x) d\mathcal{H}^{2}(x).$$

After the preliminaries are fixed, we shall proceed by analysing the asymptotic behaviour of the solution of Equation (1).

#### 3.3 | Outer expansion

We start with investigating the solutions' behaviour away from the boundary layer, that is, on a set  $\Omega_{\delta} = \Omega \setminus (N_{\delta}(\Gamma) \cup N_{\delta}(\Sigma))$  for some  $\delta > 0$ . Let  $\varphi \in \{\phi_{\varepsilon}, \psi_{\varepsilon}\}$  for the following considerations.

Due to the recovery sequence property of the initial data postulated in Assumption 1,

$$\mathcal{F}_{\varepsilon}\left[v_{\varepsilon}(0,\cdot),\phi_{\varepsilon}(0,\cdot),\psi_{\varepsilon}(0,\cdot),\rho_{a,\varepsilon}(0,\cdot)\right]\in O(1).$$

Further, the sufficiently fast decay of the species densities' time derivative, see Assumption 6 imply

$$\int_{\Omega_{\varepsilon}} g_{\varepsilon}[\phi](y) \int_{\Omega_{\varepsilon}} g_{\varepsilon}[\psi](x) \partial_{\rho_{a,\varepsilon}} c\left[\partial_{t} \rho_{a,\varepsilon}\right] d\mathcal{L}^{3}(x) d\mathcal{L}^{3}(y) \in O(1).$$

From (1c) and (1d), we also obtain

$$\varepsilon^{\alpha} \Delta \left( \nabla_{\varphi}^{L^{2}} \mathcal{S}_{\Gamma}^{\varepsilon} [\varphi] + \nabla_{\varphi}^{L^{2}} \mathcal{C}_{\varepsilon} \right) \in O(1),$$

so for  $\alpha < 1$ ,  $\nabla_{\varphi}^{L^2} S_{\Gamma}^{\varepsilon}[\varphi] + \nabla_{\varphi}^{L^2} C_{\varepsilon} \in O(1)$  (Bringing  $\varepsilon^{\alpha}$  to the right, all leading order terms of  $\Delta \left( \nabla_{\varphi}^{L^2} S_{\Gamma}^{\varepsilon}[\varphi] + \nabla_{\varphi}^{L^2} C_{\varepsilon} \right)$  from order -3 to -1 have no match on the right-hand side and thus have to be zero following the separation of scales argument. Using that the Neumann boundary conditions (1g) do not depend on  $\varepsilon$ , we can thus conclude that all these terms are of order zero.) Comparing the right-hand side of (1a) with its left-hand side, we conclude

$$\int_{\Omega_{\delta}} H_{\psi}(x) \rho_{a,\varepsilon}(t,x) \mathrm{v}_{\nu_{\psi}}(t,x) \int_{\Omega_{\delta}} g_{\varepsilon}[\phi](y) \partial_{\rho_{a,\varepsilon}} c\left(x,y,\rho_{a,\varepsilon},\nu_{\psi}\right) \, \mathrm{d}\mathcal{L}^{3}(y) \, \mathrm{d}\mathcal{L}^{3}(x) +$$

$$\int_{\Omega_{\varepsilon}} \int_{\Omega_{\varepsilon}} g_{\varepsilon} \left[ \phi_{\varepsilon} \right] (y) \nabla \left( \partial_{\rho_{a,\varepsilon}} c \left( \cdot, y, \rho_{a,\varepsilon}, \nu_{\psi} \right) \right) \cdot \upsilon_{\tau} g_{\varepsilon} [\psi] \rho_{a,\varepsilon} \, \mathrm{d} \mathcal{L}^{3}(y) \, \mathrm{d} \mathcal{L}^{3}(x) \in O(1).$$

It, thus, follows from Equation (3) that

ess 
$$\sup_{t \in [0,T]} \mathcal{F}_{\varepsilon} [\phi_{\varepsilon}, \psi_{\varepsilon}, \rho_{a}] \in O(1).$$

Therefore,  $\int_{\Omega_{\delta}} \frac{\varepsilon}{2} |\nabla \rho|^2 + \varepsilon^{-1} W(\rho) d\mathcal{L}^3 \in O(1)$  for all  $t \in [0, T]$ , and we conclude  $W(\varphi) \in O(\varepsilon)$ . Inserting the outer expansion of  $\varphi$  into  $W(\varphi)$  brings

$$W(\varphi) = \left(\left(\varphi_0^o\right)^2 - 1\right)^2 + O(\varepsilon).$$

Hence, it must hold

$$\left. \left( \left( \varphi_0^o \right)^2 - 1 \right)^2 \right|_{\Omega_s} = 0$$

for any  $\delta > 0$ . This further implies  $\varphi_0^0 \mid \Omega_\delta(t,\cdot) \in \{-1,1\}$  for all  $t \in [0,T]$ . For the initial data of  $\varphi$ , we have (cf. Assumption 2)  $\varphi_0^0(0,\cdot) = -1$  in  $\Omega_S^-$  and 1 in  $\Omega_S^+$ ,  $S \in \{\Gamma,\Sigma\}$ , so that we can argue by continuity in time that

$$\varphi_0^o\Big|_{\Omega_S^- \setminus N_\delta(S)}(t, \cdot) = -1 \text{ and } \varphi_0^o\Big|_{\Omega_S^+ \setminus N_\delta(S)}(t, \cdot) = 1 \text{ for all } t \in [0, T],$$
(20)

which is the essential result of this paragraph.

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#### 3.4 | Inner expansion

As there is no danger of confusion, we drop the subscript  $\varepsilon$  on the physical quantities. Let us first note that the result of the previous paragraph can be combined with the principle of asymtptotic matching on the phase fields such that we obtain

$$\left(\lim_{z \nearrow \infty} \hat{\phi}_0^i(\cdot, \cdot, z)\right) \circ \iota_{\varepsilon}(t, x) = \lim_{\substack{x \to \Gamma \\ x \in \Omega_{\Gamma}^+}} \phi_0^o(t, x) = 1 \tag{21}$$

for  $x \in N_{\delta}(\Gamma) \cap \Omega_{\Gamma}^+$ , that is,  $d_{\Gamma}(x) > 0$ . Analogously,

$$\left(\lim_{z \searrow -\infty} \hat{\phi}_0^i(\cdot, \cdot, z)\right) \circ \iota_{\varepsilon}(t, x) = \lim_{\substack{x \to \Gamma \\ x \in \Omega_{\Gamma}^-}} \phi_0^o(t, x) = -1$$
(22)

for  $x \in N_{\delta}(\Gamma) \cap \Omega_{\Gamma}^{-}$  and mutatis mutandis for  $\psi$ .

Remark 3.5. An immediate consequence of the matching principle and the assumption that  $q_{\ell}^o = 0$  for all  $\ell \in \{-N, ..., -1\}$  of the outer expansion is

$$\lim_{Z \to +\infty} \hat{q}_{\ell} = 0 \quad \text{for all } \ell \in \{-N, \dots, -1\}$$
 (23)

of the inner expansion. This also holds for all derivatives as long as they exist.

#### 3.5 | Properties of $\hat{v}$ and $\hat{p}$ to leading order

Let  $S \in \{\Gamma, \Sigma\}$ . To obtain insight on the higher-order coefficients in the expansion of the velocity and the pressure, we exploit the structure of the Navier–Stokes equations (1a), (1b) following Abels and Liu [16, p. 486, Section A.1.2]. Due to Assumption 8,  $\nabla_{3b}^{L^2} \mathcal{W} \in O(\varepsilon^{-3})$ . Thus, for  $N \ge 3$ , we have from Equation (1a), at order  $\varepsilon^{-N-2}$ ,

$$-\eta \hat{v}_{-N}^{\prime\prime} \circ \iota_{\varepsilon} = 0$$

With Equation (23), it further follows  $\hat{v}'_{-N} = 0$ . From  $\hat{v}'_{-N} = 0$  with Equation (23), we conclude analogously  $\hat{v}_{-N} = 0$ . At order  $\varepsilon^{-N-1}$ , the equation is

$$-\eta \hat{v}_{-N+1}^{"} \circ \iota_{\varepsilon} + \hat{p}_{-N}^{\prime} \circ \iota_{\varepsilon} \bar{\nu} = 0. \tag{24}$$

From Equation (1b) we have, using Remark 3.2 (10), to leading order  $\varepsilon^{-N}$ :

$$\hat{v}'_{-N+1} \circ \iota_{\varepsilon} \cdot \bar{\nu} = 0. \tag{25}$$

Multiplying Equation (24) by  $\bar{\nu}$ , we find with Equation (25)

$$\hat{p}'_{-N} \circ \iota_{\varepsilon} = 0. \tag{26}$$

In turn, inserting Equation (26) back into Equation (24), we obtain  $\hat{v}''_{-N+1} = 0$ , and with Equation (23) further  $\hat{v}'_{-N+1} = 0$ . From  $\hat{v}'_{-N+1} = 0$  with Equation (23), we conclude analogously  $\hat{v}_{-N+1} = 0$ . Arguing verbatim with Equations (23), (26) implies  $\hat{p}_{-N} = 0$ .

Repeating the arguments of the previous paragraph, we may from now on assume w.l.o.g.  $\hat{v}_{\ell} = 0$  for all  $\ell \leq -3$  and  $\hat{p}_{\ell} = 0$  for all  $\ell \leq -4$ .

At order  $\varepsilon^{-4}$ , we have an additional right-hand side term

$$\varepsilon^{-4} \left( -\eta \hat{v}_{-2}^{\prime\prime} \circ \iota_{\varepsilon} + \hat{p}_{-3}^{\prime} \circ \iota_{\varepsilon} \bar{\nu} \right) = \varepsilon^{-1} \left( \nabla_{\phi}^{L^{2}} \mathcal{F} \hat{\phi}_{0}^{\prime} \circ \iota_{\varepsilon} \bar{\nu} + \nabla_{\psi}^{L^{2}} \mathcal{F} \hat{\psi}_{0}^{\prime} \circ \iota_{\varepsilon} \bar{\nu} \right) - \partial_{\rho_{a}} C_{\phi} H_{\psi_{0}^{i}} \nu_{\psi_{0}^{i}} \rho_{a-1}^{i}.$$

Multiplying again by  $\bar{\nu}$  and noting that due to the previous considerations  $\hat{v}'_{-2} \circ \iota_{\varepsilon} \cdot \bar{\nu} = 0$  (25), we have

$$\varepsilon^{-4} \hat{p}_{-3}' \circ \iota_{\varepsilon} = \varepsilon^{-1} \left( \nabla_{\phi}^{L^2} \mathcal{F} \hat{\phi}_0' \circ \iota_{\varepsilon} + \nabla_{\psi}^{L^2} \mathcal{F} \hat{\psi}_0' \circ \iota_{\varepsilon} \right) - \partial_{\rho_a} C_{\phi} H_{\psi_0^i} \nu_{\psi_0^i} \cdot \bar{\nu} \rho_{a-1}^i;$$

hence,  $\hat{v}_{-2}^{\prime\prime}=0$  and we may conclude  $\hat{v}_{-2}=0$  as before.

We cannot go further now. However, in Section 3.6, we show that actually  $\nabla^{L^2}_{\rho} \mathcal{W} \in O\left(\varepsilon^{-2}\right)$  and in Section 3.7 that  $\rho^i_a \in O(1)$  – using only the results on velocity and pressure we have derived here, which gives  $\hat{p}'_{-3} \circ \iota_{\varepsilon} = 0$  and further

$$\varepsilon^{-3}\hat{p}'_{-2}\circ\iota_{\varepsilon}=\varepsilon^{-1}\left(\nabla_{\phi}^{L^{2}}\mathcal{F}\hat{\phi}'_{0}\circ\iota_{\varepsilon}+\nabla_{\psi}^{L^{2}}\mathcal{F}\hat{\psi}'_{0}\circ\iota_{\varepsilon}\right)-\partial_{\rho_{a}}C_{\phi}H_{\psi_{0}^{i}}\nu_{\psi_{0}^{i}}\cdot\bar{\nu}\rho_{a0}^{i}$$

resulting in  $\hat{v}''_{-1} = 0$  and  $\hat{v}_{-1} = 0$ . All together, we can, thus, state that

$$\hat{v}_{\ell} = 0 \text{ for all } \ell \in \{-N, ..., -1\}, \text{ and } \hat{p}_{\ell} = 0 \text{ for all } \ell \in \{-N, ..., -3\}.$$
 (27)

## 3.6 | Optimal profiles of $\hat{\psi}$ and $\hat{\phi}$ to leading order

Leading order of  $\nabla_{\psi}^{L^2} \mathcal{G}$  and  $\nabla_{\psi}^{L^2} \mathcal{C}$  is at most  $\varepsilon^{-2}$ . We consider the evolution law (1d):

$$\partial_t \psi + v \cdot \nabla \psi = \varepsilon^{\alpha} \Delta \left( \nabla_{\psi}^{L^2} \mathcal{W} + \nabla_{\psi}^{L^2} \mathcal{G} + \nabla_{\psi}^{L^2} \mathcal{C} \right).$$

The left-hand side is at most of order  $\varepsilon^{-2}$  (since the velocity is at most of order  $\varepsilon^{-1}$ , see the previous Section 3.5). So requiring  $\alpha \leq 2$ , the leading order terms of  $\varepsilon^{\alpha} \Delta \left( \nabla_{\psi}^{L^2} \mathcal{W} \right)$  are of order  $\varepsilon^{-3}$  and must be zero, which is equivalent to the equation

$$\left(\left(\hat{\psi}_{0}^{\prime\prime\prime}-W^{\prime}\left(\hat{\psi}_{0}\right)\right)^{\prime\prime}-\left(\hat{\psi}_{0}^{\prime\prime\prime}-W^{\prime}\left(\hat{\psi}_{0}\right)\right)W^{\prime\prime}\left(\hat{\psi}_{0}\right)\right)^{\prime\prime}=0.$$

We pose the additional condition  $\hat{\psi}_0(t,s,0)=0$  (otherwise, we had infinitely many solutions by shifting along the abscissa). Further, we set  $g:=\left(\hat{\psi}_0''-W'\left(\hat{\psi}_0\right)\right)''-\left(\hat{\psi}_0''-W'\left(\hat{\psi}_0\right)\right)W''\left(\hat{\psi}_0\right)$  and observe that thanks to the counterparts of Equations (21), (22) for  $\psi$ ,  $\lim_{|z|\to\infty}g=0$ . By integration, we obtain

$$0 = g'(z) - g'(0),$$

and sending  $|z| \to \infty$  gives g'(0) = 0. Conclusively, g'(z) = 0 for all  $z \in \mathbb{R}$ . Repeating the argument, we obtain

$$0 = g(z) - g(0),$$

send  $|z| \to \infty$ , conclude g(0) = 0 and thus have g(z) = 0 for all  $z \in \mathbb{R}$ . Setting  $f := (\hat{\psi}_0'' \circ \iota_{\varepsilon} - W'(\psi_0))$ , a solution to

$$(\hat{\psi}_{0}^{"} - W'(\hat{\psi}_{0}))^{"} - (\hat{\psi}_{0}^{"} - W'(\hat{\psi}_{0})) W''(\hat{\psi}_{0}) = g = 0$$

is obviously given by f = 0. From

$$f = \hat{\psi}_0^{\prime\prime} \circ \iota_{\varepsilon} - W^{\prime}(\psi_0) = 0 \tag{28}$$

we further conclude with the counterparts of Equations (21), (22) for  $\psi$  that  $\hat{\psi}_0(z) = \tanh\left(\frac{z}{\sqrt{2}}\right)$ 

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The very same argument applies verbatim for  $\phi$ .

### 3.7 | Properties of $\hat{\rho}_a$ and $\hat{\rho}_i$ to leading order

The following analysis is conducted on the example of  $\hat{\rho_a}$ , but the arguments are the same for  $\hat{\rho_i}$ . We consider Equation (1i) on  $N_{\delta}(\Sigma)$ :

$$g_{\varepsilon}[\psi]\partial_{t}\rho_{a} - \mathbf{v}_{\nu_{\psi}}H_{\psi}\rho_{a} - \nabla\cdot(g_{\varepsilon}[\psi]\eta_{a}\nabla\rho_{a}) + \nabla\cdot(g_{\varepsilon}[\psi]\rho_{a}v_{\tau}) = g_{\varepsilon}[\psi]\mathcal{R}\left[\rho_{a},\rho_{i};\phi,\nu_{\psi}\right].$$

Using Equation (16), the results from Section 3.5, (27), the optimal profile found for  $\psi$  in Section 3.6 together with Equation (18), we have

$$g_{\varepsilon}[\psi] \partial_{t} \rho_{a}^{i}, \mathbf{v}_{\nu_{v}} H_{\psi} \rho_{a}^{i}, \nabla \cdot \left( g_{\varepsilon} \left[ \psi^{i} \right] \rho_{a}^{i} v_{\tau}^{i} \right), g_{\varepsilon}[\psi] \mathcal{R} \left[ \rho_{a}, \rho_{i}; \phi, \nu_{\psi} \right] \in O \left( \varepsilon^{-N-2} \right),$$

so to leading order only the terms at  $\varepsilon^{-N-3}$  of the diffusion term matter:

$$\nabla_{x} \cdot \left( \varepsilon^{-N-2} \left( \frac{1}{2} \left( \hat{\psi}_{0}' \right)^{2} + W \left( \hat{\psi}_{0} \right) \right) \circ \iota_{\varepsilon} \eta_{a} \hat{\rho}_{a-N}' \circ \iota_{\varepsilon} \bar{\nu} \right) = \varepsilon^{-N-3} \left( \left( \frac{1}{2} \left( \hat{\psi}_{0}' \right)^{2} + W \left( \hat{\psi}_{0} \right) \right) \eta_{a} \hat{\rho}_{a-N}' \hat{\nu} \right)' \cdot \bar{\nu} + O \left( \varepsilon^{-N-2} \right) = 0.$$

Thus,  $\left(\frac{1}{2}\left(\hat{\psi}_{0}'\right)^{2} + W\left(\hat{\psi}_{0}\right)\right)\eta_{a}\hat{\rho_{a-N}}'$  has to be constant in z. However,  $\frac{1}{2}\left(\hat{\psi}_{0}'\right)^{2} + W\left(\hat{\psi}_{0}\right)$  decays due to Equations (21) and (22). Simultaneously,  $\hat{\rho}_{a-N}'$  decays as  $|z| \to \infty$ , see Equation (23). Thus, it must even hold

$$\left(\frac{1}{2}\left(\hat{\psi}_{0}^{\prime}\right)^{2}+W\left(\hat{\psi}_{0}\right)\right)\eta_{a}\hat{\rho}a_{-N}^{\prime}=0$$

and so  $\hat{\rho}_{a-N}'(s,z) = 0$  for all s,z. Consequently,  $\hat{\rho}_a - N$  is constant in z. Leveraging Equation (23) again, it follows  $\hat{\rho}_a - N = 0$ . We may repeat this argument and find

$$\hat{\rho_{a\ell}} = 0 \quad \text{for all } \ell \in \{-N, \dots, -1\}.$$

Finally, we have to leading order:

$$\left(\left(\frac{1}{2}\left(\hat{\psi}_{0}^{\prime}\right)^{2}+W\left(\hat{\psi}_{0}\right)\right)\eta_{a}\hat{\rho_{a_{0}}}^{\prime}\hat{\nu}\right)^{\prime}\cdot\bar{\nu}=0,$$

and conclude

$$\hat{\rho}_{\alpha}'(s,z) = 0 \quad \text{for all } s, z. \tag{30}$$

## 3.8 | Further properties of $\hat{\phi}$ and $\hat{\psi}$

The expansion of the Willmore-Energy gradient in interfacial coordinates shall be

$$\widehat{\nabla_{\varphi}^{L^2W}} = \sum_{k=-3}^{\infty} \varepsilon^k \hat{e}_k(s, z),$$

and in original coordinates

$$\nabla_{\varphi}^{L^2} \mathcal{W} = \sum_{k=-3}^{\infty} \varepsilon^k e_k \left( \pi_{\Phi}(x), \frac{d_{\Phi}(x)}{\varepsilon} \right). \tag{31}$$

We are going to show that  $\hat{e}_{-3} = \hat{e}_{-2} = \hat{e}_{-1} = 0$  by dint of the energy inequality. Afterwards, we are going to see that important properties of  $\hat{\varphi}_0$ ,  $\hat{\varphi}_1$  and  $\hat{\varphi}_2$  follow from these equations that we will use when passing to the limit in the next Section 4. Before going on, let us calculate

$$\nabla_{\varphi}^{L^2} \mathcal{W}[\varphi] = -\Delta(\mu[\varphi]) + \varepsilon^{-2} \mu[\varphi] W^{\prime\prime}(\varphi)$$

Thanks to the optimal profiles at leading order for both phase fields, compare Section 3.6, we have  $\nabla_{\varphi}^{L^2}\mathcal{W}[\varphi] \in O\left(\varepsilon^{-2}\right)$ , and also  $\nabla_{\varphi}^{L^2}\mathcal{G}[\varphi] \in O(1)$ . We note further

$$\nabla_{\phi}^{L^2} \mathcal{C}(y) = \mu[\phi](y) C_{\psi}(y) - \varepsilon \int_{\Omega} g_{\varepsilon}[\psi](x) \nabla_y \phi \cdot \nabla_y c\left(x,y,\rho_a,\nu_{\psi}\right) \, \mathrm{d}\mathcal{L}^3(x) \in O(1),$$

which follows from the optimal profile of  $\phi$  and  $\psi$  to leading order combined with Lemma 3.4. (The optimal profiles allow for showing the decaying condition that is the main prerequisite of Lemma 3.4.) For

$$\begin{split} \nabla_{\psi}^{L^{2}}C(x) &= \mu[\psi](x)C_{\phi}(x) - \int_{\Omega} \varepsilon g_{\varepsilon}[\phi](y)\nabla_{x}\left(c\left(x,y,\rho_{a},\nu_{\psi}\right)\right) \cdot \nabla_{x}\psi \,\mathrm{d}\mathcal{L}^{3}(y) \\ &- \int_{\Omega} g_{\varepsilon}[\phi](y)\nabla_{x} \cdot \left(g_{\varepsilon}[\psi](x)\nabla_{\nu}c\left(x,y,\rho_{a},\nu_{\psi}\right)^{T} \frac{1}{|\nabla\psi|}\mathbb{P}_{\nu_{\psi}}\right) \,\mathrm{d}\mathcal{L}^{3}(y) \in O(1), \end{split}$$

we have to additionally consider Equation (57), and note Equation (58), as well as  $\frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}} \in O(\varepsilon)$ . We conclude  $f_{N_{\delta}(S)} \nabla_{\varphi} \mathcal{F} d\mathcal{L}^3 \in O(\varepsilon^{-1})$  (again, leveraging Lemma 3.4 and using the optimal profile of  $\phi$  and  $\psi$  to verify the prerequisites). The energy inequality (3) gives us additionally

$$\int_0^T \int_{N_s(S)} \varepsilon^{\alpha} \left| \nabla \nabla_{\varphi} \mathcal{F} \right|^2 d\mathcal{L}^3 d\mathcal{L}^1 \in O(1).$$

Note that we can restrict to  $N_{\delta}(S)$  since the energies and their  $L^2$ -gradients are zero outside to leading order. Applying the Poincaré–Wirtinger inequality, we deduce,

$$\left(\int_0^T \int_{N_{\delta}(S)} \varepsilon^{\alpha} \left(\nabla_{\varphi} \mathcal{F} - \int_{N_{\delta}(S)} \nabla_{\varphi} \mathcal{F} \, \mathrm{d}\mathcal{L}^3\right)^2 \mathrm{d}\mathcal{L}^3 \, \mathrm{d}\mathcal{L}^1\right)^{\frac{1}{2}} \leq \left(\int_0^T \int_{N_{\delta}(S)} \varepsilon^{\alpha} \left|\nabla \nabla_{\varphi} \mathcal{F}\right|^2 \, \mathrm{d}\mathcal{L}^3 \, \mathrm{d}\mathcal{L}^1\right)^{\frac{1}{2}},$$

which implies, using the reversed triangle inequality for  $\|\cdot\|_{L^2(N_{\delta}(S))}$ ,

$$\left(\int_{0}^{T} \int_{N_{\delta}(S)} \varepsilon^{\alpha} \left| \nabla_{\varphi} \mathcal{F} \right|^{2} d\mathcal{L}^{3} d\mathcal{L}^{1} \right)^{\frac{1}{2}} - \sqrt{|N_{\delta}(S)|} \varepsilon^{\frac{\alpha}{2}} \int_{N_{\delta}(S)} \nabla_{\varphi} \mathcal{F} d\mathcal{L}^{3} \in O(1), \tag{32}$$

thus

$$\left(\int_{0}^{T} \int_{N_{\delta}(S)} \left| \nabla_{\varphi} \mathcal{F} \right|^{2} d\mathcal{L}^{3} d\mathcal{L}^{1} \right)^{\frac{1}{2}} - \sqrt{|N_{\delta}(S)|} \oint_{N_{\delta}(S)} \nabla_{\varphi} \mathcal{F} d\mathcal{L}^{3} \in O\left(\varepsilon^{-\frac{\alpha}{2}}\right), \tag{33}$$

SO

$$\int_0^T \int_{N_\delta(S)} \left| \nabla_\varphi \mathcal{F} \right|^2 \, \mathrm{d} \mathcal{L}^3 \, \mathrm{d} \mathcal{L}^1 \in O\left(\varepsilon^{-2}\right),$$

for  $\alpha \leq 2$ . By applying Young's inequality, we can deduce further

$$\int_{N_{\delta}(S)} \left| \nabla_{\varphi} \mathcal{F} \right|^2 \, \mathrm{d} \mathcal{L}^3 = \int_{N_{\delta}(S)} \left| \nabla_{\varphi}^{L^2} \mathcal{C} + \nabla_{\varphi}^{L^2} \mathcal{G} \right|^2 + 2 \nabla_{\varphi}^{L^2} \mathcal{W} \cdot \left( \nabla_{\varphi}^{L^2} \mathcal{C} + \nabla_{\varphi}^{L^2} \mathcal{G} \right) + \left| \nabla_{\varphi}^{L^2} \mathcal{W} \right|^2 \, \mathrm{d} \mathcal{L}^3,$$

which in turn implies

$$\frac{1}{2} \int_{N_{\delta}(S)} \left| \nabla_{\varphi}^{L^2} \mathcal{W} \right|^2 \, \mathrm{d} \mathcal{L}^3 \leq \int_{N_{\delta}(S)} \left| \nabla_{\varphi} \mathcal{F} \right|^2 + 3 \left| \nabla_{\varphi}^{L^2} \mathcal{C} + \nabla_{\varphi}^{L^2} \mathcal{G} \right|^2 \, \mathrm{d} \mathcal{L}^3,$$

so with the co-area formula, it follows

$$\varepsilon \int_{0}^{T} \int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon z}} \left| \widehat{\nabla_{\varphi}^{2} \mathcal{W}} \right|^{2} d\mathcal{H}^{2} d\mathcal{L}^{1}(z) d\mathcal{L}^{1} \in O\left(\varepsilon^{-2}\right). \tag{34}$$

From Equation (31), the expansion

$$\begin{split} \left| \widehat{\nabla L_{\varphi}^2 \mathcal{W}} \right|^2 &= \varepsilon^{-6} \hat{e}_{-3}^2 + \varepsilon^{-5} 2 \hat{e}_{-3} \hat{e}_{-2} + \varepsilon^{-4} \left( \hat{e}_{-2}^2 + 2 \hat{e}_{-3} \hat{e}_{-1} \right) + \varepsilon^{-3} \left( 2 \hat{e}_{-3} \hat{e}_0 + 2 \hat{e}_{-2} \hat{e}_{-1} \right) \\ &+ \varepsilon^{-2} \left( \hat{e}_{-1}^2 + \hat{e}_{-2} \hat{e}_0 + 2 \hat{e}_{-3} \hat{e}_1 \right) + O \left( \varepsilon^{-1} \right) \\ &= \sum_{k=-6}^{-2} \varepsilon^k f_k(s,z) + O \left( \varepsilon^{-1} \right) \end{split}$$

of the integrand follows directly. Equation (34) then requires

$$\int_0^T \int_{-\infty}^\infty \int_{\Phi} f_k \, \mathrm{d}\mathcal{H}^2 \, \mathrm{d}\mathcal{L}^1 \, \mathrm{d}\mathcal{L}^1 = 0$$

up to  $k \leq -4$ , so

$$\hat{e}_{-3}^2 = f_{-6} = 0$$
 a.e.  $\Longrightarrow \hat{e}_{-3} = 0$  a.e. 
$$\Longrightarrow \hat{e}_{-2}^2 = f_{-4} = 0$$
 a.e. 
$$\Longrightarrow \hat{e}_{-2} = 0$$
 a.e.

This in turn gives  $\nabla_{\varphi} \mathcal{F} \in O\left(\varepsilon^{-1}\right)$ , so  $f_{N_{\delta}(S)} \nabla_{\varphi} \mathcal{F} \, \mathrm{d} \mathcal{L}^3 \in O(1)$ , which we insert into Equation (32), and choose  $\alpha < 1$  to obtain

$$\int_{N_{\delta}(S)} \left| \nabla_{\varphi} \mathcal{F} \right|^2 \, \mathrm{d} \mathcal{L}^3 \in o \left( \varepsilon^{-1} \right)$$

hence,

$$\int_0^T \int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon z}} \left| \widehat{\nabla} \bar{L}_\varphi^2 \mathcal{W} \right|^2 \, \mathrm{d} \mathcal{H}^2 \, \mathrm{d} \mathcal{L}^1(z) \, \mathrm{d} \mathcal{L}^1 \in o\left(\varepsilon^{-2}\right),$$

so that  $\hat{e}_{-1} = 0$ .

Now that we have found equations  $\hat{e}_{-1} = 0$ ,  $\hat{e}_{-2} = 0$  and  $\hat{e}_{-3} = 0$ , we may derive information on  $\hat{\varphi}$  from them.

## 3.8.1 | Expansion of the $L^2$ -gradient of the Willmore energy

We recall that

$$\nabla_{\varphi}^{L_2} \mathcal{W} = -\Delta(\mu] \varphi]) + \epsilon^2 \mu [\varphi] W''(\varphi)$$
(35)

First, we expand the chemical potential,

$$\mu\left[\varphi_0 + \varepsilon e_1\right] = -\varepsilon \Delta \left(\varphi_0 + \varepsilon e_1\right) + \varepsilon^{-1} W'\left(\varphi_0 + \varepsilon e_1\right),\,$$

by expanding the Laplacian term:

$$\begin{split} \varepsilon\Delta\left(\varphi_{0}+\varepsilon e_{1}\right) = & \varepsilon^{-1}\hat{\varphi}_{0}^{\prime\prime}\circ\iota_{\varepsilon}-\hat{\varphi}_{0}^{\prime}\circ\iota_{\varepsilon}\bar{H}+\varepsilon\Delta_{\Gamma_{d(x)}}\varphi_{0} \\ & +\hat{\varphi}_{1}^{\prime\prime}\circ\iota_{\varepsilon}-\varepsilon\hat{\varphi}_{1}^{\prime}\circ\iota_{\varepsilon}\bar{H}+\varepsilon^{2}\Delta_{\Gamma_{d(x)}}\varphi_{1} \\ & +\varepsilon\hat{\varphi}_{2}^{\prime\prime}\circ\iota_{\varepsilon}-\varepsilon^{2}\hat{\varphi}_{2}^{\prime}\circ\iota_{\varepsilon}\bar{H} \\ & +\varepsilon^{2}\hat{\varphi}_{3}^{\prime\prime}\circ\iota_{\varepsilon}+O\left(\varepsilon^{3}\right) \end{split}$$

and the double well potential's first derivative:

$$\begin{split} \varepsilon^{-1}W'\left(\varphi_{0}+\varepsilon e_{1}\right) &= \varepsilon^{-1}\left(W'\left(\varphi_{0}\right)+\varepsilon W''\left(\varphi_{0}\right)e_{1}+\varepsilon^{2}W^{(3)}\left(\varphi_{0}\right)e_{1}^{2}+\varepsilon^{3}W^{(4)}\left(\varphi_{0}\right)e_{1}^{3}\right) \\ &= \varepsilon^{-1}W'\left(\varphi_{0}\right)+W''\left(\varphi_{0}\right)\left(\varphi_{1}+\varepsilon \varphi_{2}+\varepsilon^{2}\varphi_{3}\right)+\varepsilon W^{(3)}\left(\varphi_{0}\right)\left(\varphi_{1}^{2}+2\varepsilon \varphi_{1}\varphi_{2}\right)+\varepsilon^{2}W^{(4)}\left(\varphi_{0}\right)\varphi_{1}^{3} \\ &+O\left(\varepsilon^{3}\right) \\ &= \varepsilon^{-1}W'\left(\varphi_{0}\right)+W''\left(\varphi_{0}\right)\varphi_{1}+\varepsilon\left(W''\left(\varphi_{0}\right)\varphi_{2}+W^{(3)}\left(\varphi_{0}\right)\varphi_{1}^{2}\right) \\ &+\varepsilon^{2}\left(W''\left(\varphi_{0}\right)\varphi_{3}+2W^{(3)}\left(\varphi_{0}\right)\varphi_{1}\varphi_{2}+W^{(4)}\left(\varphi_{0}\right)\varphi_{1}^{3}\right)+O\left(\varepsilon^{3}\right). \end{split}$$

The expansion of the chemical potential then reads

$$\mu\left[\varphi_{0} + \varepsilon e_{1}\right] = \varepsilon^{-1}\mu_{-1}[\varphi] + \mu_{0}[\varphi] + \varepsilon\mu_{1}[\varphi] + \varepsilon^{2}\mu_{2}[\varphi] + O\left(\varepsilon^{3}\right) \tag{36}$$

with

$$\mu_{-1}[\varphi] = -\hat{\varphi}_{0}^{"} \circ \iota_{\varepsilon} + W^{\prime}(\varphi_{0}),$$

$$\mu_{0}[\varphi] = \hat{\varphi}_{0}^{\prime} \circ \iota_{\varepsilon} \bar{H} - \hat{\varphi}_{1}^{"} \circ \iota_{\varepsilon} + W^{"}(\varphi_{0}) \varphi_{1},$$

$$\mu_{1}[\varphi] = -\Delta_{\Gamma_{d(x)}} \varphi_{0} + \hat{\varphi}_{1}^{\prime} \circ \iota_{\varepsilon} \bar{H} - \hat{\varphi}_{2}^{"} \circ \iota_{\varepsilon} + W^{"}(\varphi_{0}) \varphi_{2} + W^{(3)}(\varphi_{0}) \varphi_{1}^{2},$$

$$\mu_{2}[\varphi] = -\Delta_{\Gamma_{d(x)}} \varphi_{1} + \hat{\varphi}_{2}^{\prime} \circ \iota_{\varepsilon} \bar{H} - \hat{\varphi}_{3}^{"} \circ \iota_{\varepsilon} + W^{"}(\varphi_{0}) \varphi_{3} + 2W^{(3)}(\varphi_{0}) \varphi_{1} \varphi_{2} + W^{(4)}(\varphi_{0}) \varphi_{1}^{3}.$$
(37)

*Expansion of*  $\Delta(\mu[\varphi])$ *:* 

We may rewrite  $\mu_i[\varphi] = \hat{\mu}_i[\hat{\varphi}] \circ \iota_{\varepsilon}$  and treat the Laplacian terms  $\Delta(\mu_i[\varphi])$  with Equation (8):

$$\Delta\left(\mu_{i}[\varphi]\right) = \varepsilon^{-2}\hat{\mu}_{i}[\hat{\varphi}]^{\prime\prime} \circ \iota_{\varepsilon} - \varepsilon^{-1}\hat{\mu}_{i}[\hat{\varphi}]^{\prime} \circ \iota_{\varepsilon}\bar{H} + \Delta_{\Gamma_{d(x)}}(\mu_{i}[\varphi])$$

giving

$$\begin{split} \Delta(\mu[\varphi]) = & \varepsilon^{-3} \left( \hat{\mu}_{-1}[\hat{\varphi}]'' \circ \iota_{\varepsilon} \right) + \\ & \varepsilon^{-2} \left( -\hat{\mu}_{-1}[\hat{\varphi}]' \circ \iota_{\varepsilon} \bar{H} + \hat{\mu}_{0}[\hat{\varphi}]'' \circ \iota_{\varepsilon} \right) + \\ & \varepsilon^{-1} \left( \Delta_{\Gamma_{d(x)}} \left( \mu_{-1}[\varphi] \right) - \hat{\mu}_{0}[\hat{\varphi}]' \circ \iota_{\varepsilon} \bar{H} + \hat{\mu}_{1}[\hat{\varphi}]'' \circ \iota_{\varepsilon} \right) + \\ & \Delta_{\Gamma_{d(x)}} \left( \mu_{0}[\varphi] \right) - \hat{\mu}_{1}[\hat{\varphi}]' \circ \iota_{\varepsilon} \bar{H} + \hat{\mu}_{2}[\hat{\varphi}]'' \circ \iota_{\varepsilon} + \\ & O(\varepsilon). \end{split}$$

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Expansion of  $\varepsilon^{-2}W''(\varphi)\mu[\varphi]$ :

For obtaining the expansion of  $\varepsilon^{-2}W''(\varphi)\mu[\varphi]$ , the remaining ingredient is an expansion of  $W''(\varphi)$ :

$$\varepsilon^{-2}W''(\varphi_0 + \varepsilon e_1) = \varepsilon^{-2}W''(\varphi_0) + \varepsilon^{-1}W^{(3)}(\varphi_0)\varphi_1 + W^{(3)}(\varphi_0)\varphi_2 + W^{(4)}(\varphi_0)\varphi_1^2 + \varepsilon \left(W^{(3)}(\varphi_0)\varphi_3 + 2W^{(4)}(\varphi_0)\varphi_1\varphi_2 + W^{(5)}(\varphi_0)\varphi_1^3\right) + O(\varepsilon^2).$$
(38)

Multiplication of Equations (36) and (38) gives

$$\begin{split} \varepsilon^{-2}W''(\varphi)\mu[\varphi] &= \varepsilon^{-3} \left( \mu_{-1}[\varphi]W''\left(\varphi_{0}\right) \right) + \\ \varepsilon^{-2} \left( \mu_{0}[\varphi]W''\left(\varphi_{0}\right) + \mu_{-1}[\varphi]W^{(3)}\left(\varphi_{0}\right)\varphi_{1} \right) + \\ \varepsilon^{-1} \left( \mu_{1}[\varphi]W''\left(\varphi_{0}\right) + \mu_{0}[\varphi]W^{(3)}\left(\varphi_{0}\right)\varphi_{1} + \mu_{-1}[\varphi]\left(W^{(3)}\left(\varphi_{0}\right)\varphi_{2} + W^{(4)}\left(\varphi_{0}\right)\varphi_{1}^{2}\right) \right) + \\ \mu_{2}[\varphi]W''\left(\varphi_{0}\right) + \mu_{1}[\varphi]W^{(3)}\left(\varphi_{0}\right)\varphi_{1} + \mu_{0}[\varphi]\left(W^{(3)}\left(\varphi_{0}\right)\varphi_{2} + W^{(4)}\left(\varphi_{0}\right)\varphi_{1}^{2}\right) + \\ \mu_{-1}[\varphi]\left(W^{(3)}\left(\varphi_{0}\right)\varphi_{3} + 2W^{(4)}\left(\varphi_{0}\right)\varphi_{1}\varphi_{2} + W^{(5)}\left(\varphi_{0}\right)\varphi_{1}^{3}\right) + \\ O(\varepsilon). \end{split}$$

Finally, we draw the following conclusions for  $\hat{\varphi}_0$ ,  $\hat{\varphi}_1$  and  $\hat{\varphi}_2$  by evaluating the equations  $\hat{e}_i = 0$ , for  $i \in \{-1, -2, -3\}$ :

- $\hat{e}_{-3} = 0$ : This is an equation we have already encountered in Section 3.6, and it reassures the optimal profile  $\hat{\varphi}_0(s, z) = \tanh\left(\frac{z}{\sqrt{2}}\right)$ .
- $\hat{e}_{-2} = 0$ : We use

$$0 = -\hat{\mu}_0[\hat{\varphi}]^{\prime\prime} \circ \iota_{\varepsilon} + \mu_0[\varphi]W^{\prime\prime}(\varphi_0), \tag{39}$$

and compute

$$-\hat{\mu}_{0}[\varphi]'' = -\left(\hat{\varphi}_{0}'\hat{H}\right)'' + \left(\hat{\varphi}_{1}'' - W''(\hat{\varphi}_{0})\,\hat{\varphi}_{1}\right)''$$

$$= -\hat{\varphi}_{0}^{(3)}\hat{H} - 2\hat{\varphi}_{0}''\hat{H}' - \hat{\varphi}_{0}'\hat{H}'' + \left(\hat{\varphi}_{1}'' - W''(\hat{\varphi}_{0})\,\hat{\varphi}_{1}\right)''$$
(40)

with

$$\hat{H}''(s,z) = \bar{H}(s + \varepsilon z \nu_S(s))' = \varepsilon \nabla \bar{H}(s + \varepsilon z \nu_S(s)) \cdot \nu_S(s)$$
(41)

and

$$\hat{H}''(s,z) = \bar{H}\left(s + \varepsilon z \nu_S(s)\right)'' = \varepsilon^2 \nabla^2 \bar{H}\left(s + \varepsilon z \nu_S(s)\right) : \nu_S(s) \otimes \nu_S(s). \tag{42}$$

Passing the last two terms to lower scales, we obtain from Equation (39),

$$-\bar{H}\hat{\varphi}_{0}^{(3)}\circ\iota_{\varepsilon}+\left(\hat{\varphi}_{1}^{\prime\prime}+W^{\prime\prime\prime}\left(\hat{\varphi}_{0}\right)\hat{\varphi}_{1}\right)^{\prime\prime}\circ\iota_{\varepsilon}-\left(-\bar{H}\hat{\varphi}_{0}^{\prime}\circ\iota_{\varepsilon}+\hat{\varphi}_{1}^{\prime\prime}\circ\iota_{\varepsilon}-W^{\prime\prime\prime}\left(\varphi_{0}\right)\varphi_{1}\right)W^{\prime\prime\prime}\left(\varphi_{0}\right)=0.$$

We note that from the optimal profile property  $\hat{\varphi}_0'' \circ \iota_{\varepsilon} - W'(\varphi_0) = 0$  the relation  $\hat{\varphi}_0^{(3)} = \hat{\varphi}_0'W''(\hat{\varphi}_0)$  directly follows, so we may further simplify:

$$\left(\hat{\varphi}_{1}^{\prime\prime}+W^{\prime\prime}\left(\hat{\varphi}_{0}\right)\hat{\varphi}_{1}\right)^{\prime\prime}\circ\iota_{\varepsilon}-\left(\hat{\varphi}_{1}^{\prime\prime}\circ\iota_{\varepsilon}-W^{\prime\prime}\left(\varphi_{0}\right)\varphi_{1}\right)W^{\prime\prime}\left(\varphi_{0}\right)=0,$$

which is solved by

$$\hat{\varphi}_1 = 0. \tag{43}$$

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•  $\hat{e}_{-1} = 0$ : Equation

$$0 = \bar{H}\hat{\mu}_0[\bar{\varphi}]' \circ \iota_{\varepsilon} - \hat{\mu}_1[\hat{\varphi}]'' \circ \iota_{\varepsilon} + \mu_1[\varphi]W''(\varphi_0) - 2\hat{\varphi}_0'' \circ \iota_{\varepsilon}\nabla \bar{H} \cdot \bar{\nu}(x)$$

is equivalent to

$$0 = \bar{H}^{2} \hat{\varphi}_{0}^{"} \circ \iota_{\varepsilon} - \hat{\mu}_{1}[\hat{\varphi}]^{"} \circ \iota_{\varepsilon} + \mu_{1}[\varphi] W^{"}(\varphi_{0}) - 2\hat{\varphi}_{0}^{"} \circ \iota_{\varepsilon} \nabla \bar{H} \cdot \bar{\nu}(x)$$

$$+ \varepsilon \bar{H} \hat{\varphi}_{0}^{'} \circ \iota_{\varepsilon} \nabla \bar{H} \cdot \bar{\nu}$$

$$(44)$$

using  $\hat{\varphi}_1 = 0$  so that  $\mu_0[\varphi] = \hat{\varphi}_0' \circ \iota_{\varepsilon} \bar{H}$ . We use Lemma 3.1 abbreviating  $\hat{H}(s,0) = : \hat{H}|_{\varsigma}(s)$ :

$$\nabla(\bar{H})\big|_{X} \cdot \bar{\nu}(X) = \left(\sum_{i=1}^{2} \hat{\kappa}_{i}^{2} + 2\varepsilon z \hat{\kappa}_{i}^{3} + O\left(\varepsilon^{2}\right)\right) \circ \iota_{\varepsilon}\left(\pi_{S}(X)\right)$$

$$= \left(\hat{H}\big|_{S}^{2} - 2\hat{K}\big|_{S} + 2\varepsilon z\left(\hat{H}\big|_{S}^{3} - 3\hat{H}\big|_{S}\hat{K}\big|_{S}\right) + O\left(\varepsilon^{2}\right)\right) \circ \iota_{\varepsilon}\left(\pi_{S}(X)\right)$$

$$(45)$$

and

$$\bar{H}(x)^{2} = \left(\hat{H}\Big|_{S} + \varepsilon z \left(\hat{H}\Big|_{S}^{2} - 2\hat{K}\Big|_{S}\right) + O\left(\varepsilon^{2}\right)\right)^{2} \circ \iota_{\varepsilon}(\pi_{S}(x))$$

$$= \left(\hat{H}\Big|_{S}^{2} + 2\varepsilon z \hat{H}\Big|_{S} \left(\hat{H}\Big|_{S}^{2} - 2\hat{K}\Big|_{S}\right) + O\left(\varepsilon^{2}\right)\right) \circ \iota_{\varepsilon}(\pi_{S}(x))$$
(46)

Passing all terms of lower order to the lower scales, we obtain

$$0 = \hat{H} \Big|_{S}^{2} \hat{\varphi}_{0}^{"} - \hat{\mu}_{1}[\hat{\varphi}]^{"} + \mu_{1}[\hat{\varphi}]W^{"}(\hat{\varphi}_{0}) - 2\hat{\varphi}_{0}^{"} \left(\hat{H} \Big|_{S}^{2} - 2\hat{K} \Big|_{S}\right)$$

$$= -\hat{\mu}_{1}[\hat{\varphi}]^{"} + \mu_{1}[\hat{\varphi}]W^{"}(\hat{\varphi}_{0}) - \hat{\varphi}_{0}^{"} \left(\hat{H} \Big|_{S}^{2} - 4\hat{K} \Big|_{S}\right). \tag{47}$$

We make the ansatz  $\hat{\mu}_1[\hat{\varphi}](s,z) = -\left(\hat{H}\Big|_S^2 - 4\hat{K}\Big|_S\right)(s)s_1(z)$  Then, Equation (47) becomes

$$0 = \left( \hat{H} \Big|_{S}^{2} - 4 \hat{K} \Big|_{S} \right) \left( s_{1}^{\prime \prime} - s_{1} W^{\prime \prime} \left( \hat{\varphi}_{0} \right) - \hat{\varphi}_{0}^{\prime \prime} \right).$$

Substituting  $\hat{\varphi}_{0}^{\prime\prime}=W^{\prime}\left(\hat{\varphi}_{0}\right)$ , and solving for

$$0=s_1^{\prime\prime}-s_1W^{\prime\prime}\left(\hat{\varphi}_0\right)-\hat{\varphi}_0^{\prime\prime}$$

gives  $s_1(z)=\frac{1}{2}\hat{\varphi}_0'(z)z$  as in Wang [18, Theorem 2.13, Equ. (2.29)], so

$$\hat{\mu}_1[\hat{\varphi}](s,z) = -\frac{1}{2} \left( \hat{H} \Big|_S^2 - 4\hat{K} \Big|_S \right) (s) \hat{\varphi}_0'(z) z. \tag{48}$$

### 3.9 | Revisiting $\hat{v}$ and $\hat{p}$ at leading order

The incompressibility (1b) gives with Equation (10) to leading order  $\varepsilon^{-1}$ 

$$\left(\hat{v}_0 \cdot \bar{v}\right)' = 0. \tag{49}$$

We have shown in Section 3.8 that  $\nabla_{\varphi}^{L^2} \mathcal{F} \in O(1)$ . This gives, by repeating the arguments used in Section 3.5,  $\hat{p}_{-2} = 0$ . Using Equations (9), (11) and (12), we compute for the inner expansion on  $N_{\delta}(\Gamma) \cup N_{\delta}(\Sigma)$ ,  $S \in \{\Gamma, \Sigma\}$ ,

$$\begin{split} &\partial_t v = \partial_t v_0^i - \varepsilon^{-1} \hat{v}_0' \circ \iota_\varepsilon V_\nu^\Phi + \hat{v}_1' \circ \iota_\varepsilon + O(\varepsilon), \\ &\nabla v = \varepsilon^{-1} \hat{v}_0' \circ \iota_\varepsilon \otimes \bar{v} + \nabla_{S_d} v_0^i + \hat{v}_1' \circ \iota_\varepsilon \otimes \bar{v} + O(\varepsilon) \end{split}$$

resulting in

$$(v\cdot\nabla)v=\varepsilon^{-1}\hat{v}_0'\circ\iota_\varepsilon v_0^i\cdot\bar{v}+\hat{v}_0'\circ\iota_\varepsilon v_1^i\cdot\bar{v}+\left(\nabla_{S_d}v_0^i+\hat{v}_1'\circ\iota_\varepsilon\otimes\bar{v}\right)v_0^i+O(\varepsilon),$$

and

$$\Delta v^i = \varepsilon^{-2} \hat{v}_0'' \circ \iota_{\varepsilon} + \varepsilon^{-1} \left( -\hat{v}_0' \bar{H} + \hat{v}_1'' \right) + \Delta_{\Phi_d} v_0^i - \hat{v}_1' \bar{H} + \hat{v}_2'' \circ \iota_{\varepsilon} + O(\varepsilon).$$

At leading order  $\varepsilon^{-2}$  of Equation (1a), we thus find

$$-\eta \hat{v}_0^{\prime\prime} \circ \iota_{\varepsilon} + \hat{p}_{-1}^{\prime} \circ \iota_{\varepsilon} \bar{\nu} = 0.$$

Multiplication by  $\bar{\nu}$  and using Equation (49) gives

$$\hat{p}_{-1}' = 0. (50)$$

By matching Equation (23),  $\hat{p}_{-1} = 0$ . Inserting back again, we obtain  $\hat{v}_0'' = 0$  Conclusively,  $\hat{v}_0'$  is constant in z. Matching with the outer expansion

$$\left(\lim_{z \nearrow \infty} \hat{v_0}\right) \circ \iota_{\varepsilon}(x) = \lim_{\delta \searrow 0} v_0^o \left(\pi_S(x) + \delta \nu_S \left(\pi_S(x)\right)\right)$$

and

$$\left(\lim_{z \searrow -\infty} \hat{v_0}\right) \circ \iota_{\varepsilon}(x) = \lim_{\delta \nearrow 0} v_0^o \left(\pi_S(x) + \delta \nu_S \left(\pi_S(x)\right)\right)$$

indicates that  $\hat{v_0}$  is bounded. Thus, it must hold

$$\hat{v}_0' = 0. \tag{51}$$

#### 4 | SHARP INTERFACE LIMIT

By inserting the expansions in interfacial coordinates of the components of the solution of Equation (1) into the systems' equations, we have managed to

- eliminate the velocity expansion's summands up to (and including) order  $\varepsilon^{-1}$ ,
- eliminate the pressure expansion's summands up to (and including) order  $\varepsilon^{-3}$ ,
- show that both phase fields assume the optimal profile at leading order,
- show that  $\varphi_1 = 0$ ,
- and derive Equation (48).

Before we can make use of these findings and pass to the limit  $\varepsilon \to 0$ , we compute the expansions of the remaining terms in K (see the right-hand side of Equation 1a).

## Expansion of $\nabla^{L^2}C$ and remaining force terms

We compute the asymptotic expansions of  $\nabla^{L^2}_{\phi} \mathcal{C}, \nabla^{L^2}_{\psi} \mathcal{C},$ 

$$G_{\varepsilon} := -\partial_{\rho_a} C_{\phi} H_{\psi} \rho_a \nu_{\psi} = -\rho_a H_{\psi} \int_{\Omega} g_{\varepsilon}[\phi](y) \partial_{\rho_a} c\left(x, y, \rho_a, \nu_{\psi}\right) d\mathcal{L}^3(y) \nu_{\psi},$$

and

$$H_{\varepsilon} := -g_{\varepsilon}[\psi] \mathbb{P}_{\nu_{\psi}} \nabla \partial_{\rho_{a}} C_{\phi} \rho_{a} = -\int_{\Omega} g_{\varepsilon}[\phi](y) \mathbb{P}_{\nu_{\psi}} \nabla_{x} \left( \partial_{\rho_{a}} c \left( \cdot, y, \rho_{a}, \nu_{\psi} \right) \right) g_{\varepsilon}[\psi] \rho_{a} d\mathcal{L}^{3}(y).$$

Expansion of  $\nabla^{L^2}_{\phi} \mathcal{C}$ : We recall from Equation (2d) that

$$\nabla_{\phi}^{L^2} C = A_{\varepsilon} + B_{\varepsilon} \tag{52a}$$

with

$$A_{\varepsilon}(y) = \left(-\varepsilon \Delta_{y} \phi + \varepsilon^{-1} W'(\phi)\right)(y) \int_{N_{\delta}(\Sigma)} g_{\varepsilon}[\psi](x) c\left(x, y, \rho_{a}, \nu_{\psi}\right) d\mathcal{L}^{3}(x) + O(\varepsilon),$$

$$B_{\varepsilon}(y) = -\varepsilon \nabla_{y} \phi \cdot \int_{N_{\delta}(\Sigma)} g_{\varepsilon}[\psi](x) \nabla_{y} \left(c\left(x, y, \rho_{a}, \nu_{\psi}\right)\right) d\mathcal{L}^{3}(x) + O(\varepsilon). \tag{52b}$$

We further expand

$$c\left(x,y,\rho_{a0}+\varepsilon r_{1},\nu_{\psi_{0}+\varepsilon s_{1}}\right)=c\left(x,y,\rho_{a0},\nu_{\psi_{0}}\right)+\varepsilon\nabla_{\rho_{a},\nu}c\cdot\left(r_{1},\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\nu_{\psi_{0}+\varepsilon s_{1}}\right)\Big|_{0}\right)^{T}+O\left(\varepsilon^{2}\right),$$

and note

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon} \left( \nu_{\psi_0 + \varepsilon s_1} \right) \bigg|_0 = \frac{1}{|\nabla \psi_0|} \mathbb{P}_{\nu_{\psi_0}} \nabla s_1 \in O(1), \tag{53}$$

and thus

$$\nabla_{\rho_a,\nu}c\cdot\left(r_1,\,\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\nu_{\psi_0+\varepsilon s_1}\right)\Big|_0\right)^T\in O(1).$$

By employing Equation (16), we expand  $A_{\varepsilon}$ :

$$\begin{split} &\int_{N_{\delta}(\Sigma)} g_{\varepsilon}[\psi](x) c\left(x,y,\rho_{a},\nu_{\psi}\right) \, \mathrm{d}\mathcal{L}^{3}(x) = \\ &\int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left(\frac{1}{2} \left(\hat{\psi}_{0}'\right)^{2} \circ \iota_{\varepsilon}(x) + W\left(\psi_{0}(x)\right)\right) c\left(x,y,\rho_{a0},\nu_{\psi_{0}}\right) + O(1) \, \mathrm{d}\mathcal{L}^{3}(x). \end{split}$$

Multiplication with  $\left(-\varepsilon\Delta_{y}\phi + \varepsilon^{-1}W'(\phi)\right)$  yields

$$A_{\varepsilon}(y) = \hat{\phi}_0' \circ \iota_{\varepsilon}(y) \bar{H}(y) \int_{N_{\varepsilon}(\Sigma)} \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\psi}_0' \right)^2 \circ \iota_{\varepsilon}(x) + W \left( \psi_0(x) \right) \right) c \left( x, y, \rho_{a0}, \nu_{\psi_0} \right) + O(1) \, \mathrm{d}\mathcal{L}^3(x)$$

thanks to  $\hat{\psi}_0$  being the optimal profile, and Equation (43).

In order to expand  $B_{\varepsilon}$ , we first compute

$$\nabla_{y}c\left(x,y,\rho_{a0}+\varepsilon r_{1},\nu_{\psi_{0}+\varepsilon s_{1}}\right)=\nabla_{y}c\left(x,y,\rho_{a0},\nu_{\psi_{0}}\right)+\varepsilon\nabla_{\rho_{a},\nu}\nabla_{y}c\left(\frac{r_{1}}{\frac{1}{|\psi_{0}|}\mathbb{P}_{\nu_{\psi_{0}}}\nabla s_{1}}\right)+O\left(\varepsilon^{2}\right).$$

Therefore, using Equation (16), we find

$$\begin{split} &\int_{N_{\delta}(\Sigma)} g_{\varepsilon}[\psi] \nabla_{y} c\left(x, y, \rho_{a}, \nu_{\psi}\right) \, \mathrm{d}\mathcal{L}^{3}(x) = \\ &\int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left(\frac{1}{2} \left(\hat{\psi}_{0}'\right)^{2} \circ \iota_{\varepsilon}(x) + W\left(\psi_{0}(x)\right)\right) \nabla_{y} c\left(x, y, \rho_{a0}, \nu_{\psi_{0}}\right) + O(1) \, \mathrm{d}\mathcal{L}^{3}(x). \end{split}$$

Multiplication with  $-\varepsilon \nabla \phi$  gives

$$B_{\varepsilon}(y) = -\hat{\phi}_0' \circ \iota_{\varepsilon}(y) \int_{N_{\varepsilon}(\Sigma)} \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\psi}_0' \right)^2 \circ \iota_{\varepsilon}(x) + W \left( \psi_0(x) \right) \right) \bar{\nu}(y) \cdot \nabla_y c \left( x, y, \rho_{a0}, \nu_{\psi_0} \right) + O(1) \, \mathrm{d} \mathcal{L}^3(x).$$

Expansion of  $\nabla_{\psi}^{L^2}C$ : We recall Equation (2e),

$$\nabla_{\psi}^{L^2C} = C_{\varepsilon} + D_{\varepsilon} + E_{\varepsilon} \tag{54a}$$

with

$$C_{\varepsilon}(x) = \left(-\varepsilon \Delta_{x} \psi + \varepsilon^{-1} W'(\psi)\right)(x) \int_{N_{\delta}(\Gamma)} g_{\varepsilon}[\phi](y) c\left(x, y, \rho_{a}, \nu_{\psi}\right) d\mathcal{L}^{3}(y),$$

$$D_{\varepsilon}(x) = -\varepsilon \nabla_{x} \psi \cdot \int_{N_{\delta}(\Gamma)} g_{\varepsilon}[\phi](y) \nabla_{x} \left(c\left(x, y, \rho_{a}, \nu_{\psi}\right)\right) d\mathcal{L}^{3}(y),$$

$$E_{\varepsilon}(x) = -\int_{N_{\varepsilon}(\Gamma)} g_{\varepsilon}[\phi](y) \nabla_{x} \cdot \left(g_{\varepsilon}[\psi] \nabla_{\nu} c^{T} \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}}\right) d\mathcal{L}^{3}(y).$$
(54b)

Before we start expanding these terms, we prove the following formulae:

Lemma 4.1. It holds.

$$\frac{\nabla \psi}{|\nabla \psi|} = \bar{\nu} + O\left(\varepsilon^2\right) \tag{55}$$

$$\nabla^2 \psi = \varepsilon^{-2} \hat{\psi}_0^{\prime\prime} \circ \iota_{\varepsilon} \bar{\nu} \otimes \bar{\nu} + \varepsilon^{-1} \hat{\psi}_0^{\prime} \circ \iota_{\varepsilon} \nabla \bar{\nu} + \hat{\psi}_2^{\prime\prime} \circ \iota_{\varepsilon} \bar{\nu} \otimes \bar{\nu} + O(\varepsilon). \tag{56}$$

*Proof.* Ad (55): Due to  $\hat{\psi}_0$  being the optimal profile and it thus being independent of the tangential variable s, and considering Equation (43), we have

$$\nabla \psi = \varepsilon^{-1} \hat{\psi}_0' \circ \iota_{\varepsilon} \bar{\nu} + \nabla_{\Sigma_d} \hat{\psi}_0 + \hat{\psi}_1' \circ \iota_{\varepsilon} \bar{\nu} + O(\varepsilon) = \varepsilon^{-1} \hat{\psi}_0' \circ \iota_{\varepsilon} \bar{\nu} + O(\varepsilon).$$

This observation brings the claimed expansion for the product of  $\nabla \psi$  and  $|\nabla \psi|^{-1}$  using Equation (19). Ad (56):

$$\begin{split} \nabla \left( \partial_i \psi \right) &= \varepsilon^{-2} \hat{\psi}_0^{\prime\prime} \circ \iota_{\varepsilon} \bar{\nu} \bar{\nu}_i + \varepsilon^{-1} \nabla_{\Sigma_d} \left( \hat{\psi}_0^{\prime} \circ \iota_{\varepsilon} \right) \bar{\nu}_i + \varepsilon^{-1} \hat{\psi}_0^{\prime} \circ \iota_{\varepsilon} \nabla \bar{\nu}_i \\ &+ \nabla_{\Sigma_d} \left( \varepsilon^{-1} \hat{\psi}_0^{\prime} \circ \iota_{\varepsilon} \bar{\nu}_i + \nabla_{\Sigma_d} \left( \psi_0 \right) (i) \right) + \nabla \left( \hat{\psi}_1^{\prime} \circ \iota_{\varepsilon} \nabla \nu_i + \varepsilon \nabla_{\Sigma_d} \hat{\psi}_1 (i) \right) \\ &+ \hat{\psi}_0^{\prime\prime} \circ \iota_{\varepsilon} \bar{\nu} \bar{\nu}_i + O(\varepsilon). \end{split}$$

We again use the optimal profile and Equation (43) to conclude

$$\varepsilon^{-1}\nabla_{\Sigma_{d}}\left(\hat{\psi}_{0}'\circ\iota_{\varepsilon}\right)\nu_{i}=\nabla_{\Sigma_{d}}\left(\varepsilon^{-1}\hat{\psi}_{0}'\circ\iota_{\varepsilon}\nu_{i}+\nabla_{\Sigma_{d}}\left(\psi_{0}\right)\left(i\right)\right)=\nabla\left(\hat{\psi}_{1}'\circ\iota_{\varepsilon}\nabla\nu_{i}+\varepsilon\nabla_{\Sigma_{d}}\hat{\psi}_{1}(i)\right)=0,$$

and the claim follows.

 $C_{\varepsilon}$  is expanded just like  $A_{\varepsilon}$ :

$$C_{\varepsilon}(x) = \hat{\psi}_0' \circ \iota_{\varepsilon}(x) \bar{H}(x) \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\phi}_0' \right)^2 \circ \iota_{\varepsilon}(x) + W \left( \phi_0(x) \right) \right) c \left( x, y, \rho_{a0}, \nu_{\psi_0} \right) + O(1) \, \mathrm{d}\mathcal{L}^3(y).$$

We continue by expanding  $D_{\varepsilon}$ : First note

$$\varepsilon \nabla_{x} \psi \cdot \nabla_{x} \left( c \left( \cdot, y, \rho_{a}, \nu_{\psi} \right) \right) = \varepsilon \nabla_{x} \psi \cdot \left( \nabla_{x} c + \partial_{\rho_{a}} c \nabla_{x} \rho_{a} + \nabla \nu_{\eta}^{T} \nabla_{\nu} c \right).$$

Then we observe  $\varepsilon \nabla_x \psi^T \nabla \nu_{\psi}^T = O(\varepsilon)$ , so

$$\varepsilon \nabla_x \psi \cdot \nabla_x c = \left(\hat{\psi}_0' \circ \iota_{\varepsilon} \bar{\nu} + O(\varepsilon)\right) \cdot \left(\nabla_x c + \partial_{\rho_a} c \nabla \rho_a\right) = \hat{\psi}_0' \circ \iota_{\varepsilon} \bar{\nu} \cdot \left(\nabla_x c + \partial_{\rho_a} c \nabla \rho_a\right) + O(\varepsilon),$$

where the last equality is justified by Equation (30). Then,

$$D_{\varepsilon}(x) = -\int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\phi}_0' \right)^2 \circ \iota_{\varepsilon}(y) + W \left( \phi_0(y) \right) \right) \left( \hat{\psi}_0' \circ \iota_{\varepsilon} \bar{\nu} \cdot \left( \nabla_x c + \partial_{\rho_a} c \nabla \rho_a \right) + O(\varepsilon) \right) + O(\varepsilon) \, \mathrm{d}\mathcal{L}^3(y).$$

At last, we turn to  $E_{\varepsilon}$  and compute

$$\nabla_{x} \cdot \left( g_{\varepsilon}[\psi] \nabla_{\nu} c^{T} \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}} \right) = \nabla_{x} \left( g_{\varepsilon}[\psi] \right) \cdot \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}}^{T} \nabla_{\nu} c + g_{\varepsilon}[\psi] \nabla \cdot \left( \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}}^{T} \nabla_{\nu} c \right)$$

$$= \nabla_{\nu} c^{T} \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}} \nabla_{x} \left( g_{\varepsilon}[\psi] \right)$$

$$+ g_{\varepsilon}[\psi] \left( \frac{1}{|\nabla \psi|} \nabla \left( \nabla_{\nu} c \right) : \mathbb{P}_{\nu_{\psi}} + \nabla_{\nu} c \cdot \nabla \cdot \left( \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}} \right) \right). \tag{57}$$

On the first term, we use Equations (56) and (43) (for the expansion of the double well potential) to obtain

$$\begin{split} \nabla \left( g_{\varepsilon}[\psi] \right) &= \left( \varepsilon \nabla^{2} \psi + \varepsilon^{-1} W'(\psi) \right) \nabla \psi \\ &= \left( \varepsilon^{-1} \hat{\psi}_{0}'' \circ \iota_{\varepsilon} \bar{\nu} \otimes \bar{\nu} + \hat{\psi}_{0}' \circ \iota_{\varepsilon} \nabla \bar{\nu} + \varepsilon^{-1} W'(\psi_{0}) + O(\varepsilon) \right) \left( \varepsilon^{-1} \hat{\psi}_{0}' \circ \iota_{\varepsilon} \bar{\nu} + O(\varepsilon) \right) \\ &= \varepsilon^{-2} \left( \hat{\psi}_{0}'' \circ \iota_{\varepsilon} \hat{\psi}_{0}' \circ \iota_{\varepsilon} \bar{\nu} + W'(\psi_{0}) \hat{\psi}_{0}' \circ \iota_{\varepsilon} \bar{\nu} \right) + O(1). \end{split}$$

Since  $\mathbb{P}_{\nu_{tb}}\bar{\nu} \in O\left(\varepsilon^2\right)$  thanks to Equation (55), we have

$$\nabla_{\nu} c^{T} \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}} \nabla \left( g_{\varepsilon} [\psi] \right) \in O(\varepsilon). \tag{58}$$

Second, we calculate

$$\begin{split} g_{\varepsilon}[\psi] \frac{1}{|\nabla \psi|} \nabla \left( \nabla_{\nu} c \right) \, \colon \, \mathbb{P}_{\nu_{\psi}} &= \left( \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\psi}_{0}' \right)^{2} \circ \iota_{\varepsilon} + W \left( \psi_{0} \right) \right) + O(\varepsilon) \right) \frac{1}{|\nabla \psi|} \left( \nabla \left( \nabla_{\nu} c \right) \, \colon \, \mathbb{P}_{\bar{\nu}} + O \left( \varepsilon^{2} \right) \right) \\ &= \varepsilon^{-1} \frac{1}{|\nabla \psi|} \left( \frac{1}{2} \left( \hat{\psi}_{0}' \right)^{2} \circ \iota_{\varepsilon} + W \left( \psi_{0} \right) \right) \nabla_{\Sigma_{d(x)}} \cdot \left( \nabla_{\nu} c \right) + O \left( \varepsilon^{2} \right). \end{split}$$

Third.

$$\nabla \cdot \left( \frac{1}{|\nabla \psi|} \mathbb{P}_{\nu_{\psi}} \right) = \mathbb{P}_{\nu_{\psi}} \nabla \left( \frac{1}{|\nabla \psi|} \right) + \frac{1}{|\nabla \psi|} \nabla \cdot \mathbb{P}_{\nu_{\psi}},$$

We further compute

$$\nabla\left(\frac{1}{|\nabla\psi|}\right) = -\frac{1}{|\nabla\psi|^3}\nabla^2\psi\nabla\psi = -\frac{1}{|\nabla\psi|^2}\nabla^2\psi\bar{\nu},$$

and using Equation (56), we find

$$\nabla_{\boldsymbol{\nu}} \boldsymbol{c} \cdot \nabla \cdot \left( \frac{1}{|\nabla \psi|} \mathbb{P}_{\boldsymbol{\nu}_{\psi}} \right) = \nabla_{\boldsymbol{\nu}} \boldsymbol{c} \cdot \mathbb{P}_{\boldsymbol{\nu}_{\psi}} \nabla \left( \frac{1}{|\nabla \psi|} \right) + \nabla_{\boldsymbol{\nu}} \boldsymbol{c} \cdot \frac{1}{|\nabla \psi|} \nabla \cdot \mathbb{P}_{\boldsymbol{\nu}_{\psi}} = \nabla_{\boldsymbol{\nu}} \boldsymbol{c} \cdot \frac{1}{|\nabla \psi|} \nabla \cdot \mathbb{P}_{\boldsymbol{\nu}_{\psi}} + O\left(\varepsilon^{3}\right).$$

Finally,

$$\nabla \cdot \mathbb{P}_{\nu,_{h}} = -(\nabla \bar{\nu}\bar{\nu} + \bar{\nu}\nabla \cdot \bar{\nu} + O(\varepsilon)) = \bar{H}\bar{\nu} + O(\varepsilon),$$

SO

$$\begin{split} E_{\varepsilon}(x) &= -\frac{\varepsilon^{-1}}{|\nabla_{x}\psi|} \left(\frac{1}{2} \left(\hat{\psi}_{0}'\right)^{2} \circ \iota_{\varepsilon}(x) + W\left(\psi_{0}(x)\right)\right). \\ &\cdot \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \left(\frac{1}{2} \left(\hat{\phi}_{0}'\right)^{2} \circ \iota_{\varepsilon}(y) + W\left(\phi_{0}(y)\right)\right) \left(\nabla_{\Sigma_{d(x)}} \cdot (\nabla_{\nu}c) + \nabla_{\nu}c \cdot \bar{H}(x)\bar{\nu}(x)\right) \, \mathrm{d}\mathcal{L}^{3}(y) + O(1). \end{split}$$

#### Expansion of $G_{\varepsilon}$ :

We use Equations (16), (18) and (55) in connection with Equation (43) to obtain

$$\begin{split} G_{\varepsilon} &= -\int_{\Omega} g_{\varepsilon}[\phi](y) \rho_{a} H_{\psi} \partial_{\rho_{a}} c\left(\cdot, y, \rho_{a}, \nu_{\psi}\right) \nu_{\psi} \, \mathrm{d}\mathcal{L}^{3}(y) = \\ &- \varepsilon^{-1} \rho_{a0} \left(\hat{\psi}_{0}^{\prime}\right)^{2} \bar{H} \bar{\nu} \int_{N_{\tau}(\Gamma)} \varepsilon^{-1} \left(\frac{1}{2} \left(\hat{\phi}_{0}^{\prime}\right)^{2} \circ \iota_{\varepsilon}(y) + W\left(\phi_{0}(y)\right)\right) \partial_{\rho_{a}} c\left(\cdot, y, \rho_{a0}, \nu_{\psi_{0}}\right) \, \mathrm{d}\mathcal{L}^{3}(y) + O(1). \end{split}$$

#### Expansion of $H_{\varepsilon}$ :

As before, we employ Equations (16) and (55) to obtain

$$\begin{split} H_{\varepsilon} &= -\int_{\Omega} g_{\varepsilon}[\phi](y) \mathbb{P}_{\nu_{\psi}} \nabla_{x} \left( \partial_{\rho_{a}} c \left( \cdot, y, \rho_{a}, \nu_{\psi} \right) \right) g_{\varepsilon}[\psi] \rho_{a} \, \mathrm{d}\mathcal{L}^{3}(y) = -\varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\phi}'_{0} \right)^{2} \circ \iota_{\varepsilon} + W \left( \psi_{0} \right) \right) \\ & \cdot \int_{\Omega} \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\psi}'_{0} \right)^{2} \circ \iota_{\varepsilon}(y) + W \left( \phi_{0}(y) \right) \right) \nabla_{\Sigma_{d}} \left( \partial_{\rho_{a}} c \left( \cdot, y, \rho_{a0}, \nu_{\psi_{0}} \right) \right) \rho_{a0} \, \mathrm{d}\mathcal{L}^{3}(y) + O(1). \end{split}$$

We now show, using the results of the analysis in the previous sections, that classical solutions of Equation (1) converge formally to solutions of Equation (4) for  $\varepsilon \searrow 0$ . In the following, we will often use that

$$\left(\hat{\varphi}_0'(z)\right)^2 = \left(\hat{\psi}_0'(z)\right)^2 = \left(\tanh\left(\frac{z}{\sqrt{2}}\right)'\right)^2 = \frac{1}{2}\left(1 - \tanh\left(\frac{z}{\sqrt{2}}\right)^2\right)^2$$

is integrable, and we will abbreviate

$$Z := \frac{1}{2} \int_{-\infty}^{\infty} \left( 1 - \tanh\left(\frac{z}{\sqrt{2}}\right)^{2} \right)^{2} d\mathcal{L}^{1}(z).$$

We also partition all integrals over  $\Omega$  into an interal over  $N_{\delta}(S)$  and one over  $\Omega_{\delta} = \Omega \setminus N_{\delta}(S)$ . In the latter region, the outer expansions hold, and thus the integrands are all of lower order vanishing in the limit, so we can neglect them.

#### 4.2 | Momentum balance and mass conservation

#### 4.2.1 | Outer region

At order  $\varepsilon^0$ , we find with the results of Section 3.3 (causing all the energy gradient terms on the right to vanish)

$$\rho\left(\partial_{t}v_{0}^{o}+\left(v_{0}^{o}\cdot\nabla\right)v_{0}^{o}\right)-\nabla\cdot\left(\eta\left(\nabla v_{0}^{o}+\nabla v_{0}^{oT}\right)\right)+\nabla p_{0}^{o}=0,$$

and for the incompressibility condition

$$\nabla \cdot v_0^o = 0.$$

This gives Equations (4a) and (4b).

#### 4.2.2 | Inner region

Let  $S \in \{\Gamma, \Sigma\}$ . We note that the matching conditions for the velocity state the no-jump conditions (4d), (4e). Plugging further the inner expansion into Equation (1a) and using Equations (50) and (51), we find

$$\begin{split} -\varepsilon^{-1} \left( \left( \hat{\eta} \hat{v}_1' \right)' + \left( \widehat{\nabla_{\Phi_d} v_0}^T \hat{\eta}^T \right)' \hat{v} + \hat{v} \otimes \hat{v}_1'' \hat{v} \right) \circ \iota_{\varepsilon} + \varepsilon^{-1} \hat{p}_0' \circ \iota_{\varepsilon} \bar{v} + r = \\ \varepsilon^{-1} \left( \nabla_{\phi}^{L^2} \mathcal{F} \hat{\phi}_0' \circ \iota_{\varepsilon} + \nabla_{\psi}^{L^2} \mathcal{F} \hat{\psi}_0' \circ \iota_{\varepsilon} \right) \bar{v} - \partial_{\rho_a} C_{\phi} H_{\psi_0^i} v \psi_0^i \rho_{a0}^i, \end{split}$$

where  $r = \hat{r} \circ \iota_{\varepsilon}$  with  $\hat{r} \in O(1)$ . For understanding the limit of this equation, let us consider its variational formulation with test functions  $w \in [H^1(\Omega)]^3$ . The left-hand side then reads

$$\varepsilon^{-1} \int_{N_{\delta}(\Gamma) \cup N_{\delta}(\Sigma)} \left( -\left( \hat{\eta} \hat{v}_{1}' \right)' \circ \iota_{\varepsilon} + \left( \widehat{\nabla_{\Phi_{d}} v_{0}}^{T} \hat{\eta}^{T} \right)' \bar{v} \circ \iota_{\varepsilon} \bar{v} + \bar{v} \otimes \hat{v}_{1}'' \circ \iota_{\varepsilon} \bar{v} + \hat{p}_{0}' \circ \iota_{\varepsilon} \bar{v} \right) \cdot w \, d\mathcal{L}^{3} =$$

$$\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Gamma_{\varepsilon z} \cup \Sigma_{\varepsilon z}} \left( \left( -\left( \hat{\eta} \hat{v}_{1}' \right)' + \left( \widehat{\nabla_{\Phi_{\varepsilon z}} v_{0}}^{T} \hat{\eta}^{T} \right)' \hat{v} + \hat{v} \otimes \hat{v}_{1}'' \hat{v} \right) (\pi_{\Sigma \cup \Gamma}(\sigma), z) + \hat{p}_{0}' (\pi_{\Sigma \cup \Gamma}(\sigma), z) \, \bar{v}(\sigma) \right) \cdot w \, d\mathcal{H}^{2}(\sigma) \, dz =$$

$$\int_{\Gamma_{\varepsilon z} \cup \Sigma_{\varepsilon z}} \left( \left[ -\hat{\eta} \hat{v}_{1}' + \left( \widehat{\nabla_{\Phi_{\varepsilon z}} v_{0}}^{T} \hat{\eta}^{T} \right) \hat{v} + \hat{v} \otimes \hat{v}_{1}' \hat{v} \right]_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} (\pi_{\Sigma \cup \Gamma}(\sigma)) + \left[ \hat{p}_{0} \right]_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} (\pi_{\Sigma \cup \Gamma}(\sigma)) \, \bar{v}(\sigma) \right) \cdot w \, d\mathcal{H}^{2}(\sigma). \tag{59}$$

We can rewrite the integral of  $-\hat{\eta}\hat{v}_1' + \left(\widehat{\nabla_{\Phi_{\varepsilon z}}}_{0}\hat{\eta}^T\right)\hat{v} + \hat{v}\otimes\hat{v}_1'\hat{v}$  in z by looking at the expansions of  $\nabla v\bar{v}$  and of  $\nabla v^T\bar{v}$  in interfacial coordinates:

$$\begin{split} \nabla \left( \hat{v} \circ \iota_{\varepsilon} \right) \bar{\nu} &= \varepsilon^{-1} \hat{v}_{0}' \circ \iota_{\varepsilon} + \hat{v}_{1}' \circ \iota_{\varepsilon} + O(\varepsilon) \\ &= \hat{v}_{1}' \circ \iota_{\varepsilon} + O(\varepsilon), \end{split}$$

and

$$\begin{split} \nabla \left( \hat{v} \circ \iota_{\varepsilon} \right)^{T} \bar{v} &= \varepsilon^{-1} \bar{v} \otimes \bar{v}_{0}' \circ \iota_{\varepsilon} \bar{v} + \nabla_{\Phi_{d}} v_{0}^{T} \bar{v} \otimes \bar{v}_{1}' \circ \iota_{\varepsilon} \bar{v} + O(\varepsilon) \\ &= \nabla_{\Phi_{d}} v_{0}^{T} \bar{v} + \bar{v} \otimes \bar{v}_{1}' \circ \iota_{\varepsilon} \bar{v} + O(\varepsilon), \end{split}$$

respectively (following with Equations 11 and 51). With the matching conditions for  $\nabla v \bar{v}$  and  $\nabla v^T \bar{v}$ , we further obtain

$$\lim_{\alpha \searrow 0} (\nabla v_0 \bar{v}) (\pi_S(x) + \alpha v_S(\pi_S(x))) = \left(\lim_{z \nearrow \infty} \hat{v}_1'\right) \circ \iota_{\varepsilon}(x),$$

$$\lim_{\alpha \searrow 0} (\nabla v_0^T \bar{v}) (\pi_S(x) + \alpha v_S(\pi_S(x))) = \lim_{z \nearrow \infty} \left(\widehat{\nabla_{\Phi_d} v_0}^T\right) \circ \iota_{\varepsilon} \bar{v} + \bar{v} \otimes \lim_{z \nearrow \infty} (\hat{v}_1') \circ \iota_{\varepsilon} \bar{v}.$$
(60)

The computations go analogously for the limits  $\alpha \nearrow 0$  and  $z \searrow -\infty$ . Together, both limits form a jump  $[\cdot]$ . Now we pass  $\varepsilon \searrow 0$  in Equation (59) and insert the matching condition for the pressure and Equation (60). This reveals

$$\varepsilon^{-1} \int_{N_{\delta}(\Gamma) \cup N_{\delta}(\Sigma)} \left( -\left( \hat{\eta} \hat{v}_{1}^{\prime} \right)^{\prime} \circ \iota_{\varepsilon} + \left( \widehat{\nabla_{\Phi_{d}} v_{0}}^{T} \hat{\eta}^{T} \right)^{\prime} \bar{\nu} \circ \iota_{\varepsilon} \bar{\nu} + \bar{\nu} \otimes \hat{v}_{1}^{\prime \prime} \circ \iota_{\varepsilon} \bar{\nu} + \hat{p}_{0}^{\prime} \circ \iota_{\varepsilon} \bar{\nu} \right) \cdot w \, d\mathcal{L}^{3} \xrightarrow{\varepsilon > 0} \\
\int_{\Gamma \cup \Sigma} -\left[ \left[ \eta \left( \nabla v_{0} + \nabla v_{0}^{T} \right) - p_{0} \right] \nu \cdot w \, d\mathcal{H}^{2}, \tag{61}$$

where  $\nu \in {\{\nu_{\Gamma}, \nu_{\Sigma}\}}$  depending on what surface the integrand is to be understood.

The right-hand side of Equation (1a) in variational form is

$$f(w) = \left(\nabla_{\phi}^{L^{2}} \mathcal{W}[\phi] + \nabla_{\phi}^{L^{2}} \mathcal{G}[\phi] + \nabla_{\phi}^{L^{2}} \mathcal{C}[\phi, \psi, \rho_{a}], \nabla \phi \cdot w\right)_{L^{2}(N_{\delta}(\Gamma))}$$

$$+ \left(\nabla_{\psi}^{L^{2}} \mathcal{W}[\psi] + \nabla_{\psi}^{L^{2}} \mathcal{G}[\psi] + \nabla_{\psi}^{L^{2}} \mathcal{C}[\phi, \psi, \rho_{a}], \nabla \psi \cdot w\right)_{L^{2}(N_{\delta}(\Sigma))}$$

$$- \left(\int_{\Omega} g_{\varepsilon}[\phi](y) \mathbb{P}_{\nu_{\psi}} \nabla \left(\partial_{\rho_{a}} c\left(\cdot, y, \rho_{a}, \nu_{\psi}\right)\right) g_{\varepsilon}[\psi] \rho_{a} \, d\mathcal{L}^{3}(y), w\right)_{\left[L^{2}(N_{\delta}(\Sigma))\right]^{3}}$$

$$- \left(\int_{N_{\delta}(\Gamma)} g_{\varepsilon}[\phi](y) \rho_{a} H_{\psi} \partial_{\rho_{a}} c \, d\mathcal{L}^{3}(y), w \cdot \nu_{\psi}\right)_{L^{2}(N_{\epsilon}(\Sigma))}.$$

$$(62)$$

Note that we can rewrite

$$-\left(\int_{N_{\delta}(\Gamma)} g_{\varepsilon}[\phi](y) \rho_{a} H_{\psi} \partial_{\rho_{a}} c \, d\mathcal{L}^{3}(y), w \cdot \nu_{\psi}\right)_{L^{2}(N_{\delta}(\Sigma))} = -\left(\partial_{\rho_{a}} C_{\phi} H_{\psi} \rho_{a}, w \cdot \nu_{\psi}\right)_{L^{2}(N_{\delta}(\Sigma))}$$

and

$$\begin{split} -\left(\int_{\Omega}g_{\varepsilon}[\phi](y)\mathbb{P}_{\nu_{\psi}}\nabla\left(\partial_{\rho_{a}}c\left(\cdot,y,\rho_{a},\nu_{\psi}\right)\right)g_{\varepsilon}[\psi]\rho_{a}\,\mathrm{d}\mathcal{L}^{3}(y),w\right)_{\left[L^{2}(N_{\delta}(\Sigma))\right]^{3}} = \\ -\left(g_{\varepsilon}[\psi]\mathbb{P}_{\nu_{\psi}}\nabla\partial_{\rho_{a}}C_{\phi}\rho_{a},w\right)_{\left[L^{2}(N_{\delta}(\Sigma))\right]^{3}}, \end{split}$$

which we use in the following as abbreviation.

To pass Equation (62) to the limit, we treat the gradients of the energies separately. The gradients of  $\mathcal{W}$  and  $\mathcal{G}$  have the same structure for both  $\phi$  and  $\psi$ , and can, therefore, be treated verbatim. For  $\mathcal{C}$ , we distinguish the derivatives w.r.t.  $\phi$  and  $\psi$ . Let us start our analysis with  $\nabla^{L^2}_{\varphi}\mathcal{W}$ .

## 4.2.3 | Force terms of $\nabla^{L^2}_{\varphi} \mathcal{W}$

In this section, we show the following theorem:

**Theorem 4.2.** Let  $S \in \{\Gamma, \Sigma\}$  and  $\varphi \in \{\phi, \psi\}$  such that S is the boundary layer for  $\varphi$ . The following limit holds true:

$$\beta \int_{N_{\delta}(\Phi)} \left( -\Delta(\mu[\varphi]) + \mu[\varphi] \varepsilon^{-2} W''(\varphi) \right) \nabla \varphi \cdot w \, d\mathcal{L}^{3} \xrightarrow{\varepsilon \to 0} -C \int_{\Phi} \left( 2\Delta_{\Phi} H_{\Phi} + H_{\Phi} \left( H_{\Phi}^{2} - 4K_{\Phi} \right) \right) \nu_{S} \cdot w \, d\mathcal{H}^{2}$$

for a constant C.

The strategy of the proof is as follows: In Section 3.8, we have expanded the gradient  $\nabla_{\varphi}^{L^2}\mathcal{W}$  and concluded from the energy inequality that all its terms up to order  $\varepsilon^{-1}$  must equal zero. The terms remaining on order  $\varepsilon^0$  are shifted to order  $\varepsilon^{-1}$  by multiplication with  $\nabla \varphi \cdot w$ , which is just the right scaling for obtaining the claimed limit using Lemma 3.4.

*Proof of* 4.2. Collect all the terms of  $\left(\nabla_{\varphi}^{L^2} \mathcal{W}, \nabla_{\varphi} \cdot w\right)_{L^2(N_{\delta}(\Phi))}$  on order  $\varepsilon^{-1}$ :

$$\begin{split} \left(\nabla_{\varphi}^{L^{2}}\mathcal{W},\nabla\varphi\cdot w\right)_{L^{2}(N_{\delta}(\Phi))} &= \varepsilon^{-1}\int_{N_{\delta}(\Phi)}\left(-\Delta_{\Phi_{d(x)}}\left(\mu_{0}[\varphi]\right) + \hat{\mu}_{1}[\hat{\varphi}]'\circ j\bar{H} - \hat{\mu}_{2}[\hat{\varphi}]''\circ \iota_{\varepsilon} \right. \\ &+ \left. \mu_{2}[\varphi]W''\left(\varphi_{0}\right) + \mu_{0}[\varphi]W^{(3)}\left(\varphi_{0}\right)\varphi_{2} \\ &+ \left. \hat{\varphi}_{0}'\circ\iota_{\varepsilon}\nabla\bar{H}\cdot\bar{\nu}\bar{H} + 2\varepsilon^{-1}d(x)\hat{\varphi}_{0}''\circ\iota_{\varepsilon}\bar{H}\right|_{\Phi}\left(\left.\bar{H}\right|_{\Phi}^{2} - 2\bar{K}\right|_{\Phi}\right) \\ &\left. -\hat{\varphi}_{0}'\circ\iota_{\varepsilon}\nabla^{2}\bar{H}: \left.\bar{\nu}\otimes\bar{\nu} - 4\varepsilon^{-1}d(x)\hat{\varphi}_{0}''\circ\iota_{\varepsilon}\left(\left.\bar{H}\right|_{\Phi}^{3} - \left.\bar{3}\bar{H}\right|_{\Phi}\bar{K}\right|_{\Phi}\right)\right)\hat{\varphi}_{0}'\circ\iota_{\varepsilon}\nu_{\varphi}\cdot w\,\mathrm{d}\mathcal{L}^{3}(x) \\ &+ O(\varepsilon). \end{split}$$

The terms on the first and second line are from the expansion of the chemical potential and the double well potential. The left summand on line three stems from Equation (44), the right one from Equation (46). The left summand on line four is taken from Equation (40) (note (42)); the right summand is from (44) (note Equation 45). First, we substitute some expressions using Lemma 3.1 and Equation 43:

$$\begin{split} \left(\nabla_{\varphi}^{L^{2}}\mathcal{W},\nabla\varphi\cdot w\right)_{L^{2}(N_{\delta}(\Phi))} &= \varepsilon^{-1}\int_{N_{\delta}(\Phi)}\left(-\hat{\varphi}_{0}'\circ\iota_{\varepsilon}\Delta_{\Phi_{d(x)}}\bar{H} + \hat{\mu}_{1}[\hat{\varphi}]'\circ\iota_{\varepsilon}\bar{H} - \hat{\mu}_{2}[\hat{\varphi}]''\circ\iota_{\varepsilon} \right. \\ &+ \mu_{2}[\varphi]W''\left(\varphi_{0}\right) + \mu_{0}[\varphi]W^{(3)}\left(\varphi_{0}\right)\varphi_{2} \\ &+ \hat{\varphi}_{0}'\circ\iota_{\varepsilon}\bar{H}\left(\bar{H}^{2} - 2\bar{K}\right) + 2\varepsilon^{-1}d(x)\hat{\varphi}_{0}''\circ\iota_{\varepsilon}\bar{H}\Big|_{\Phi}\left(\bar{H}\Big|_{\Phi}^{2} - 2\bar{K}\Big|_{\Phi}\right) \\ &\left. - 2\hat{\varphi}_{0}'\circ\iota_{\varepsilon}\left(\bar{H}^{3} - 3\bar{H}\bar{K}\right) - 4\varepsilon^{-1}d(x)\hat{\varphi}_{0}''\circ\iota_{\varepsilon}\left(\bar{H}\Big|_{\Phi}^{3} - 3\bar{H}\Big|_{\Phi}\bar{K}\Big|_{\Phi}\right)\right)\hat{\varphi}_{0}'\circ\iota_{\varepsilon}\nu\varphi\cdot w\,\mathrm{d}\mathcal{L}^{3}(x) \\ &+ O(\varepsilon). \end{split}$$

Second, we transform the integral using the co-area formula. We denote  $j(\sigma, z) = (\pi_{\Phi}(\sigma), z)$ .

$$\begin{split} \left(\nabla_{\varphi}^{L^{2}}\mathcal{W},\nabla\varphi\cdot w\right)_{L^{2}(N_{\delta}(\Phi))} &= \int_{-\frac{\delta}{\varepsilon}}^{\frac{\varepsilon}{\varepsilon}} \int_{\Phi_{\varepsilon}} \left(-\hat{\varphi}_{0}'\circ j\Delta_{\Phi_{\varepsilon}z}\bar{H} + \hat{\mu}_{1}[\hat{\varphi}]'\circ j\bar{H} - \hat{\mu}_{2}[\hat{\varphi}]''\circ j \right. \\ &+ \left. \mu_{2}[\varphi]W''\left(\varphi_{0}\right) + \mu_{0}[\varphi]W^{(3)}\left(\varphi_{0}\right)\varphi_{2} \\ &+ \left. \hat{\varphi}_{0}'\circ j\bar{H}\left(\bar{H}^{2} - 2\bar{K}\right) + 2z\hat{\varphi}_{0}''\circ j\bar{H}\Big|_{\Phi} \left(\bar{H}\Big|_{\Phi}^{2} - 2\bar{K}\Big|_{\Phi}\right) \\ &- 2\hat{\varphi}_{0}'\circ j\left(\bar{H}^{3} - 3\bar{H}\bar{K}\right) - 4z\hat{\varphi}_{0}''\circ j\left(\bar{H}\Big|_{\Phi}^{3} - 3\bar{H}\Big|_{\Phi}\bar{K}\Big|_{\Phi}\right) \quad \left. \right)\hat{\varphi}_{0}'\circ j\nu_{\varphi}\cdot w\,\mathrm{d}\mathcal{H}^{2}(\sigma)\,\mathrm{d}\mathcal{L}^{1}(z) \\ &+ O(\varepsilon). \end{split}$$

With integration by parts, it follows directly that  $\int_{-\infty}^{\infty} z \hat{\varphi}_0'' \hat{\varphi}_0' dz = -\frac{1}{2} \int_{-\infty}^{\infty} \left(\hat{\varphi}_0'\right)^2 dz$  Exploiting this property and the independence of  $\hat{\varphi}_0$  of the first argument of j, we obtain

$$\begin{split} &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon z}} \left( \hat{\varphi}_0' \circ j \bar{H} \left( \bar{H}^2 - 2 \bar{K} \right) + 2 z \hat{\varphi}_0'' \circ j \bar{H} \Big|_{\Phi} \left( \bar{H} \Big|_{\Phi}^2 - 2 \bar{K} \Big|_{\Phi} \right) \right) \hat{\varphi}_0' \circ j \, \mathrm{d} \mathcal{H}^2(\sigma) \, \mathrm{d} \mathcal{L}^1(z) = \\ &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \left( \hat{\varphi}_0' \right)^2 \int_{\Phi_{\varepsilon z}} \bar{H} \left( \bar{H}^2 - 2 \bar{K} \right) \, \mathrm{d} \mathcal{H}^2(\sigma) \, \mathrm{d} \mathcal{L}^1(z) - \int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \left( \hat{\varphi}_0' \right)^2 \, \mathrm{d} \mathcal{L}^1(z) \int_{\Phi} \bar{H} \left|_{\Phi} \left( \bar{H} \Big|_{\Phi}^2 - 2 \bar{K} \Big|_{\Phi} \right) \, \mathrm{d} \mathcal{H}^2(\sigma). \end{split}$$

Thanks to Lemma 3.4, we know that this difference converges to zero as  $\varepsilon \setminus 0$ . The same reasoning applies for

$$\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon z}} \left( -2\hat{\varphi}_0' \circ j \left( \bar{H}^3 - 3\bar{H}\bar{K} \right) - 4z\hat{\varphi}_0'' \circ j \left( \bar{H} \big|_{\Phi}^3 - \left. 3\bar{H} \big|_{\Phi} \bar{K} \right|_{\Phi} \right) \right) \hat{\varphi}_0' \circ j \, \mathrm{d}\mathcal{H}^2 \, \mathrm{d}\mathcal{L}^1(z).$$

The remaining terms are treated as follows: We recall  $\hat{H}' \in O(\varepsilon)$  and  $\hat{H}'' \in O(\varepsilon^2)$  (cf. Equations 41 and 42) and

$$\hat{\mu}_{2}[\hat{\varphi}] = \hat{\varphi}_{2}' \hat{H} - \hat{\varphi}_{3}'' + \hat{\varphi}_{3} W''(\hat{\varphi}_{0})$$

(cf. Equation 37 with  $\varphi_1 = 0$ ). Thus, the following expansion holds:

$$\hat{\mu}_2[\hat{\varphi}]'' = \hat{\varphi}_2^{(3)} \hat{H} - \hat{q}'' + O(\varepsilon),$$

where

$$\hat{q} = \hat{\varphi}_3^{\prime\prime} - \hat{\varphi}_3 W^{\prime\prime}(\hat{\varphi}_0).$$

This way we see with  $\mu_0[\varphi] = \bar{H}\hat{\varphi}_0' \circ \iota_{\varepsilon}$  and  $\hat{\mu}_1[\hat{\varphi}] = -\hat{\varphi}_2'' + W''(\hat{\varphi}_0)\hat{\varphi}_2$  (cf. Equation 37 with  $\varphi_1 = 0$ ) that

$$\begin{split} -\hat{\mu}_{2}[\hat{\varphi}]'' \circ j + \mu_{2}[\varphi]W''(\varphi_{0}) + \mu_{0}[\varphi]W^{(3)}(\varphi_{0}) \, \varphi_{2} &= -\bar{H}\hat{\varphi}_{2}^{(3)} \circ j + \bar{H}W''(\varphi_{0}) \, \hat{\varphi}_{2}' \circ j + \mu_{0}[\varphi]W^{(3)}(\varphi_{0}) \, \varphi_{2} \\ &\quad + \hat{q}'' \circ j - qW''(\varphi_{0}) + O(\varepsilon) \\ &\quad = \bar{H} \left( -\hat{\varphi}_{2}'' + W''(\hat{\varphi}_{0}) \, \hat{\varphi}_{2} \right)' \circ j + \hat{q}'' \circ j - qW''(\hat{\varphi}_{0}) \circ j + O(\varepsilon) \\ &\quad = \bar{H}\hat{\mu}_{1}[\hat{\varphi}]' \circ j + \hat{q}'' \circ j - qW''(\hat{\varphi}_{0}) \circ j + O(\varepsilon), \end{split}$$

where we used  $\mu_0[\varphi]W^{(3)}(\varphi_0)\varphi_2 = \varphi_0' \circ jW^{(3)}(\varphi_0)\varphi_2 \bar{H} = (W''(\hat{\varphi}_0))' \circ j\varphi_2 \bar{H}$ . We, therefore, obtain,

$$\begin{split} &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon z}} \left( -\hat{\varphi}_0' \circ j \Delta_{\Phi_{\varepsilon z}} \bar{H} + \bar{H} \hat{\mu}_1[\hat{\varphi}]' \circ j - \hat{\mu}_2[\hat{\varphi}]'' \circ j \right. \\ &+ \mu_2[\varphi] W''(\varphi_0) + \mu_0[\varphi] W^{(3)}(\varphi_0) \varphi_2 \right) \hat{\varphi}_0' \circ j \nu_\varphi \cdot w \, \mathrm{d} \mathcal{H}^2 \, \mathrm{d} \mathcal{L}^1(z) = \\ &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon z}} \left( -\hat{\varphi}_0' \circ j \Delta_{\Phi_{\varepsilon z}} \bar{H} + 2\bar{H}_1[\hat{\varphi}]' \circ j + \hat{q}'' \circ j - \hat{q} \circ j W''(\hat{\varphi}_0) \circ j \right) \hat{\varphi}_0' \circ j \nu_\varphi \cdot w \, \mathrm{d} \mathcal{H}^2(\sigma) \, \mathrm{d} \mathcal{L}^1(z) + O(\varepsilon). \end{split}$$

To treat  $\int_{-\frac{\delta}{\varepsilon}}^{\frac{\sigma}{\varepsilon}} \hat{\varphi}'_0 \int_{\Phi_{\varepsilon z}} \hat{q}'' \circ j\nu_{\varphi} \cdot w \, d\mathcal{H}^2(\sigma) \, d\mathcal{L}^1(z)$ , we take a global parametrisation  $\gamma : \mathbb{R}^2 \to \Phi$  (this is w.l.o.g. since in case there is no global parametrisation, we make all the following calculations locally and patch the integrals together

afterwards), and define  $\gamma_{\varepsilon z}(s) = \gamma(s) + \varepsilon z \nu_S(\gamma(s))$ . With the area formula, we obtain

$$\begin{split} &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \hat{\varphi}_0'(z) \int_{\Phi_{\varepsilon z}} \hat{q}'' \circ j \nu_{\varphi} \cdot w \, \mathrm{d}\mathcal{H}^2(\sigma) \, \mathrm{d}\mathcal{L}^1(z) = \\ &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \hat{\varphi}_0'(z) \int_{\mathbb{R}^2} \hat{q}''(\gamma(s), z) \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z} J \left[ \gamma_{\varepsilon z} \right] \, \mathrm{d}\mathcal{L}^2(s) \, \mathrm{d}\mathcal{L}^1(z). \end{split}$$

Note that  $j(\gamma_{\varepsilon z}(s), z) = (\gamma(s), z)$ . We further integrate by parts

$$\begin{split} &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \hat{\varphi}_0'(z) \int_{\mathbb{R}^2} \hat{q}''(\gamma(s),z) J\left[\gamma_{\varepsilon z}\right] \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z} \, \mathrm{d}\mathcal{L}^2(s) \, \mathrm{d}\mathcal{L}^1(z) = \\ &- \int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \hat{\varphi}_0''(z) \int_{\mathbb{R}^2} \hat{q}'(\gamma(s),z) J\left[\gamma_{\varepsilon z}\right] \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z} \, \mathrm{d}\mathcal{L}^2(s) \, \mathrm{d}\mathcal{L}^1(z) \\ &+ \int_{\mathbb{R}^2} \left[ \hat{q}'(\gamma(s),\cdot) \hat{\varphi}_0' J\left[\gamma_{\varepsilon z}\right] \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z} \right]_{-\delta/\varepsilon}^{\delta/\varepsilon} \, \mathrm{d}\mathcal{L}^2(s) \\ &+ \int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \hat{\varphi}_0'' \int_{\mathbb{R}^2} \hat{q}'(\gamma(s),z) J\left[\gamma_{\varepsilon z}\right] \left(\nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z}\right)' \, \mathrm{d}\mathcal{L}^2(s) \, \mathrm{d}\mathcal{L}^1(z) + O(\varepsilon). \end{split}$$

We observe

$$\begin{split} \left(\nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z}\right)' &= \varepsilon \nabla \nu_{\varphi}^{T} \circ \gamma_{\varepsilon z} \nu_{\Phi} \circ \gamma \cdot w \circ \gamma_{\varepsilon z} + \varepsilon \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot \nabla w^{T} \circ \gamma_{\varepsilon z} \nu_{\Phi} \circ \gamma \\ &= \varepsilon \left(\frac{1}{|\varphi|} \nabla^{2} \varphi^{T} \mathbb{P}_{\nu_{\varphi}}\right) \circ \gamma_{\varepsilon z} \nu_{\Phi} \circ \gamma \cdot w \circ \gamma_{\varepsilon z} + O(\varepsilon), \end{split}$$

and we have  $\mathbb{P}_{\nu_{\omega}} \circ \gamma_{\varepsilon z} \nu_{\Phi} \in O\left(\varepsilon^{2}\right) \circ \gamma$  (see Equation 55), so

$$\int_{-\frac{\delta}{2}}^{\frac{\delta}{\varepsilon}} \hat{\varphi}_0'' \int_{\mathbb{R}^2} \hat{q}' J\left[\gamma_{\varepsilon z}\right] \left(\nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z}\right)' \, \mathrm{d}\mathcal{L}^2(s) \, \mathrm{d}\mathcal{L}^1(z) \in O(\varepsilon).$$

With Jacobi's formula for derivatives of determinants, it can be seen that the derivative of the Jacobian w.r.t z is also in  $O(\varepsilon)$ . Integrating by parts, one more time leads us, therefore, to

$$\begin{split} &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \hat{\varphi}_0'(z) \int_{\mathbb{R}^2} \hat{q}''(\gamma(s),z) J\left[\gamma_{\varepsilon z}\right] \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z} \, \mathrm{d}\mathcal{L}^2(s) \, \mathrm{d}\mathcal{L}^1(z) = \\ &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \hat{\varphi}_0^{(3)}(z) \int_{\mathbb{R}^2} \hat{q}(\gamma(s),z) \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z} J\left[\gamma_{\varepsilon z}\right] \, \mathrm{d}\mathcal{L}^2(s) \, \mathrm{d}\mathcal{L}^1(z) \\ &+ \int_{\mathbb{R}^2} \left[ \hat{q}'(\gamma(s),\cdot) \hat{\varphi}_0' \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z} J\left[\gamma_{\varepsilon z}\right] \right]_{-\delta/\varepsilon}^{\delta/\varepsilon} \, \mathrm{d}\mathcal{L}^2(s) \\ &- \int_{\mathbb{R}^2} \left[ \hat{q}(\gamma(s),\cdot) \hat{\varphi}_0'' \nu_{\varphi} \circ \gamma_{\varepsilon z} \cdot w \circ \gamma_{\varepsilon z} J\left[\gamma_{\varepsilon z}\right] \right]_{-\delta/\varepsilon}^{\delta/\varepsilon} \, \mathrm{d}\mathcal{L}^2(s) + O(\varepsilon). \end{split}$$

The last integrals vanish for  $\varepsilon \searrow 0$  since  $\hat{\varphi}'_0$  and  $\hat{\varphi}''_0$  vanish for  $z \to \pm \infty$  (see Equations 21 and 22). Hence,

$$\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon}} \left( \hat{q}'' - \hat{q} W''(\hat{\varphi}_{0}) \right) \hat{\varphi}'_{0} \nu_{\varphi} \cdot w \, d\mathcal{H}^{2}(\sigma) \, d\mathcal{L}^{1}(z) \xrightarrow{\varepsilon \searrow_{0}} \int_{-\infty}^{\infty} \hat{\varphi}_{0}^{(3)} - \hat{\varphi}'_{0} W''(\hat{\varphi}_{0}) \, d\mathcal{L}^{1}(z) \int_{\Phi} q \nu_{\varphi} \cdot w \, d\mathcal{H}^{2}(s).$$

Note that  $\hat{\varphi}_0^{(3)} - \hat{\varphi}_0' W''(\hat{\varphi}_0) = 0$  (property of the optimal profile), so the whole integral vanishes in the limit. The last term we need to investigate is  $2\hat{H}\hat{\mu}_1[\hat{\varphi}]'$  and we already know (see Equation 48)

$$2\hat{H}\hat{\mu}_{1}[\hat{\varphi}]'=-\hat{H}\left(\left.\hat{H}\right|_{\Phi}^{2}-4\hat{K}\right|_{\Phi}\right)\left(\hat{\varphi}_{0}'z\right)'=-\hat{H}\left(\left.\hat{H}\right|_{\Phi}^{2}-4\hat{K}\right|_{\Phi}\right)\left(\hat{\varphi}_{0}''z+\hat{\varphi}_{0}'\right).$$

Now we observe

$$\begin{split} &\int_{-\frac{\delta}{\varepsilon}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon z}} -\bar{H} \left( \left. \bar{H} \right|_{\Phi}^{2} - 4\bar{K} \right|_{\Phi} \right) \left( \hat{\varphi}_{0}^{\prime\prime} \circ jz + \hat{\varphi}_{0}^{\prime} \circ j \right) \hat{\varphi}_{0}^{\prime} \circ j\nu_{\varphi} \cdot w \, \mathrm{d}\mathcal{H}^{2}(\sigma) \, \mathrm{d}\mathcal{L}^{1}(z) \overset{\varepsilon \searrow 0}{\longrightarrow} \\ &- \int_{-\infty}^{\infty} \hat{\varphi}_{0}^{\prime\prime} \hat{\varphi}_{0}^{\prime} z + \left( \hat{\varphi}_{0}^{\prime} \right)^{2} \, \mathrm{d}\mathcal{L}^{1}(z) \int_{\Phi} \hat{H} \left( \left. \hat{H} \right|_{\Phi}^{2} - 4\hat{K} \right|_{\Phi} \right) \nu_{\varphi} \cdot w \, \mathrm{d}\mathcal{H}^{2}(\sigma), \end{split}$$

and finally use  $\int_{-\infty}^{\infty} \hat{\varphi}_0'' \hat{\varphi}_0' z + \left(\hat{\varphi}_0'\right)^2 d\mathcal{L}^1(z) = \frac{1}{2} \int_{-\infty}^{\infty} \left(\hat{\varphi}_0'\right)^2 d\mathcal{L}^1(z)$ .

## 4.2.4 | Force terms of $\nabla^{L^2}_{\omega} \mathcal{G}$

A small calculation reveals

$$\nabla_{\varphi}^{L^2} \mathcal{G}[\varphi] = \gamma \mu[\varphi],$$

and from Equation (36) we have with  $\hat{\varphi}_0'' \circ \iota_{\varepsilon} - W'(\varphi_0) = 0$  and Equation (43)

$$\mu[\varphi] = \gamma \hat{\varphi}_0' \circ \iota_{\varepsilon} \bar{H} + O(\varepsilon).$$

So convergence under the integral follows by Lemma 3.4:

$$\int_{N_\delta(\Phi)} \left(\hat{\varphi}_0'\right)^2 \circ \iota_\varepsilon \gamma \bar{H} \nu_\varphi \cdot w \, \mathrm{d}\mathcal{L}^3 + O(\varepsilon) \xrightarrow{\varepsilon \searrow 0} Z \int_\Phi \gamma \bar{H} \nu_\Phi \cdot w \, \mathrm{d}\mathcal{H}^2.$$

#### 4.2.5 | Coupling energy force terms

We now come to the limit of the terms

$$\begin{split} \left(\nabla_{\phi}^{L^2}C, \nabla\phi\cdot w\right)_{L^2(N_{\delta}(\Gamma))}, \\ \left(\nabla_{\psi}^{L^2}C, \nabla\psi\cdot w\right)_{L^2(N_{\delta}(\Sigma))}, \\ \bar{G}_{\varepsilon} := -\left(\partial_{\rho_a}C_{\phi}H_{\psi}\rho_a, w\cdot \nu_{\psi}\right)L_{L^2(N_{\delta}(\Sigma))}, \text{ and } \\ \bar{H}_{\varepsilon} := -\left(g_{\varepsilon}[\psi]\mathbb{P}_{\nu_{\psi}}\nabla\partial_{\rho_a}C_{\phi}\rho_a, w\right)_{\left[L^2(N_{\delta}(\Sigma))\right]^3} \end{split}$$

in Equation (62).

Limit of 
$$\left( 
abla_{\phi}^{L^2} \mathcal{C}, 
abla \phi \cdot w \right)_{L^2(N_{\delta}(\Gamma))}$$
:

Recall Equation (52) with the term abbreviations introduced therein. Then,

$$\left(\nabla_{\phi}^{L^{2}C,\nabla\phi\cdot w}\right)_{L^{2}(N_{\delta}(\Gamma))} = \left(|\nabla\phi|\left(A_{\varepsilon} + B_{\varepsilon}\right), \nu_{\phi}\cdot w\right)_{L^{2}(N_{\delta}(\Gamma))} = : \bar{A}_{\varepsilon} + \bar{B}_{\varepsilon}. \tag{63}$$

We further define

$$\tilde{A}_{\varepsilon} = \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \frac{1}{2} \left( \hat{\psi}_0'(\iota(x)) \right)^2 + W \left( \psi_0(x) \right) \right) c \left( x, \cdot, \rho_{a0}, \nu_{\psi_0} \right) + O(1) \, \mathrm{d}\mathcal{L}^3(x)$$

so that

$$A_{\varepsilon} = \hat{\phi}_0' \circ \iota_{\varepsilon} \bar{H} \tilde{A}_{\varepsilon}. \tag{64}$$

Due to the optimal profile for  $\psi_0$ , it holds  $W(\psi_0) = (\hat{\psi}_0')^2$ , and applying Lemma 3.4, we have as  $\varepsilon \setminus 0$ ,

$$\begin{split} \tilde{A}_{\varepsilon} &= \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\psi}_{0}'(\iota(x)) \right)^{2} c \left( x, \cdot, \rho_{a0}, \nu_{\psi_{0}} \right) + O(1) \, \mathrm{d}\mathcal{L}^{3}(x) \\ &\to \frac{3Z}{2} \int_{\Sigma} c \left( x, \cdot, \rho_{a0}, \nu_{\Sigma} \right) \, \mathrm{d}\mathcal{H}^{2}(x). \end{split}$$

In order to apply Lemma 3.4 on  $\bar{A}_{\varepsilon}$ , we shall show that for  $y_{\varepsilon}$  converging to y,  $\tilde{A}_{\varepsilon}(y_{\varepsilon})$  converges. To this purpose, we write  $\tilde{A}_{\varepsilon}(y) = F_{\varepsilon}[c(\cdot, y, \rho_{a0}, \psi_0)]$  for all  $y \in \Omega$ , where  $F_{\varepsilon}: L^2(\Omega) \to \mathbb{R}$  is linear and continuous.  $\tilde{A}_{\varepsilon}(y_{\varepsilon})$  converging is then equivalent to  $F_{\varepsilon}[c_{\varepsilon}] = \tilde{A}_{\varepsilon}(y_{\varepsilon})$  converging for  $c_{\varepsilon} = c(\cdot, y_{\varepsilon}, \rho_{a0}, \psi_0)$ . We calculate

$$|F_{\varepsilon}[c_{\varepsilon}] - F_0[c_0]| \le |F_{\varepsilon}[c_{\varepsilon} - c_0]| + |F_{\varepsilon}[c_0] - F_0[c_0]|. \tag{65}$$

The previous calculations directly show  $|F_{\varepsilon}[c_0] - F_0[c_0]| \to 0$ . For the other summand, it holds  $|F_{\varepsilon}[c_{\varepsilon} - c_0]| \le \|F_{\varepsilon}\| \|c_{\varepsilon} - c_0\|_{L^2(\Omega)}$  Since we have convergence of  $F_{\varepsilon}[f]$  for every  $f \in L^2(\Omega)$ , the Banach–Steinhaus theorem implies  $\|F_{\varepsilon}\| < \infty$ . Also, the last term converges to zero (c is continuous in c), and so the left-hand side of Equation (65) converges to zero. Then, as  $c \setminus 0$ ,

$$\begin{split} \bar{A}_{\varepsilon} &= \int_{N_{\delta}(\Gamma)} \left| \nabla_{y} \phi(y) \right| A_{\varepsilon}(y) \nu_{\phi}(y) \cdot w(y) \, \mathrm{d} \mathcal{L}^{3}(y) \\ &= \varepsilon^{-1} \int_{N_{\delta}(\Gamma)} \left( \hat{\phi}'_{0}(\iota(y)) \right)^{2} \bar{H}(y) \tilde{A}_{\varepsilon}(y) \nu_{\phi}(y) \cdot w(y) \, \mathrm{d} \mathcal{L}^{3}(y) + O(\varepsilon) \\ &\to Z \int_{\Gamma} H_{\Gamma}(y) \tilde{A}_{0}(y) \nu_{\Gamma}(y) \cdot w(y) \, \mathrm{d} \mathcal{H}^{2}(y) \\ &= \frac{3Z^{2}}{2} \int_{\Gamma} H_{\Gamma}(y) \int_{\Sigma} c\left( x, y, \rho_{a0}, \nu_{\Sigma} \right) \, \mathrm{d} \mathcal{H}^{2}(x) \nu_{\Gamma}(y) \cdot w(y) \, \mathrm{d} \mathcal{H}^{2}(y). \end{split}$$

Concerning  $\bar{B}_{\varepsilon}$  one argues analogously, as  $\varepsilon \setminus 0$ ,

$$\begin{split} \bar{B}_{\varepsilon} &= \int_{N_{\delta}(\Gamma)} \left| \nabla_{y} \phi(y) \right| B_{\varepsilon}(y) \nu_{\phi}(y) \cdot w(y) \, \mathrm{d}\mathcal{L}^{3}(y) \\ &= -\varepsilon^{-1} \int_{N_{\delta}(\Gamma)} \left( \hat{\phi}'_{0} \circ \iota_{\varepsilon} \right)^{2} \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\psi}'_{0}(\iota_{\varepsilon}(x)) \right)^{2} \bar{\nu}(y) \cdot \nabla_{y} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) + O(1) \, \mathrm{d}\mathcal{L}^{3}(x) \nu_{\phi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(y) \\ &\to -\frac{3Z^{2}}{2} \int_{\Gamma} \nu_{\Gamma} \cdot \int_{\Sigma} \nabla_{y} c \left( x, y, \rho_{a0}, \nu_{\Sigma} \right) \, \mathrm{d}\mathcal{H}^{2}(x) \nu_{\Gamma} \cdot w \, \mathrm{d}\mathcal{H}^{2}(y). \end{split}$$

Limit of 
$$\left( 
abla_{\psi}^{L^2} \mathcal{C}, 
abla \psi \cdot w \right)_{L^2(N_{\delta}(\Sigma))}$$
:

We recall Equation (54) and write

$$\left(\nabla_{\psi}^{L^{2}(\Omega)}C, \nabla\psi \cdot w\right)_{L^{2}(N_{\delta}(\Sigma))} = \left(|\nabla\psi|\left(C_{\varepsilon} + D_{\varepsilon} + E_{\varepsilon}\right), \nu_{\psi} \cdot w\right)_{L^{2}(N_{\delta}(\Sigma))} + O(\varepsilon) = \bar{C}_{\varepsilon} + \bar{D}_{\varepsilon} + \bar{E}_{\varepsilon} + O(\varepsilon). \tag{66}$$

The term  $\bar{C}_{\varepsilon}$  is treated just like  $\bar{A}_{\varepsilon}$ , so we obtain in the limit  $\varepsilon \searrow 0$ 

$$\begin{split} \tilde{C}_{\varepsilon} &= \int_{N_{\delta}(\Sigma)} \left( -\varepsilon \Delta \psi + \varepsilon^{-1} W'(\psi) \right) \int_{N_{\delta}(\Gamma)} g_{\varepsilon}[\phi](y) c\left(x, y, \rho_{a}, \nu_{\psi}\right) d\mathcal{L}^{3}(y) \nu_{\psi}(x) \cdot w(x) d\mathcal{L}^{3}(x) \\ &\rightarrow \frac{3Z^{2}}{2} \int_{\Sigma} H_{\Sigma}(x) \int_{\Gamma} c\left(x, y, \rho_{a0}, \nu_{\Sigma}\right) d\mathcal{H}^{2}(y) \nu_{\Sigma}(x) \cdot w(x) d\mathcal{H}^{2}(x). \end{split}$$

Using the expansion of  $D_{\varepsilon}$ , we compute further

$$\begin{split} &\bar{D}_{\varepsilon} = -\int_{N_{\delta}(\Sigma)} |\nabla \psi| \varepsilon \nabla \psi \cdot \int_{N_{\delta}(\Gamma)} g_{\varepsilon}[\phi](y) \nabla_{x} \left( c \left( x, y, \rho_{a}, \nu_{\psi} \right) \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) \\ &= -\int_{N_{\delta}(\Sigma)} |\nabla \psi| \hat{\psi}'_{0} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} g_{\varepsilon}[\phi](y) \nabla_{x} c \left( x, y, \rho_{a}, \nu_{\psi} \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) \\ &- \int_{N_{\delta}(\Sigma)} |\nabla \psi| \hat{\psi}'_{0} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} g_{\varepsilon}[\phi](y) \partial_{\rho_{a}} c \left( x, y, \rho_{a}, \nu_{\psi} \right) \nabla_{x} \rho_{a0} \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) + O(\varepsilon) \\ &= -\int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \hat{\psi}'_{0} \right)^{2} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}'_{0} \left( \iota_{\varepsilon}(y) \right) \right)^{2} \nabla_{x} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) \\ &- \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \hat{\psi}'_{0} \right)^{2} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}'_{0} \left( \iota_{\varepsilon}(y) \right) \right)^{2} \partial_{\rho_{a}} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \nabla_{x} \rho_{a0} \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) + O(\varepsilon) \\ &\stackrel{(1)}{=} - \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \hat{\psi}'_{0} \right)^{2} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}'_{0} \left( \iota_{\varepsilon}(y) \right) \right)^{2} \nabla_{x} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) + O(\varepsilon) \\ &\stackrel{(1)}{=} - \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \hat{\psi}'_{0} \right)^{2} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}'_{0} \left( \iota_{\varepsilon}(y) \right) \right)^{2} \nabla_{x} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) + O(\varepsilon) \\ &\stackrel{(1)}{=} - \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \hat{\psi}'_{0} \right)^{2} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}'_{0} \left( \iota_{\varepsilon}(y) \right) \right)^{2} \nabla_{x} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) + O(\varepsilon) \\ &\stackrel{(1)}{=} - \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \hat{\psi}'_{0} \right)^{2} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\psi}'_{0} \left( \iota_{\varepsilon}(y) \right) \right)^{2} \nabla_{x} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) + O(\varepsilon) \\ &\stackrel{(1)}{=} - \int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \left( \hat{\psi}'_{0} \right)^{2} \circ \iota_{\varepsilon} \bar{\nu} \cdot \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \left( \hat{\psi}'_{0} \left( \iota_{\varepsilon}(y) \right) \right)^{2} \nabla_{x} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal$$

where for Equation (1), we observe that due to Equation (30),  $\nabla_x \rho_{a0} = \nabla_{\Sigma_d} \rho_{a0}$ , thus  $\bar{\nu} \cdot \nabla_x \rho_{a0} = 0$ . At last, we turn to  $\bar{E}_{\varepsilon}$ :

$$\begin{split} \bar{E}_{\varepsilon} &= -\int_{\Omega} \varepsilon^{-1} \frac{3}{2} \left( \hat{\psi}_{0}' \right)^{2} \circ \iota_{\varepsilon} \int_{\Omega} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}_{0}' \left( \iota_{\varepsilon}(y) \right) \right)^{2} \nabla_{\Sigma} \cdot \left( \nabla_{\nu} c \right) \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) \\ &- \int_{\Omega} \varepsilon^{-1} \frac{3}{2} \left( \hat{\psi}_{0}' \right)^{2} \circ \iota_{\varepsilon} \int_{\Omega} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}_{0}' \left( \iota_{\varepsilon}(y) \right) \right)^{2} \nabla_{\nu} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \cdot \bar{H}(x) \bar{\nu}(x) \, \mathrm{d}\mathcal{L}^{3}(y) \nu_{\psi} \cdot w \, \mathrm{d}\mathcal{L}^{3}(x) \\ &\rightarrow - \left( \frac{3Z}{2} \right)^{2} \int_{\Sigma} \int_{\Gamma} \nabla_{\Sigma} \cdot \left( \nabla_{\nu} c \right) (x, y, \rho_{a0}, \nu_{\Sigma}) + \nabla_{\nu} c \left( x, y, \rho_{a0}, \nu_{\Sigma} \right) \cdot H_{\Sigma}(x) \nu_{\Sigma}(x) \, \mathrm{d}\mathcal{H}^{2}(y) \nu_{\Sigma} \cdot w \, \mathrm{d}\mathcal{H}^{2}(x) \, \mathrm{as} \, \varepsilon \searrow 0. \end{split}$$

Limit of  $\bar{G}_{\varepsilon}$ :

Using the expansion we computed before, we obtain

$$\begin{split} \bar{G}_{\varepsilon} &= -\int_{N_{\delta}(\Sigma)} \rho_{a0} \varepsilon^{-1} \left( \hat{\psi}_{0}' \circ \iota_{\varepsilon} \right)^{2} \bar{H} \bar{\nu} \cdot w \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}_{0}' \circ \iota_{\varepsilon} \right)^{2} \partial_{\rho_{a}} c \left( x, y, \rho_{a0}, \nu_{\psi_{0}} \right) \, \mathrm{d} \mathcal{L}^{3}(y) \, \mathrm{d} \mathcal{L}^{3}(x) + O(\varepsilon) \\ &\rightarrow -\frac{3Z^{2}}{2} \int_{\Sigma} \rho_{a0} H_{\Sigma} \nu_{\Sigma} \cdot w \int_{\Gamma} \partial_{\rho_{a}} c \left( x, y, \rho_{a0}, \nu_{\Sigma} \right) \, \mathrm{d} \mathcal{H}^{2}(y) \, \mathrm{d} \mathcal{H}^{2}(x) \, \mathrm{as} \, \varepsilon \searrow 0. \end{split}$$

Limit of  $\bar{H}_{\varepsilon}$ :

On the expansion derived before, we use  $W(\psi_0) = (\hat{\psi}_0')^2$ , and then pass to the limit  $\varepsilon \searrow 0$ :

$$\begin{split} \bar{H}_{\varepsilon} &= -\int_{N_{\delta}(\Sigma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\psi}_{0}' \right)^{2} \circ \iota_{\varepsilon}(x) \int_{N_{\delta}(\Gamma)} \varepsilon^{-1} \frac{3}{2} \left( \hat{\phi}_{0}' \right)^{2} \circ \iota_{\varepsilon}(y) \nabla_{\Sigma_{d}} \left( \partial_{\rho_{a}} c \left( \cdot, y, \rho_{a0}, \nu_{\psi_{0}} \right) \right) \cdot w \rho_{a0} \, \mathrm{d}\mathcal{L}^{3}(y) \, \mathrm{d}\mathcal{L}^{3}(x) \\ &+ O(\varepsilon) \\ & \to - \left( \frac{3Z}{2} \right)^{2} \int_{\Sigma} \int_{\Gamma} \nabla_{\Sigma_{d}} \left( \partial_{\rho_{a}} c \left( \cdot, y, \rho_{a0}, \nu_{\psi_{0}} \right) \right) \cdot w \rho_{a0} \, \mathrm{d}\mathcal{H}^{2} \, \mathrm{d}\mathcal{H}^{2}. \end{split}$$

### Deriving the jump conditions

We now observe that all the previously computed limits have equal, corresponding terms in the right hand sides of Equations (4f) and (4g). Note that these appear with a minus on the right-hand side of the momentum balance, so we negate them here accordingly. We start by labelling them (here in variational form):

$$\begin{split} &\bar{I}_0 = \int_{\Gamma} \left( -\nabla_y C_\Sigma^0 \cdot \nu_\Gamma + H_\Gamma C_\Sigma^0 \right) w \cdot \nu_\Gamma \, \mathrm{d}\mathcal{H}^2, \\ &\bar{J}_0 = \int_{\Sigma} \left( -\nabla_x C_\Gamma^0 \cdot \nu_\Sigma + H_\Sigma C_\Gamma^0 \right) w \cdot \nu_\Sigma \, \mathrm{d}\mathcal{H}^2, \\ &\bar{K}_0 = -\int_{\Sigma} \partial_{\rho_a} C_\Gamma^0 H_\Sigma \rho_a w \cdot \nu_\Sigma \, \mathrm{d}\mathcal{H}^2, \\ &\bar{L}_0 = -\int_{\Sigma} \nabla_\Sigma \left( \partial_{\rho_a} C_\Gamma^0 \right) \cdot \rho_a w \, \mathrm{d}\mathcal{H}^2, \\ &\bar{M}_0 = -\int_{\Sigma} \left( \nabla_\Sigma \cdot \left( \nabla_\nu C_\Gamma^0 \right) + H_\Sigma \left( \nabla_\nu C_\Gamma^0 \cdot \nu_\Sigma \right) \right) w \cdot \nu_\Sigma \, \mathrm{d}\mathcal{H}^2. \end{split}$$

We see immediately that  $\bar{B}_0 + \bar{A}_0 = \frac{3Z^2}{2}\bar{I}_0$ . Further,

$$\bar{D}_0 + \bar{C}_0 = -\frac{3Z^2}{2} \int_{\Sigma} \int_{\Gamma} \nu_{\Sigma} \cdot \nabla_x c \nu_{\Sigma} \cdot w \, d\mathcal{H}^2 \, d\mathcal{H}^2 + \frac{3Z^2}{2} \int_{\Sigma} H_{\Sigma} \int_{\Gamma} c \, d\mathcal{H}^2 \nu_{\Sigma} \cdot w \, d\mathcal{H}^2 = \frac{3Z^2}{2} \bar{J}_0.$$

Clearly, 
$$\bar{G}_0 = \frac{3Z^2}{2}\bar{K}_0$$
,  $\bar{H}_0 = \left(\frac{3Z}{2}\right)^2\bar{L}_0$  and  $\bar{E}_0 = (\frac{3Z}{2})^2\bar{M}_0$ .

Clearly,  $\bar{G}_0 = \frac{3Z^2}{2}\bar{K}_0$ ,  $\bar{H}_0 = \left(\frac{3Z}{2}\right)^2\bar{L}_0$  and  $\bar{E}_0 = (\frac{3Z}{2})^2\bar{M}_0$ . Equating Equation (61) on the left and the limit of Lemma 4.2, as well as the terms for the Ginzburg–Landau energy gradient and  $\bar{A}_0 + \bar{B}_0 + \bar{C}_0 + \bar{D}_0 + \bar{E}_0 + \bar{G}_0 + \bar{H}_0$  on the right, we find Equations (4f) and (4g).

#### 4.3 Phase field evolution equations

Equations (1c) and (1d) are just the tautologies 0 = 0 in the outer region, so we are only concerned with them close to the boundary layers. On their left-hand sides, we find at leading order  $\varepsilon^{-1}$ 

$$-V_{\nu}^{\Phi}\hat{\varphi}_{0}^{\prime}\circ\iota_{\varepsilon}+\upsilon_{0}\cdot\bar{\nu}\hat{\varphi}_{0}^{\prime}\circ\iota_{\varepsilon}\tag{67}$$

for  $\varphi \in \{\phi, \psi\}$  with corresponding boundary layer  $\Phi \in \{\Gamma, \Sigma\}$ .

From the energy inequality, the following bound holds,

$$\varepsilon^{\alpha} \int_{0}^{T} \int_{N_{\delta}(\Phi)} \left| \nabla \nabla_{\varphi}^{L^{2}} \mathcal{F} \right|^{2} d\mathcal{L}^{3} dt \in O(1).$$
 (68)

We have found in Section 3.8 that  $\nabla_{\varphi}^{L^2} \mathcal{F}[\varphi] \in O(1)$ , so

$$\nabla \nabla_{\varphi}^{L^{2}} \mathcal{F} = \sum_{i=-1}^{2} \varepsilon^{i} \hat{f}_{i} \circ \iota_{\varepsilon} + O\left(\varepsilon^{3}\right).$$

Thus,

$$\left| \nabla \widehat{\nabla L_{\varphi}^2} \mathcal{F} \right|^2 = \varepsilon^{-2} \hat{f}_{-1}^2 + 2\varepsilon^{-1} \hat{f}_{-1} \hat{f}_0 + \left( \hat{f}_0^2 + \hat{f}_{-1} \hat{f}_1 \right) + \varepsilon \left( 2\hat{f}_{-1} \hat{f}_2 + 2\hat{f}_0 \hat{f}_1 \right) + \varepsilon^2 \left( \hat{f}_1^2 + 2\hat{f}_{-1} \hat{f}_3 + 2\hat{f}_0 \hat{f}_2 \right) + O(1).$$

Equation (68) directly implies

$$\int_0^T \int_{-\frac{\delta}{z}}^{\frac{\delta}{\varepsilon}} \int_{\Phi_{\varepsilon z}} \left| \widehat{\nabla \nabla_{\varphi}^{L^2}} \mathcal{F} \right|^2 (\pi_{\Phi}(\sigma), z) \; \mathrm{d}\mathcal{H}^2(\sigma) \, \mathrm{d}z \, \mathrm{d}t \in O\left(\varepsilon^{-\alpha - 1}\right).$$

Since  $\alpha < 1$  (required in Section 3.8),  $\hat{f}_{-1} = 0$ , so  $\widehat{\nabla \nabla_{\varphi}^{L^2}} \mathcal{F} \in O(1)$ . Further,  $\nabla \cdot \left( \varepsilon^{\alpha} \nabla \left( \nabla_{\varphi}^{L^2} \mathcal{F} \right) \right) \in O\left( \varepsilon^{-1+\alpha} \right)$ , which is of lower order than the left-hand side (67) for  $\alpha > 0$ , so we obtain from the phase field evolution to leading order

$$v_0 \cdot \bar{v} = V_{\nu}^{\Phi} \tag{69}$$

meaning that the interface  $\Phi$  is driven purely by the fluid's velocity in normal direction, and this is equivalent to the Hamilton–Jacobi equations (4h) and (4i).

#### 4.4 | Species subsystem

Like the phase field equations, the species subsystem (1i), (1j) is meaningless in the outer region. For reasons of symmetry, it suffices to conduct the asymptotic analysis for the equation of  $\rho_a$ : it carries over to  $\rho_i$  verbatim.

We start our analysis by expanding the term  $\nabla \cdot (g_{\varepsilon}[\psi]\eta_a \nabla \rho_a)$ . W.l.o.g., we assume that  $\hat{\eta}_a' = 0$ . First we derive from Equation (7) and using Equation (30)

$$\begin{split} \eta_a \nabla \rho_a &= \varepsilon^{-1} \eta_a \hat{\rho}'_{a0} \circ \iota_{\varepsilon} \bar{\nu} + \eta_a \nabla_{\Sigma_d} \rho_{a0} + \eta_a \hat{\rho}'_{a1} \circ \iota_{\varepsilon} \bar{\nu} + \varepsilon \eta_a \nabla_{\Sigma_d} \rho_{a1} + O\left(\varepsilon^2\right) \\ &= \eta_a \nabla_{\Sigma_d} \rho_{a0} + \eta_a \hat{\rho}'_{a1} \circ \iota_{\varepsilon} \bar{\nu} + \varepsilon \eta_a \nabla_{\Sigma_d} \rho_{a1} + O\left(\varepsilon^2\right). \end{split}$$

With Equation (16) and thanks to Equation (43) and  $\hat{\psi}_0$  being the optimal profile, we have also

$$g_{\varepsilon}[\psi] = \varepsilon^{-1} \frac{3}{2} \left( \hat{\psi}_0' \right)^2 \circ \iota_{\varepsilon} + O(\varepsilon).$$

Multiplying both equations gives

$$g_{\varepsilon}[\psi]\eta_{a}\nabla\rho_{a} = \varepsilon^{-1}\frac{3}{2}\left(\hat{\psi}_{0}'\right)^{2} \circ \iota_{\varepsilon}\eta_{a}\left(\nabla_{\Sigma_{d}}\rho_{a0} + \hat{\rho}_{a1}'\circ\iota_{\varepsilon}\bar{\nu}\right) + \frac{3}{2}\left(\hat{\psi}_{0}'\right)^{2} \circ \iota_{\varepsilon}\eta_{a}\nabla_{\Sigma_{d}}\rho_{a1} + O(\varepsilon). \tag{70}$$

We also expand

$$\nabla \cdot (g_{\varepsilon}[\psi]\rho_{a}v_{\tau}) = \nabla \cdot \left(\varepsilon^{-1}\frac{3}{2}\left(\hat{\psi}_{0}^{\prime}\right)^{2} \circ \iota_{\varepsilon}\rho_{a0}\left(v_{0}\right)_{\tau} + \frac{3}{2}\left(\hat{\psi}_{0}^{\prime}\right)^{2} \circ \iota_{\varepsilon}\left(\rho_{a1}\left(v_{0}\right)_{\tau} + \rho_{a0}\left(v_{1}\right)_{\tau}\right) + O(\varepsilon)\right)$$

$$= \varepsilon^{-2}\left(\frac{3}{2}\left(\hat{\psi}_{0}^{\prime}\right)^{2}\hat{\rho}_{a0}\left(\hat{v}_{0}\right)_{\tau}\right)^{\prime} \circ \iota_{\varepsilon} \cdot \bar{v} + \varepsilon^{-1}\left(\frac{3}{2}\left(\hat{\psi}_{0}^{\prime}\right)^{2}\left(\hat{\rho}_{a1}\left(\hat{v}_{0}\right)_{\tau} + \hat{\rho}_{a0}\left(\hat{v}_{1}\right)_{\tau}\right)\right)^{\prime} \circ \iota_{\varepsilon} \cdot \bar{v}$$

$$+ \varepsilon^{-1}\nabla_{\Sigma_{d}} \cdot \left(\frac{3}{2}\left(\hat{\psi}_{0}^{\prime}\right)^{2} \circ \iota_{\varepsilon}\rho_{a0}\left(v_{0}\right)_{\tau}\right) + O(1). \tag{71}$$

The first and second summands vanish since  $(\hat{v}_i)_{\tau} \cdot \hat{v} = \hat{v}_i^T \mathbb{P}_{\nu_{\hat{\psi}}} \hat{v} = O\left(\epsilon^2\right), i \in \{1, 2\}$ , thanks to Equation (55). Second, we compute (making again use of Equation 30)

$$\begin{split} \nabla \cdot \left( g_{\varepsilon}[\psi] \eta_{a} \nabla \rho_{a} \right) &= \varepsilon^{-2} \frac{3}{2} \left( \left( \hat{\psi}_{0}^{\prime} \right)^{2} \right)^{\prime} \circ \iota_{\varepsilon} \eta_{a} \left( \nabla_{\Sigma_{d}} \rho_{a0} + \hat{\rho}_{a1}^{\prime} \circ \iota_{\varepsilon} \bar{\nu} \right) \cdot \bar{\nu} + \varepsilon^{-2} \frac{3}{2} \left( \hat{\psi}_{0}^{\prime} \right)^{2} \circ \iota_{\varepsilon} \eta_{a} \hat{\rho}_{a1}^{\prime\prime} \circ \iota_{\varepsilon} \\ &+ O \left( \varepsilon^{-1} \right) \\ &= \varepsilon^{-2} \frac{3}{2} \left( \left( \left( \hat{\psi}_{0}^{\prime} \right)^{2} \right)^{\prime} \circ \iota_{\varepsilon} \hat{\rho}_{a1}^{\prime} \circ \iota_{\varepsilon} + \left( \hat{\psi}_{0}^{\prime} \right)^{2} \circ \iota_{\varepsilon} \eta_{a} \hat{\rho}_{a1}^{\prime\prime} \circ \iota_{\varepsilon} \right) \\ &= \varepsilon^{-2} \frac{3}{2} \eta_{a} \left( \left( \hat{\psi}_{0}^{\prime} \right)^{2} \hat{\rho}_{a1}^{\prime} \right)^{\prime} \circ \iota_{\varepsilon} + O \left( \varepsilon^{-1} \right). \end{split}$$

All other terms in Equation (1i) are in  $O(\varepsilon^{-1})$ . Thus,  $(\hat{\psi}'_0)^2 \hat{\rho}'_{a1}$  is constant in z. We observe that  $(\hat{\psi}'_0)^2$  decays for large |z|, and for the expression to remain constant,  $\hat{\rho}'_{a1}$  must either blow up or be zero constantly. We can exclude the former case by matching, so

$$\hat{\rho}'_{a1} = 0.$$

Then, Equation (70) simplifies and we obtain

$$\begin{split} \nabla \cdot \left(g_{\varepsilon}[\psi] \eta_{a} \nabla \rho_{a}\right) &= \varepsilon^{-1} \frac{3}{2} \left( \left( \left( \hat{\psi}_{0}' \right)^{2} \right)' \circ \iota_{\varepsilon} \eta_{a} \nabla_{\Sigma_{d}} \rho_{a1} \cdot \bar{\nu} \right. \\ &+ \left( \hat{\psi}_{0}' \right)^{2} \circ \iota_{\varepsilon} \left( \nabla_{\Sigma_{d}} \cdot \left( \eta_{a} \nabla_{\Sigma_{d}} \rho_{a0} \right) + \eta_{a} \left( \widehat{\nabla_{\Sigma_{d}} \rho_{a}} \right)' \circ \iota_{\varepsilon} \cdot \bar{\nu} \right) \right) + O(1) \\ &= \varepsilon^{-1} \frac{3}{2} \left( \hat{\psi}_{0}' \right)^{2} \circ \iota_{\varepsilon} \nabla_{\Sigma_{d}} \cdot \left( \eta_{a} \nabla_{\Sigma_{d}} \rho_{a0} \right). \end{split}$$

Finally, we find in Equation (1i) (note Equations 71 and 18, and the independence of  $\hat{\psi}_0$  from the tangential variable due to its being the optimal profile) to leading order  $\varepsilon^{-1}$ 

$$\begin{split} \frac{3}{2} \left( \hat{\psi}_{0}^{\prime} \right)^{2} &\circ \iota_{\varepsilon} \left( \partial_{t} \rho_{a0} - \nabla_{\Sigma_{d}} \cdot \left( \eta_{a} \nabla_{\Sigma_{d}} \rho_{a0} \right) \right) - \left( \hat{\psi}_{0}^{\prime} \right)^{2} \circ \iota_{\varepsilon} \rho_{a0} \bar{H} v_{0} \cdot \bar{v} + \frac{3}{2} \left( \hat{\psi}_{0}^{\prime} \right)^{2} \circ \iota_{\varepsilon} \nabla_{\Sigma_{d}} \cdot \left( \rho_{a0} \left( v_{0} \right)_{\tau} \right) = \\ \frac{3}{2} \left( \hat{\psi}_{0}^{\prime} \right)^{2} \circ \iota_{\varepsilon} \mathcal{R} \left[ \rho_{a0}, \rho_{i0}; \phi_{0}, \nu_{\psi_{0}} \right], \end{split}$$

which is Equation (4j) up to constants. On the right-hand side, we used the expansion

$$\mathcal{R}\left[\rho_{a},\rho_{i};\phi,\nu_{\psi}\right] = \mathcal{R}\left[\rho_{a0},\rho_{i0};\phi_{0},\nu_{\psi_{0}}\right] + O(\varepsilon),$$

which holds with Equation (53) and

$$\nabla_{\rho_a}^{L^2} \mathcal{R}, \nabla_{\rho_i}^{L^2} \mathcal{R}, \nabla_{\phi}^{L^2} \mathcal{R}, \nabla_{\nu}^{L^2} \mathcal{R} \in O(1).$$

So altogether, we could argue with the help of formally matched asymptotic expansions that solutions of the PDE system (1), under suitable Assumptions Assumptions 1–8, converge to solutions of Equation (4) as  $\varepsilon \setminus 0$ .

#### **5** | CONCLUSION

We have made plausible that both the diffuse and sharp interface modelling approaches are compatible in the sense that their solutions are approximations of each other. To arrive at this conclusion, we leveraged the method of formal asymptotic analysis.

From a mathematical perspective, it is desirable to prove that this result rigorously like Abels and Liu [16] or Fei and Liu [17] did for related PDE systems. The main problems to deal with will likely be analysing the leading order terms in the expansion of the Canham–Helfrich energy and controlling the pressure, showing it does not blow up near the diffuse layers. An excellent stock of techniques for analysing the Canham–Helfrich energy is already provided in [17]. However, they analyse the pure Willmore flow problem, and so there is no coupling with a fluid, nor with a species subsystem like in the PDE system (1) investigated here, which poses additional problems like possible pressure blow-ups. Controlling the pressure for a phase-field-Navier–Stokes coupling is investigated in Abels and Liu [16]. A step towards a rigorous analysis of Equation (1) might, therefore, be possible by uniting the results of both works and leaving the species subsystem aside.

From a modelling perspective, our results increase the confidence that qualitatively both abstractions – the sharp interface or diffuse layer abstraction – are equivalent and the focus can now be more on other aspects like numerical feasibility.

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#### REFERENCES

- [1] Charras, G.T., Paluch, E.: Blebs lead the way: how to migrate without lamellipodia. Nat. Rev. Mol. Cell Biol. 9, 730-736 (2008)
- [2] Paluch, E.K., Raz, E.: The role and regulation of blebs in cell migration. Curr. Opin. Cell Biol. 25, 582-590 (2013)
- [3] Othmer, H.G.: Eukaryotic cell dynamics from crawlers to swimmers. WIREs Comput. Mol. Sci. 9, e1376 (2018)
- [4] Lavi, I., Goudarzi, M., Raz, E., Gov, N.S., Voituriez, R., Sens, P.: Cellular blebs and membrane invaginations are coupled through membrane tension buffering. Biophys. J. 117, 1485–1495 (2019)
- [5] Strychalski, W.: 3D computational modeling of bleb initiation dynamics. Front. Phys. Sec. Biophys. 9, 775465 (2021)
- [6] Lim, F.Y., Chiam, K.-H., Mahadevan, L.: The size, shape, and dynamics of cellular blebs. Europhys. Lett. 100, 28004 (2012)
- [7] Strychalski, W., Guy, R.D.: A computational model of bleb formation. Math. Med. Biol. 30, 115-130 (2013)
- [8] Strychalski, W., Copos, C.A., Lewis, O.L., Guy, R.D.: A poroelastic immersed boundary method with applications to cell biology. J. Comput. Phys. 282, 77–97 (2015)
- [9] Alert, R., Casademunt, J., Brugués, J., Sens, P.: Model for probing membrane-cortex adhesion by micropipette aspiration and fluctuation spectroscopy. Biophys. J. 108, 1878–1886 (2015)
- [10] Alert, R., Casademunt, J.: Bleb nucleation through membrane peeling. Phys. Rev. Lett. 116, 068101 (2016)
- [11] Stinner, B., Dedner, A., Nixon, A.: A finite element method for a fourth order surface equation with application to the onset of cell blebbing. Front. Appl. Math. Stat. 6, 21 (2020)
- [12] Werner, P., Burger, M., Pietschmann, J.: A PDE model for bleb formation and interaction with linker proteins. Trans. Math. Appl. 4, 1 (2020)
- [13] Werner, P., Burger, M., Frank, F., Garcke, H.: A diffuse interface model for cell blebbing including membrane-cortex coupling with linker dynamics. SIAM J. Appl. Math. 82, 1091–1112 (2022)
- [14] Werner, P.: Sharp and diffuse interface models for the evolution of surfaces that are immersed in fluids and coupled through surfactants. Ph.D. thesis, Friedrich-Alexander-Universität Erlangen-Nürnberg (2021)
- [15] Caginalp, G., Fife, P.: Phase-field methods for interfacial boundaries. Phys. Rev. B 33, 7792 (1986)
- [16] Abels, H., Liu, Y.: Sharp interface limit for a Stokes/Allen-Cahn system. Arch. Ration. Mech. Anal. 229, 417–502 (2018)
- [17] Fei, M., Liu, Y.: Phase-field approximation of the Willmore flow. Arch. Ration. Mech. Anal. 241, 1655–1706 (2021)

- [18] Wang, X.: Asymptotics analysis of phase field formulations of bending elasticity models. SIAM J. Math. Anal. 39, 1367–1401 (2008)
- [19] Gilbarg, D., Trudinger, N.S.: Elliptic partial differential equations of second order. Grundlehren der mathematischen wissenschaften, vol. 224, 3rd edn. Springer, Berlin (2010)
- [20] Onsager, L.: Reciprocal relations in irreversible processes. I. Phys. Rev. 37, 405–426 (1931)
- [21] Qian, T., Wang, X.-P., Shen, P.: A variational approach to moving contact line hydrodynamics. J. Fluid Mech. 564, 333–360 (2006)
- [22] Canham, P.B.: The minimum energy of bending as a possible explanation of the bioconcave shape of the human red blood cell. J. Theor. Biol. 26, 61-81 (1970)
- [23] Helfrich, W.: Elastic properties of lipid bilayers: theory and possible experiments. Zeitung für Naturforschung 28, 693–703 (1973)
- [24] Du, Q., Liu, C., Ryham, R., Wang, X.: Energetic variational approaches in modeling vesicle and fluid interactions. Physica D 238, 923–930 (2009)
- [25] Eckhaus, W.: Asymptotic analysis of singular perturbations. Studies in mathematics and its applications, vol. 9. North-Holland Publishing Company, Amsterdam (1979)
- [26] Holmes, M.J.: Introduction to perturbation methods. Texts in applied mathematics, vol. 20. Springer, New York (1995)

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