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John W. Barrett, Harald Garcke and Robert Nürnberg

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ON SHARP INTERFACE LIMITS OF ALLEN–CAHN/CAHN–HILLIARD VARIATIONAL INEQUALITIES

John W. Barrett
Department of Mathematics
Imperial College London
South Kensington Campus
London, SW7 2AZ, United Kingdom

Harald Garcke
NWF I - Mathematik
Universität Regensburg
93040 Regensburg, Germany

Robert Nürnberg
Department of Mathematics
Imperial College London
South Kensington Campus
London, SW7 2AZ, United Kingdom

1. **Introduction.** Two approaches to model curvature dependent interface motion are sharp interface models and phase field models. Sharp interface models describe the interface as a hypersurface, whereas in phase field models a diffusive layer with positive thickness is used to model the interface. In the limit, when the thickness of the diffusive layer tends to zero, one would like to recover a sharp interface limit. In the case of phase field models for two phases such asymptotic limits are by now well understood. Less is known if more than two physical states are present. In this paper we study the sharp interface limit of an Allen–Cahn/Cahn–Hilliard system which can be viewed as a phase field system modelling the electromigration of intergranular voids. The Allen–Cahn/Cahn–Hilliard system has been recently introduced by the authors, see [1], extending previous work by Mahadevan and Bradley [12], and Cahn and Novick-Cohen [5, 6] For further details on phase field equations and sharp interface models we refer to Elliott [7].

1.1. **The Allen–Cahn/Cahn–Hilliard variational inequality.** The model we consider is based on a Ginzburg–Landau type energy of the form

$$\mathcal{E}(u,v) := \int_\Omega (\tfrac{\gamma}{2}\,|\nabla u|^2 + \tfrac{\gamma}{2}\,|\nabla v|^2 + \gamma^{-1}\Psi(u,v))\,\mathrm{d}x, \tag{1}$$

where (u,v) are the phase fields, Ω is a domain in $\mathbb{R}^d$ (d being the spatial dimension) and γ is a positive parameter which will be related to the interfacial thickness. The

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potential Ψ is of the following obstacle type

$$\Psi(r,s) := \begin{cases} \psi(r,s) & \text{if } (r,s) \in \mathcal{K}, \\ \infty & \text{if } (r,s) \notin \mathcal{K}, \end{cases} \qquad \text{with } \psi \in C^2(\mathcal{K}),$$

where $\mathcal{K}$ is a closed equilateral triangle with corners $A = (-1,0)$, $B = (1, -\frac{2}{\sqrt{3}})$ and $C = (1, \frac{2}{\sqrt{3}})$. The function ψ is assumed to be smooth, non-negative with global minima at the points A, B and C. Here $(u,v) = A$ represents the void, while the grains B and C make up the material of the conductor, see [1] for more details.

To simplify the presentation in this paper, we will take ψ to be of the form

$$\psi(r,s) := \tfrac{8}{9} - \tfrac{1}{2}\left[(r - \tfrac{1}{3})^2 + (1-\mu)\, s^2 + \tfrac{2}{3}\,\mu\,(r+1)\right], \tag{2}$$

where $\mu < 1$ is constant; although more general forms of ψ are possible.

The Allen–Cahn/Cahn–Hilliard variational inequality introduced in [1] now has the following form. We search for functions u, v, w, z, ϕ defined in Ω and for all $t > 0$ such that for all $x \in \Omega$, $t > 0$ we have $(u,v) \in \mathcal{K}$ and and for all $(\eta_1, \eta_2) \in \mathcal{K}$

$$\gamma\, \tfrac{\partial u}{\partial t} - \nabla\,.\,(b(u)\, \nabla[w + \alpha\, \phi]\,) = 0\,, \tag{3a}$$

$$\ell(\gamma)\, \tfrac{\partial v}{\partial t} + z = 0\,, \tag{3b}$$

$$(-\gamma\, \Delta u + \gamma^{-1}\, \psi_{,u}(u,v) - w)\,(\eta_1 - u) + (-\gamma\, \Delta v + \gamma^{-1}\, \psi_{,v}(u,v) - z)\,(\eta_2 - v) \geq 0\,, \tag{3c}$$

$$\nabla\,.\,(c(u)\, \nabla \phi) = 0\,. \tag{3d}$$

In addition, we require on $\partial\Omega$, the boundary of Ω, that for $t > 0$

$$b(u)\, \tfrac{\partial[w + \alpha\, \phi]}{\partial \nu} = 0 \qquad \text{and} \qquad c(u)\, \tfrac{\partial \phi}{\partial \nu} = g$$

for a given function g. Homogeneous Neumann boundary conditions for u, v are also weakly enforced via (3c). Furthermore, initial data $(u^0, v^0) \in \mathcal{K}$, for all $x \in \Omega$, are also imposed on (u,v). Here $b(u) := 1 - u^2$ is the degenerate mobility (note that $|u| \leq 1$), $\alpha > 0$ is a constant, ϕ is the electric potential, $\ell(\gamma) := \beta\, \gamma$ or $\ell(\gamma) := \beta\, \gamma^2$ where $\beta > 0$ is constant. Furthermore, $c(u) := 1 + u$ and ν is the outward unit normal to $\partial\Omega$. For details on the physical background of the above system we refer to [1]. It can be shown that an energy inequality involving the Ginzburg–Landau energy (1) holds (see [1]).

1.2. **The sharp interface limit.** After a short time, solutions to the problem (3a-d) have the following structure. In most of Ω the solution (u,v) attains one of the values A, B or C. The regions in which one of these constants are attained are separated by layers of a thickness proportional to γ. Three of these layers might meet at triple junctions. In Section 2 we will show that in the sharp interface limit, $\gamma \searrow 0$, the following problem is obtained. Denoting by Γ^A, Γ^B and Γ^C the interfaces separating phases (B,C), (C,A) and (A,B) with normals pointing into C, A and B, respectively; we obtain for the scaling $\ell(\gamma) := \beta\, \gamma^2$:

$$\begin{aligned} \mathcal{V}^C &= -\tfrac{M^C}{2}\, \partial_{ss}\big(\tfrac{\sigma^C}{2}\, \kappa^C + \alpha\, \phi^C\big) && \text{on } \Gamma^C, \\ \mathcal{V}^B &= -\tfrac{M^B}{2}\, \partial_{ss}\big(\tfrac{\sigma^B}{2}\, \kappa^B - \alpha\, \phi^B\big) && \text{on } \Gamma^B, \\ 0 &= \kappa^A && \text{on } \Gamma^A. \end{aligned} \tag{4}$$

Here $\mathcal{V}^i$ denotes the normal velocity of interface Γ^i, ∂_{ss} denotes the second derivative with respect to arc-length, κ^i is the curvature of interface Γ^i, ϕ^i is the value of ϕ

on Γ^i, and finally M^i, σ^i are constants to be specified in Section 2. For the scaling $\ell(\gamma) := \beta\,\gamma$ we obtain that

$$\begin{aligned} \pm 2\,\mathcal{V}^i &= M^i\,\partial_{ss}\,(w^i + \alpha\,\phi^i) && \text{on } \Gamma^i \quad \text{for } i \in \{B, C\}, \\ \beta\,\omega^i\,\mathcal{V}^i &= \sigma^i\,\kappa^i \pm 2\,w^i && \text{on } \Gamma^i \quad \text{for } i \in \{B, C\}, \\ \beta\,\omega^A\,\mathcal{V}^A &= \sigma^A\,\kappa^A && \text{on } \Gamma^A; \end{aligned} \tag{5}$$

where w^i is value of the chemical potential w on Γ^i, ω^i are constants to be specified in Section 2, and in the $\pm$ option we take the top for $i = B$ and the bottom for $i = C$. For both scalings, the limiting electric potential fulfils

$$\Delta\phi = 0 \quad \text{in} \quad \Omega \setminus \overline{\Omega^A(t)}\,, \qquad \tfrac{\partial\phi}{\partial n_\Gamma} = 0 \quad \text{on} \quad \Gamma^B \cup \Gamma^C;$$

where $\Omega^A(t)$ is the region with $(u, v) = A$ and boundary $\Gamma^B \cup \Gamma^C$, and n_Γ is a normal to this interface.

Moreover, at triple junctions we obtain, for both scalings, Young's law

$$\frac{\sin\theta^A}{\sigma^A} = \frac{\sin\theta^B}{\sigma^B} = \frac{\sin\theta^C}{\sigma^C}, \tag{6}$$

where θ^A, θ^B and θ^C are the angles that the regions A, B and C form at the triple junction (see also [3, 2, 9]). Furthermore, a flux balance condition

$$M^C\,\partial_s(w^C + \alpha\,\phi^C) + M^B\,\partial_s(w^B + \alpha\,\phi^B) = 0 \tag{7}$$

and a continuity condition for chemical potentials

$$w^C = w^B \tag{8}$$

has to hold. Finally, when an interface meets the external boundary, $\partial\Omega$, a 90° angle condition has to be required. In addition, at points where the material boundary intersects $\partial\Omega$, we have

$$\partial_s(w^i + \alpha\,\phi^i) = 0 \quad \text{for} \quad i \in \{B, C\}\,.$$

1.3. **Conservation and decay properties.** The total area occupied by the void (and hence also the total area occupied by the material) is conserved by the above flows. Let $a(t)$ be the total volume of the void at time t. Using a transport theorem for area, see e.g. [11], we obtain that

$$\begin{aligned} \tfrac{d}{dt}a(t) &= -\int_{\Gamma^B(t)} \mathcal{V}^B\,\mathrm{d}s + \int_{\Gamma^C(t)} \mathcal{V}^C\,\mathrm{d}s \\ &= -\tfrac{1}{2}\int_{\Gamma^B(t)} M^B\,\partial_{ss}(w^B + \alpha\,\phi^B)\,\mathrm{d}s - \tfrac{1}{2}\int_{\Gamma^C(t)} M^C\,\partial_{ss}(w^C + \alpha\,\phi^C)\,\mathrm{d}s = 0 \end{aligned}$$

by the flux condition (7) and the no flux condition at the outer boundary.

The surface energy of the system at time t is given by

$$E^s(t) := \sum_{i\in\{A,B,C\}} \int_{\Gamma^i} \sigma^i\,\mathrm{d}s\,.$$

We now want to show that in the absence of an electric field, i.e. $\alpha = 0$, the total surface energy is a Lyapunov functional. Firstly, we consider the case of $\ell(\gamma) := \beta\,\gamma$. Using a transport theorem for integrals over the interface, see e.g. [11], (5), (6) and the angle condition at the outer boundary, we obtain (for more details in a related situation see [9, 13])

$$\begin{aligned}
\tfrac{d}{dt}E^s(t) &= -\sum_{i\in\{A,B,C\}} \int_{\Gamma^i(t)} \sigma^i\,\kappa^i\,\mathcal{V}^i\,\mathrm{d}s \\
&= -\beta \sum_{i\in\{A,B,C\}} \omega^i \int_{\Gamma^i(t)} [\mathcal{V}^i]^2\,\mathrm{d}s + 2\left[\int_{\Gamma^B(t)} w^B\,\mathcal{V}^B\,\mathrm{d}s - \int_{\Gamma^C(t)} w^C\,\mathcal{V}^C\,\mathrm{d}s\right] \\
&\leq -\sum_{i\in\{B,C\}} \int_{\Gamma^i(t)} M^i\,|\partial_s\,w^i|^2\,\mathrm{d}s \leq 0. \qquad (9)
\end{aligned}$$

In the above computation the term $[\,M^B\,w^B\,\partial_s\,w^B + M^C\,w^C\,\partial_s\,w^C\,]$ resulting from integration by parts vanishes at the outer boundary and at the triple junction due to the flux condition (7), the continuity condition (8) and the no flux condition at the outer boundary. The argument in (9) is easily adapted to the scaling $\ell(\gamma) := \beta\,\gamma^2$ on replacing the use of (5) by (4). In conclusion we have for both motions that $\frac{d}{dt}E^s(t) \leq 0$.

In Section 2 we will present the matched asymptotic expansion procedure relating the degenerate Allen–Cahn/Cahn–Hilliard variational inequality to the sharp interface model. A similar sharp interface asymptotics has been performed by Novick-Cohen [13] using a different scaling and obtaining a different sharp interface limit. Our sharp interface limit, (5), couples the so-called surface attachment limited kinetics (SALK) and surface diffusion (see e.g. [14, 8] for more information on this flow).

We obtain also another sharp interface problem, (4), where the grain boundaries Γ^A fulfil a quasi-static evolution equation and the void boundaries Γ^B, Γ^C move by surface diffusion. It requires further study to show a well-posedness result for this problem.

Let us remark also that we introduce a new methodology, to tackle matched asymptotic expansions for variational inequalities with triple junctions. To our knowledge, this work is the first to study this type of problem. We conclude with a short section on numerical simulations for the degenerate Allen–Cahn/Cahn–Hilliard variational inequality.

2. **Asymptotic expansions.**

We will use the method of formally matched asymptotic expansions to identify the sharp interface limit. Three different types of expansions will be used. In regions where either a grain or the void is present, we use an outer expansion. Close to interfaces separating either a void and a grain or two grains, an inner expansion is used. A third type of expansion has to be performed at a triple junction. All these expansions have to be matched.

The equations for the outer expansion imply that the vector (u, v) attains one of the values A, B, C. That is, in the sharp interface limit (u, v) will be either A, B or C and there are interfaces separating these regions. For the electric potential ϕ we obtain that it solves Laplace's equation in the regions where (u, v) is either B or C.

2.1. **Inner expansions (leading order).**

Now the inner expansion has to be used to determine the governing equations on the interface. There are three interfaces (curves in two space dimensions) for which we seek these laws. Let $\Gamma^{ij} = (\Gamma^{ij}(t))_{t\geq 0}$ with either $(i, j) = (A, B)$, (B, C) or (C, A) be an interface between regions occupied by i and j, which is assumed to be a smooth evolving curve in the sense of [11]; and let $X^{ij}(s,t)$ be a parameterization of Γ^{ij}, where s is an arc-length parameter. We define the unit tangent $\tau_\Gamma^{ij} := \partial_s X^{ij}$ and the unit normal n_Γ^{ij} such that $(n_\Gamma^{ij}, \tau_\Gamma^{ij})$ is positively orientated, i.e. $\tau_\Gamma^{ij} = R\, n_\Gamma^{ij}$, where R is the clockwise rotation through $\frac{\pi}{2}$. We define the direction of increasing s such that n_Γ^{ij} points into the region occupied by j. From now on we will suppress the superscripts, when no confusion can arise.

The curvature κ is defined to be positive if Γ is curved in the direction of the normal. With this choice the Frenet formulas read as

$$\partial_s n_\Gamma = -\kappa\, \tau_\Gamma, \qquad \partial_s \tau_\Gamma = \kappa\, n_\Gamma. \tag{10}$$

Since Γ is smooth, there exist functions $s(x,t)$ and $d(x,t)$ defined in a neighbourhood of Γ such that

$$x = X(s(x,t),t) + d(x,t)\, n_\Gamma(s(x,t),t);$$

see e.g. [10, §14.6]. The quantity $d(x,t)$ is the distance of the point x to $\Gamma(t)$ (note that $(x - X(s,t))\,.\,\tau_\Gamma(s,t) = 0$). In the following we will make use of the coordinate change

$$(x,t) \mapsto (\rho(x,t), s(x,t), t)\,,$$

where $\rho(x,t) = \gamma^{-1} d(x,t)$ is the re-scaled distance to Γ. This change of variables is a diffeomorphism flattening the interface Γ.

Straightforward computations yield that

$$\nabla_x s\,.\,\nabla_x d = 0\,, \qquad |\nabla_x d| = 1 \qquad \text{and} \qquad |\nabla_x s| = \tfrac{1}{1-d\,\kappa}\,. \tag{11}$$

Defining the normal velocity of Γ as $\mathcal{V} := \partial_t X\,.\,n_\Gamma$, we obtain in addition that

$$\mathcal{V} = -\partial_t d\,. \tag{12}$$

Using the new coordinates (ρ, s, t), we obtain the following identities for a scalar quantity $a(x,t) \equiv \widehat{a}(\rho(x,t), s(x,t), t)$

$$\nabla_x a(x,t) = \gamma^{-1}\partial_\rho \widehat{a}\, \nabla_x d + \partial_s \widehat{a}\, \nabla_x s \;\text{ and }\; \partial_t a(x,t) = \gamma^{-1}\partial_\rho \widehat{a}\, \partial_t d + \partial_s \widehat{a}\, \partial_t s + \partial_t \widehat{a}\,. \tag{13}$$

For a vector function $\underline{a}(x,t) \equiv \underline{\widehat{a}}(\rho(x,t), s(x,t), t)$ we obtain that

$$\nabla_x \cdot \underline{a}(x,t) = \gamma^{-1}\partial_\rho \underline{\widehat{a}}\,.\,\nabla_x d + \partial_s \underline{\widehat{a}}\,.\,\nabla_x s\,. \tag{14}$$

Using (10), (11), (13) and (14) we obtain the following representation of Δ_x in the new coordinates

$$\begin{aligned}\Delta_x a(x,t) &= \gamma^{-2}\partial_{\rho\rho}\widehat{a} - \gamma^{-1}\partial_\rho \widehat{a}\, \tfrac{\kappa}{1-\gamma\,\rho\,\kappa} + \partial_{ss}\widehat{a}\, |\nabla_x s|^2 + \partial_s \widehat{a}\, \tfrac{\gamma\,\partial_s(\rho\,\kappa)}{(1-\gamma\,\rho\,\kappa)^3} \\ &= \gamma^{-2}\partial_{\rho\rho}\widehat{a} - \gamma^{-1}\partial_\rho \widehat{a}\, \tfrac{\kappa}{1-\gamma\,\rho\,\kappa} + \partial_{ss}\widehat{a} + \mathcal{O}(\gamma)\,. \end{aligned} \tag{15}$$

We now assume that there exist expansions of u, v, w, z and ϕ in these new variables, i.e. for example

$$u(x,t) = \widehat{u}(\rho, s, t) = \widehat{u}_0(\rho, s, t) + \gamma\, \widehat{u}_1(\rho, s, t) + \dots\,.$$

In the following we drop the $\widehat{}$ for notational convenience. For reasons that will become clear later, we assume that $\mu \in (-2, \frac{4}{7})$, recall (2).

Considering (3c) to leading order, we obtain that $(u_0, v_0) : \mathbb{R} \to \mathcal{K}$ has to solve for all $(\eta_1, \eta_2) : \mathbb{R} \to \mathcal{K}$ the inequality

$$(-\partial_{\rho\rho} u_0 + \psi_{,u}(u_0, v_0))\,(\eta_1 - u_0) + (-\partial_{\rho\rho} v_0 + \psi_{,v}(u_0, v_0))\,(\eta_2 - v_0) \geq 0\,. \tag{16}$$

This variational inequality has the following solutions. At a grain boundary with

$$\lim_{\rho\to-\infty} (u_0, v_0)(\rho) = B = (1, -\tfrac{2}{\sqrt{3}}) \qquad \text{and} \qquad \lim_{\rho\to\infty} (u_0, v_0)(\rho) = C = (1, \tfrac{2}{\sqrt{3}})\,,$$

we obtain that $(u_0, v_0) = (1, \bar{v})$ with

$$\bar{v}(\rho) = \tfrac{2}{\sqrt{3}} \begin{cases} 1 & \text{if} \quad \rho > \rho_g := \frac{\pi}{2\sqrt{1-\mu}}\,, \\ \sin(\frac{\pi}{2}\,\frac{\rho}{\rho_g}) & \text{if} \quad |\rho| \leq \rho_g\,, \\ -1 & \text{if} \quad \rho < -\rho_g \end{cases}$$

is a solution, since $\mu \in (-2, \frac{4}{7})$. Similarly, at a material boundary with

$$\lim_{\rho\to-\infty} (u_0, v_0)(\rho) = A = (-1, 0) \qquad \text{and} \qquad \lim_{\rho\to\infty} (u_0, v_0)(\rho) = B = (1, -\tfrac{2}{\sqrt{3}})\,,$$

we obtain that $(u_0, v_0) = (\bar{u}, -\frac{1+\bar{u}}{\sqrt{3}})$ with

$$\bar{u}(\rho) = \begin{cases} 1 & \text{if} \quad \rho > \rho_m := \frac{\pi}{\sqrt{4-\mu}}\,, \\ \sin(\frac{\pi}{2}\,\frac{\rho}{\rho_m}) & \text{if} \quad |\rho| \leq \rho_m\,, \\ -1 & \text{if} \quad \rho < -\rho_m \end{cases} \tag{17}$$

is a solution of the variational inequality (16). The solution of the material boundary CA is then given, through symmetry, as $(u_0, v_0)(\rho) = (\bar{u}, \frac{1+\bar{u}}{\sqrt{3}})(-\rho)$.

For later use we compute the energy of the leading order interfacial layer

$$\begin{aligned}\sigma &= \int_{-\infty}^{\infty} \left[\tfrac{1}{2}((\partial_\rho u_0)^2 + (\partial_\rho v_0)^2) + \Psi(u_0, v_0)\right] \mathrm{d}\rho = \int_{-\infty}^{\infty} \left[(\partial_\rho u_0)^2 + (\partial_\rho v_0)^2\right] \mathrm{d}\rho \\ &= 2 \int_{-\infty}^{\infty} \sqrt{(\partial_\rho u_0)^2 + (\partial_\rho v_0)^2}\,\sqrt{\tfrac{1}{2}\,\Psi(u_0, v_0)}\,\mathrm{d}\rho \end{aligned} \tag{18}$$

of the solutions (u_0, v_0) above. For the solutions $(u_0, v_0) = (1, \bar{v})$ at the grain boundary, and $(u_0, v_0) = (\bar{u}, \pm\frac{1+\bar{u}}{\sqrt{3}})$ at the material boundary we obtain that

$$\sigma_{grain} = \tfrac{2}{3}\,\pi\,(1-\mu)^{\frac{1}{2}} \qquad \text{and} \qquad \sigma_{mat} = \tfrac{2}{3}\,\pi\,(1-\tfrac{\mu}{4})^{\frac{1}{2}}\,, \tag{19}$$

respectively.

2.2. **Inner expansions (1^{st} order).** Next we derive an equation for the grain boundary in the sharp interface limit. First of all we require that

$$(u_0, v_0) + \gamma\,(u_1, v_1) + \gamma^2\,(u_2, v_2) + \ldots \in \mathcal{K} \tag{20}$$

to all orders. Since $(u_0, v_0) = (1, \overline{v})$ we obtain to the order $\mathcal{O}(\gamma)$ that $u_1 \leq 0$. In addition we obtain that

$$-u_1 \pm \sqrt{3}\,v_1 \leq 0 \quad \text{if} \quad (u_0, v_0) = (1, \pm\tfrac{2}{\sqrt{3}})\,.$$

This ensures that (20) is fulfilled if (u_0, v_0) lies in a corner. Above and in what follows we will always consider the two void/grain interfaces in combination. If a choice has to be made for the sign we always take the upper sign for the CA interface and the lower sign for the AB interface.

We now plug the asymptotic ansatz for u, v, w and z into the variational inequality (3c) and require that it holds for all

$$(\eta_1, \eta_2) = (\eta_{10}, \eta_{20}) + \gamma\,(\eta_{11}, \eta_{21}) + \gamma^2\,(\eta_{12}, \eta_{22}) + \ldots\,,$$

which are assumed to have, to all orders, values in $\mathcal{K}$. To the order $\mathcal{O}(1)$ we obtain, on noting (15), that $(u_1, v_1) : \mathbb{R} \to \mathbb{R}^2$ has to fulfil $(u_0, v_0) + \gamma\,(u_1, v_1) \in \mathcal{K}$ to the order $\mathcal{O}(\gamma)$ and

$$
\begin{aligned}
&(-\partial_{\rho\rho} u_1 + \kappa\, \partial_\rho u_0 + \psi_{,uu}(u_0, v_0)\, u_1 + \psi_{,uv}(u_0, v_0)\, v_1 - w_0)\, (\eta_{10} - u_0) \\
&\quad + (-\partial_{\rho\rho} v_1 + \kappa\, \partial_\rho v_0 + \psi_{,uv}(u_0, v_0)\, u_1 + \psi_{,vv}(u_0, v_0)\, v_1 - z_0)\, (\eta_{20} - v_0) \\
&\quad + (-\partial_{\rho\rho} u_0 + \psi_{,u}(u_0, v_0))\, (\eta_{11} - u_1) + (-\partial_{\rho\rho} v_0 + \psi_{,v}(u_0, v_0))\, (\eta_{21} - v_1) \geq 0 \quad (21)
\end{aligned}
$$

for all $(\eta_{10}, \eta_{20}) : \mathbb{R} \to \mathcal{K}$ and $(\eta_{11}, \eta_{21}) : \mathbb{R} \to \mathbb{R}^2$ which fulfil $(\eta_{10}, \eta_{20}) + \gamma\, (\eta_{11}, \eta_{21}) \in \mathcal{K}$ to the order $\mathcal{O}(\gamma)$. Choosing $(\eta_{10}, \eta_{20}) = (u_0, v_0)$, and using $u_0 = 1$, we obtain that

$$\psi_{,u}(1, v_0)\, (\eta_{11} - u_1) + (-\partial_{\rho\rho} v_0 + \psi_{,v}(1, v_0))\, (\eta_{21} - v_1) \geq 0 \quad (22)$$

for all $(\eta_{11}, \eta_{21}) : \mathbb{R} \to \mathbb{R}^2$ with $\eta_{11} \leq 0$. In addition, we have to impose that

$$-\eta_{11} \pm \sqrt{3}\, \eta_{21} \leq 0 \quad \text{if} \quad (u_0, v_0) = (1, \pm\tfrac{2}{\sqrt{3}})\,. \quad (23)$$

If $|v_0| < \frac{2}{\sqrt{3}}$, we have that $-\partial_{\rho\rho} v_0 + \psi_{,v}(u_0, v_0) = 0$ and it follows from (22) that

$$0 \leq \psi_{,u}(1, v_0)\, (\eta_{11} - u_1) = -\tfrac{1}{3}\, (2 + \mu)\, (\eta_{11} - u_1) \qquad \forall\ \eta_{11} \leq 0;$$

which implies that $u_1 = 0$ as $\mu > -2$. In the interior of the set $\{|v_0| = \frac{2}{\sqrt{3}}\}$, we obtain from (22) that

$$
\begin{aligned}
0 &\leq \psi_{,u}(1, \pm\tfrac{2}{\sqrt{3}})\, (\eta_{11} - u_1) + \psi_{,v}(1, \pm\tfrac{2}{\sqrt{3}})\, (\eta_{21} - v_1) \\
&= -\tfrac{1}{3}\, (2 + \mu)\, (\eta_{11} - u_1) - (1 - \mu)\, (\pm\tfrac{2}{\sqrt{3}})\, (\eta_{21} - v_1)
\end{aligned}
$$

for all (η_{11}, η_{21}) that fulfil $\eta_{11} \leq 0$ and (23). We seek a solution (u_1, v_1) of this variational inequality in the cone $\{(u_1, v_1) : u_1 \leq 0, -u_1 \pm \sqrt{3}\, v_1 \leq 0\}$, where this constraint on (u_1, v_1) follows from the $\mathcal{O}(\gamma)$ condition in (20). It is easily deduced that only the trivial solution $(0, 0)$ exists if $\mu \in (-2, \frac{4}{7})$. Hence we obtain that $(u_1, v_1) = (0, 0)$ if $(u_0, v_0) = (1, \pm\frac{2}{\sqrt{3}})$.

For points in the set $\{|v_0| < \frac{2}{\sqrt{3}}\}$ we now choose $(\eta_{11}, \eta_{21}) = (0, 0)$ and $(\eta_{10}, \eta_{20}) = (u_0, v_0 + \delta)$ with some small $\delta \in \mathbb{R}$ in the variational inequality (21). This yields that

$$-\partial_{\rho\rho} v_1 + \kappa\, \partial_\rho v_0 + \psi_{,vv}(u_0, v_0)\, v_1 - z_0 = 0 \quad \text{in} \quad \{|v_0| < \tfrac{2}{\sqrt{3}}\}\,.$$

Multiplying this identity by $\partial_\rho v_0$, leads after integration, and integration by parts, to

$$\kappa \int_{-\infty}^{\infty} (\partial_\rho v_0)^2\, \mathrm{d}\rho = \int_{-\infty}^{\infty} z_0\, \partial_\rho v_0\, \mathrm{d}\rho\,; \quad (24)$$

where we have used the facts that $\partial_\rho u_0 = 0$, that $-\partial_{\rho\rho} v_0 + \psi_{,v}(u_0, v_0) = 0$ and that $v_1 = 0$ on $\{|v_0| = \frac{2}{\sqrt{3}}\}$. On noting (13) and (12), equation (3b) to the order $\mathcal{O}(1)$ now gives

$$z_0 = 0 \quad \text{if} \quad \ell(\gamma) := \beta\, \gamma^2 \qquad \text{and} \qquad z_0 = \beta\, \mathcal{V}\, \partial_\rho v_0 \quad \text{if} \quad \ell(\gamma) := \beta\, \gamma\,. \quad (25)$$

Therefore, depending on the scaling in (3b), we obtain on the grain boundary that

$$\kappa = 0 \quad \text{if} \quad \ell(\gamma) := \beta\, \gamma^2 \qquad \text{and} \qquad \beta\, \omega\, \mathcal{V} = \sigma\, \kappa \quad \text{if} \quad \ell(\gamma) := \beta\, \gamma\,; \quad (26)$$

where $\omega := \int_{-\infty}^{\infty} (\partial_\rho v_0)^2\, \mathrm{d}\rho = \sigma_{grain} = \frac{2}{3}\, \pi\, (1 - \mu)^{\frac{1}{2}}$, on recalling (18)–(19). Obviously, the factors ω and σ cancel in (26). However, for later developments, concerning triple junctions, we do not remove them.

Let us remark on the scaling $\ell(\gamma) := \beta\, \gamma^2$. In order to derive an asymptotic expansion around a sharp interface solution we require zero curvature, $\kappa = 0$, of the grain boundaries. Finally we point out that (3a) degenerates on grain boundaries, i.e. we obtain $\frac{\partial u}{\partial t} = 0$, and (3d) has no interfacial structure on grain boundaries since $c(u_0)$ is constant.

Deriving the governing equation for the void boundaries is more involved. From (13), (14) and (11) we obtain, on dropping the $\widehat{}$ notation, that

$$\nabla_x \,.\, (b(u) \nabla_x w) \\ = \gamma^{-2}\, \partial_\rho (b(u)\, \partial_\rho w) + \gamma^{-1}\, b(u)\, \partial_\rho w\, \partial_s (\nabla_x d) \,.\, \nabla_x s + \partial_s (b(u)\, \partial_s w\, \nabla_x s) \,.\, \nabla_x s. \quad (27)$$

Similar expressions can be obtained for $\nabla\,.\,(b(u)\,\nabla\phi)$ and $\nabla\,.\,(c(u)\,\nabla\phi)$. Hence on noting (27) and (13), the equations (3a) and (3d) to the order $\mathcal{O}(\gamma^{-2})$ imply on integrating with respect to ρ and matching that

$$\partial_\rho (w_0 + \alpha\, \phi_0) = 0 \qquad \text{and} \qquad \partial_\rho \phi_0 = 0\,.$$

As $\partial_\rho w_0 = 0$, similarly we obtain to the order $\mathcal{O}(\gamma^{-1})$ that

$$\partial_\rho (w_1 + \alpha\, \phi_1) = 0 \qquad \text{and} \qquad \partial_\rho \phi_1 = 0\,.$$

To the order $\mathcal{O}(1)$ we obtain from (3a), (13), (12), (27) and (11), since u_0 does not depend on s, that

$$-\mathcal{V}\, \partial_\rho u_0 = \partial_\rho (b(u_0)\, \partial_\rho (w_2 + \alpha\, \phi_2)) + b(u_0)\, \partial_{ss} (w_0 + \alpha\, \phi_0)\,.$$

After integration with respect to ρ we obtain

$$-\mathcal{V}\, [u_0]_i^j = M\, \partial_{ss} (w_0 + \alpha\, \phi_0) \quad (28)$$

where $[u_0]_i^j$ denotes the jump across the interface Γ^{ij} (the value for $\rho \to \infty$ minus the value for $\rho \to -\infty$) and $M := \int_{-\infty}^{\infty} b(u_0(\rho))\, \mathrm{d}\rho = \rho_m = \pi\,(4-\mu)^{-\frac{1}{2}}$.

It remains to exploit (21) at a void interface. At a void interface we have

$$-u_0 \pm \sqrt{3}\, v_0 = 1\,. \quad (29)$$

Let us first consider points such that $|u_0| < 1$. In order to fulfil (20) to the order $\mathcal{O}(\gamma)$ we need to have

$$-u_1 \pm \sqrt{3}\, v_1 \leq 0\,. \quad (30)$$

Choosing $(\eta_{10}, \eta_{20}) = (u_0, v_0) = (\bar{u}, \pm\frac{1+\bar{u}}{\sqrt{3}})$ in (21) we obtain that

$$(-\partial_{\rho\rho} u_0 + \psi_{,u}(u_0,v_0))\,(\eta_{11} - u_1) + (-\partial_{\rho\rho} v_0 + \psi_{,v}(u_0,v_0))\,(\eta_{21} - v_1) \geq 0 \quad (31)$$

for all $(\eta_{11}, \eta_{21}) : \mathbb{R} \to \mathbb{R}^2$ with

$$-\eta_{11} \pm \sqrt{3}\, \eta_{21} \leq 0,$$

which in addition fulfil $\eta_{11} \leq 0$ if $(u_0, v_0) = (1, \pm\frac{2}{\sqrt{3}})$ or $\eta_{11} \geq 0$ if $(u_0, v_0) = (-1, 0)$. The variational inequality (16), recall (17), implies that

$$-\partial_{\rho\rho} (\sqrt{3}\, u_0 \pm v_0) + \sqrt{3}\, \psi_{,u}(u_0,v_0) \pm \psi_{,v}(u_0,v_0) = 0 \quad \text{in} \quad \{|u_0| < 1\}\,. \quad (32)$$

Taking second derivatives in (29), we obtain from (32), after solving a linear system for $(\partial_{\rho\rho} u_0, \partial_{\rho\rho} v_0)$, that

$$\partial_{\rho\rho} u_0 = \pm\sqrt{3}\, \partial_{\rho\rho} v_0 = \tfrac{1}{4} (3\, \psi_{,u} \pm \sqrt{3}\, \psi_{,v})\,. \quad (33)$$

Hence (31) yields if $|u_0| < 1$ that

$$(\psi_{,u}(u_0,v_0) \mp \sqrt{3}\, \psi_{,v}(u_0,v_0))\,(\eta_{11} - u_1) + (\mp\sqrt{3}\, \psi_{,u} + 3\, \psi_{,v})\,(\eta_{21} - v_1) \geq 0 \quad (34)$$

for all (η_{11}, η_{21}) with $-\eta_{11} + \sqrt{3}\, \eta_{21} \leq 0$. Now we represent (u_1, v_1) as

$$\begin{pmatrix} u_1 \\ v_1 \end{pmatrix} = \omega_1 \begin{pmatrix} -1 \\ \pm\sqrt{3} \end{pmatrix} + \omega_2 \begin{pmatrix} \sqrt{3} \\ \pm 1 \end{pmatrix},$$

and note that (30) implies that $\omega_1 \leq 0$. Choosing $(\eta_{11}, \eta_{21}) = \omega_2\,(\sqrt{3}, \pm 1)$ in (34) yields that

$$\begin{aligned} 0 &\geq \omega_1\,(-\psi_{,u} \pm \sqrt{3}\,\psi_{,v} - 3\,\psi_{,u} \pm 3\sqrt{3}\,\psi_{,v})(u_0, v_0) \\ &= 4\,\omega_1\,(-\psi_{,u} \pm \sqrt{3}\,\psi_{,v})(u_0, v_0) = 4\,\omega_1\,(-\tfrac{4}{3}(1-\mu) + \mu\,u_0)\,. \end{aligned}$$

The term in the last bracket is always negative provided that $\mu < \frac{4}{7}$. This implies that $\omega_1 \geq 0$, and hence $\omega_1 = 0$, which in turn leads to $-u_1 \pm \sqrt{3}\,v_1 = 0$.

For points that lie in the interior of the set $\{(u_0, v_0) = (1, \pm\frac{2}{\sqrt{3}})\}$ we can argue as in the case of a grain boundary to obtain that $(u_1, v_1) = (0, 0)$. Now we consider points that lie in the interior of the set $\{(u_0, v_0) = (-1, 0)\}$. For these points the inequality (21) yields on choosing $(\eta_{10}, \eta_{20}) = (u_0, v_0)$

$$0 \leq \psi_{,u}(-1,0)\,(\eta_{11} - u_1) + \psi_{,v}(-1,0)\,(\eta_{21} - v_1) = \tfrac{1}{3}(4-\mu)\,(\eta_{11} - u_1),$$

which has to hold for all (η_{11}, η_{21}) fulfilling $\sqrt{3}\,|\eta_{21}| \leq \eta_{11}$. Since by (20) the solution (u_1, v_1) has to satisfy $\sqrt{3}\,|v_1| \leq u_1$, we obtain that $(u_1, v_1) = (0, 0)$ is the only solution to the above variational inequality.

For points in the set $\{|u_0| < 1\}$ we now choose $(\eta_{11}, \eta_{21}) = (0, 0)$ and $(\eta_{10}, \eta_{20}) = (u_0 + \sqrt{3}\,\delta, v_0 \pm \delta)$ with some small $\delta \in \mathbb{R}$ in the variational inequality (21). This yields that

$$\begin{aligned} -\,\partial_{\rho\rho}(\sqrt{3}\,u_1 \pm v_1) + \kappa\,\partial_\rho(\sqrt{3}\,u_0 \pm v_0) + (\sqrt{3}\,\psi_{,uu}(u_0, v_0)\,u_1 + \sqrt{3}\,\psi_{,uv}(u_0, v_0)\,v_1 \\ \pm\,\psi_{,vu}(u_0, v_0)\,u_1 \pm \psi_{,vv}(u_0, v_0)\,v_1) - \sqrt{3}\,w_0 \mp z_0 = 0\,. \end{aligned}$$

As $-u_0 \pm \sqrt{3}\,v_0 = 1$ and $-u_1 \pm \sqrt{3}\,v_1 = 0$, it follows from the above that

$$-4\,\partial_{\rho\rho}u_1 + 4\,\kappa\,\partial_\rho u_0 - 3\,u_1 - (1-\mu)\,u_1 - 3\,w_0 \mp \sqrt{3}\,z_0 = 0\,.$$

Similarly to (24), on multiplying the above identity by $\partial_\rho u_0$, integrating, performing integration by parts; we obtain, on noting (17) and (33) that

$$\begin{aligned} &4\,\kappa \int_{-\infty}^{\infty} (\partial_\rho u_0)^2\,\mathrm{d}\rho - 3\int_{-\infty}^{\infty} w_0\,\partial_\rho u_0\,\mathrm{d}\rho \mp \sqrt{3}\int_{-\infty}^{\infty} z_0\,\partial_\rho u_0\,\mathrm{d}\rho \\ &\quad = 3\,\kappa \int_{-\infty}^{\infty} [(\partial_\rho u_0)^2 + (\partial_\rho v_0)^2]\,\mathrm{d}\rho - 3\,w_0\,[u_0]_i^j \mp \sqrt{3}\int_{-\infty}^{\infty} z_0\,\partial_\rho u_0\,\mathrm{d}\rho = 0\,. \end{aligned}$$

Equation (3b) gives to the order $\mathcal{O}(1)$ the identities (25) and hence we get, on recalling (18),

$$\sigma\,\kappa = [u_0]_i^j\,w_0 \;\text{ if }\; \ell(\gamma) := \beta\,\gamma^2 \quad\text{and}\quad \sigma\,\kappa = [u_0]_i^j\,w_0 + \beta\,\omega\,\mathcal{V} \;\text{ if }\; \ell(\gamma) := \beta\,\gamma\,; \tag{35}$$

where $\omega := \int_{-\infty}^{\infty} (\partial_\rho v_0)^2\,\mathrm{d}\rho = \frac{1}{4}\,\sigma_{mat} = \frac{\pi}{6}\,(1 - \frac{\mu}{4})^{\frac{1}{2}}$.

For the material interfaces $(i, j) = (A, B)$, (C, A), and the grain interface (B, C), we derive from (26), (28) and (35) for the scaling $\ell(\gamma) := \beta\,\gamma$ that

$$-2\,\mathcal{V}^{AB} = M^{AB}\,\partial_{ss}(w_0^{AB} + \alpha\,\phi_0^{AB}) \quad\text{and}\quad 2\,w_0^{AB} + \beta\,\omega^{AB}\,\mathcal{V}^{AB} = \sigma^{AB}\,\kappa^{AB}, \tag{36a}$$

$$2\,\mathcal{V}^{CA} = M^{CA}\,\partial_{ss}(w_0^{CA} + \alpha\,\phi_0^{CA}) \quad\text{and}\quad -2\,w_0^{CA} + \beta\,\omega^{CA}\,\mathcal{V}^{CA} = \sigma^{CA}\,\kappa^{CA}, \tag{36b}$$

$$\beta\,\omega^{BC}\,\mathcal{V}^{BC} = \sigma^{BC}\,\kappa^{BC}; \tag{36c}$$

where, on recalling (19), we have that

$$\omega^{BC} = \sigma^{BC} = \sigma_{grain} = \tfrac{2}{3}\,\pi\,(1-\mu)^{\frac{1}{2}}\,, \qquad M^{AB} = M^{CA} = \pi\,(4-\mu)^{-\frac{1}{2}}\,,$$
$$4\,\omega^{AB} = 4\,\omega^{CA} = \sigma^{AB} = \sigma^{CA} = \sigma_{mat} = \tfrac{2}{3}\,\pi\,(1-\tfrac{\mu}{4})^{\frac{1}{2}}\,.$$

The evolution laws (36a,b) for the material interfaces combine surface diffusion and surface attachment limited kinetics (SALK), which was discussed in [14]; see also [8].

If we choose the scaling $\ell(\gamma) := \beta\,\gamma^2$ instead of $\ell(\gamma) := \beta\,\gamma$ in the evolution equation (3b) we derive from (28), (26) and (35) that

$$\mathcal{V}^{AB} = -\tfrac{M^{AB}}{2}\,\partial_{ss}(\tfrac{\sigma^{AB}}{2}\kappa^{AB} + \alpha\,\phi_0^{AB}), \qquad \mathcal{V}^{CA} = -\tfrac{M^{CA}}{2}\,\partial_{ss}(\tfrac{\sigma^{CA}}{2}\kappa^{CA} - \alpha\,\phi_0^{CA}),$$
$$\sigma^{BC}\,\kappa^{BC} = 0.$$

Therefore under this scaling the evolution of the void surface is given by surface diffusion, see [4], whereas the grain boundaries have zero mean curvature, i.e. they are in equilibrium.

2.3. **Expansions close to the triple junction.** It remains to derive the equations at a triple junction. From now on, we will always denote by superscripts A, B and C quantities that are defined on the interfaces BC, CA and AB, respectively. In particular, we have that the normals n_Γ^A, n_Γ^B and n_Γ^C are such that n_Γ^A points into C, n_Γ^B points into A and n_Γ^C points into B. At a triple junction $m(t)$ we choose at a fixed time t a triangle T_γ, whose midpoint coincides with the triple junction. In addition it is assumed that the sides of the triangle intersect the interfaces to leading order perpendicularly and have to leading order a length which is proportional to $\gamma^{\frac{1}{2}}$. We now introduce the stretched variable $y = \gamma^{-1}(x - m(t))$, and make the asymptotic ansatz

$$(u,v)(x,t) = (U_0,V_0)(y,t) + \gamma\,(U_1,V_1)(y,t) + \ldots .$$

Then (3c) gives to leading order that the following variational inequality has to hold almost everywhere on $\widetilde{T}_\gamma := \{y \in \mathbb{R}^2 \mid m(t) + \gamma\,y \in T_\gamma\}$:

$$(-\Delta_y U_0 + \psi_{,u}(U_0,V_0))\,(\eta_1 - U_0) + (-\Delta_y V_0 + \psi_{,u}(U_0,V_0))\,(\eta_2 - V_0) \geq 0 \qquad (37)$$

for all $(\eta_1,\eta_2) : \widetilde{T}_\gamma \to \mathcal{K}$. We now want to derive a solvability condition for (37), which will lead to an angle condition at the triple junction. The ansatz $(\eta_1,\eta_2) = (U_0,V_0) \pm \delta(\partial_{y_l}U_0, \partial_{y_l}V_0)$, $l = 1$, 2, leads to values in $\mathcal{K}$ for small δ in the following cases. If $(U_0,V_0)(y,t)$ lies in the interior of $\mathcal{K}$, then this is obviously true. If $(U_0,V_0)(y,t)$ lies in the interior of one of the sets $\{(u,v) = i\}$ with $i \in \{A,B,C\}$, we obtain $\nabla_y U_0 = 0$ and hence $(\eta_1,\eta_2) = (U_0,V_0)$. In the case of points that lie in the interior of one of the three sets $\{(u,v) : -u \pm \sqrt{3}\,v = 1 \text{ and } |u| < 1\}$ and $\{(u,v) : u = 1 \text{ and } |v| < \frac{2}{\sqrt{3}}\}$, we obtain also that $(\eta_1,\eta_2) \in \mathcal{K}$ for small δ. For example, if $|U_0| < 1$ and $-U_0 \pm \sqrt{3}\,V_0 = 1$ in a neighbourhood of (y,t), then we obtain $-\partial_{y_l}U_0 \pm \sqrt{3}\,\partial_{y_l}V_0 = 0$ and hence $(U_0,V_0) \pm \delta(\partial_{y_l}U_0,\partial_{y_l}V_0) \in \mathcal{K}$ if δ is sufficiently small.

Assuming that the complement of the sets considered above has measure zero, which is supported by numerical experiments, we obtain from (37) with $(\eta_1,\eta_2) = (U_0,V_0) \pm \delta\,(\partial_{y_l}U_0, \partial_{y_l}V_0)$, $l = 1$, 2, that

$$(\nabla_y U_0)^T(-\Delta_y U_0 + \psi_{,u}(U_0,V_0)) + (\nabla_y V_0)^T(-\Delta_y V_0 + \psi_{,v}(U_0,V_0)) = 0$$

almost everywhere; where $\nabla_y\cdot = (\partial_{y_1}\cdot, \partial_{y_2}\cdot)^T$. Defining $\Lambda_0 := (U_0, V_0)^T$ and using the identity

$$-(\nabla_y\Lambda_0)^T(\Delta_y\Lambda_0) = -\nabla_y \,.\, (\,(\nabla_y\Lambda_0)^T(\nabla_y\Lambda_0)) + \tfrac{1}{2}\,(\nabla_y[\,|\nabla_y\Lambda_0|^2]) \,;$$

we obtain, after integration over $\widetilde{T}_\gamma$, that the following identity holds

$$\begin{aligned}
0 &= \int_{\widetilde{T}_\gamma} \left[-(\nabla_y\Lambda_0)^T(\Delta_y\Lambda_0) + (\nabla_y\Lambda_0)^T[(\psi_{,u}, \psi_{,v})(\Lambda_0)]^T\,\right]\,\mathrm{d}y \\
&= \int_{\widetilde{T}_\gamma} \left[-\nabla_y \,.\, (\,(\nabla_y\Lambda_0)^T(\nabla_y\Lambda_0)) + \nabla_y(\tfrac{1}{2}\,|\nabla_y\Lambda_0|^2 + \psi(\Lambda_0))\right]\,\mathrm{d}y \\
&= -\int_{\partial\widetilde{T}_\gamma} (\nabla_y\Lambda_0)^T\,(\nabla_y\Lambda_0)\,n_{\partial T}\,\mathrm{d}s_T + \int_{\partial\widetilde{T}_\gamma} (\tfrac{1}{2}\,|\nabla_y\Lambda_0|^2 + \psi(\Lambda_0))\,n_{\partial T}\,\mathrm{d}s_T \,;
\end{aligned}$$

where we have applied the Gauss theorem to obtain the last identity. Moreover, $n_{\partial T}$ is the outer unit normal to $\partial\widetilde{T}_\gamma$. Since we chose the triangle T_γ such that ∂T_γ intersects the interfaces asymptotically perpendicularly, we obtain that the term $\int_{\partial\widetilde{T}_\gamma}(\nabla_y\Lambda_0)^T(\nabla_y\Lambda_0)\,n_{\partial T}\,\mathrm{d}s_T$ vanishes asymptotically. Recalling (18), matching Λ_0 and the standing wave (u_0, v_0), and noting that asymptotically $n_{\partial T}$ equals τ_Γ^i along the different sides for $i \in \{A, B, C\}$, we obtain that

$$0 = \sum_{i\in\{A,B,C\}} \sigma^i\,\tau_\Gamma^i \,.$$

This is the force balance at the triple junction and a simple computation shows that the above identity is equivalent to Young's law (6).

To obtain a flux balance condition we consider the mass balance (3a). We observe that only the second term on the left hand side of (3a) gives a contribution to leading order. Integrating the leading order term over $\widetilde{T}_\gamma$, we obtain that

$$0 = \int_{\widetilde{T}_\gamma} \nabla_y \,.\, (\,b(U_0)\,\nabla_y[W_0 + \alpha\,\Phi_0])\,\mathrm{d}y = \int_{\partial\widetilde{T}_\gamma} b(U_0)\,\nabla_y[W_0 + \alpha\,\Phi_0]\,.\,n_{\partial T}\,\mathrm{d}s_T.$$

The right hand side gives a contribution only if $b(U_0) \neq 0$, which means only on the material interfaces, AB and CA. Matching with the inner solutions, using (13) and $\nabla_x s = n_{\partial T} + \mathcal{O}(\gamma)$, we obtain that

$$\left[\int_{-\infty}^{\infty} b(u_0^C(\rho))\,\mathrm{d}\rho\right]\partial_s(w_0^C + \alpha\,\phi_0^C) + \left[\int_{-\infty}^{\infty} b(u_0^B(\rho))\,\mathrm{d}\rho\right]\partial_s(w_0^B + \alpha\,\phi_0^B) = 0,$$

where u_0^C, w_0^C, ϕ_0^C and u_0^B, w_0^B, ϕ_0^B are the inner leading order solutions at the interfaces AB and CA, respectively. Altogether at the triple junction we obtain the flux balance condition (7).

It remains to determine an additional condition at the triple junction, which is related to the fact that the chemical potential is continuous. Neglecting lower order terms in (3a), we obtain close to the triple junction that

$$\begin{aligned}
0 &= \int_{\widetilde{T}_\gamma} [\nabla_y \,.\, (b(U_0)\,\nabla_y(W_0 + \alpha\,\Phi_0))\,]\,(W_0 + \alpha\,\Phi_0)\,\mathrm{d}y \\
&= -\int_{\widetilde{T}_\gamma} b(U_0)\,|\nabla_y(W_0 + \alpha\,\Phi_0)|^2\,\mathrm{d}y \\
&\qquad + \int_{\partial\widetilde{T}_\gamma} b(U_0)\,(W_0 + \alpha\,\Phi_0)\,\nabla_y(W_0 + \alpha\,\Phi_0)\,.\,n_{\partial T}\,\mathrm{d}s_T \,.
\end{aligned}$$

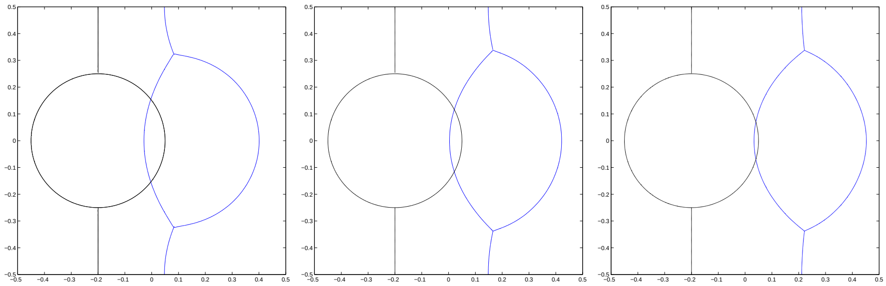

FIGURE 1. Results for the scaling $\ell(\gamma) := \gamma^2$ for $\gamma = \frac{1}{12\pi}$, $\frac{1}{24\pi}$ and $\frac{1}{48\pi}$.

The choice of $\widetilde{T}_\gamma$ yields that $\nabla_y(W_0 + \alpha\,\Phi_0)\,.\,n_{\partial T}$ results in a partial derivative along the interface. Since the s-variable in the inner expansion is scaled in a different way, we obtain from matching the inner expansion to the triple junction expansion that $\nabla_y(W_0 + \alpha\,\Phi_0)\,.\,n_{\partial T}$ has to vanish to leading order. Hence, to leading order at the triple junction, $W_0 + \alpha\,\Phi_0$ is constant on the support of $b(U_0)$, which is assumed to be connected. By matching the solution close to the triple junction with the inner solution, we obtain that the limit for $w_0 + \alpha\,\phi_0$ coming from the AB interface has to equal that coming from the CA interface. Assuming that the ϕ equation has a continuous solution up to the boundary, we obtain that at the triple junction

$$w_0^C = w_0^B\,. \tag{38}$$

We remark that the choice of scaling $\ell(\gamma) := \beta\,\gamma$ or $\beta\,\gamma^2$ does not effect the conditions (6), (7) and (38) at the triple junction, as the equation (3b) was not used to derive them. Of course, under the scaling $\ell(\gamma) := \beta\,\gamma^2$ we deduce from (35) and (38) that at the triple junction

$$\sigma^C\,\kappa^C = -\sigma^B\,\kappa^B\,.$$

Finally, when an interface meets the external boundary, further boundary conditions have to hold (see §1.2); and these can be derived as in [9, 13]. We note that the ideas presented above can also be used to handle more general potentials Ψ including situations in which Ψ is smooth. In particular, the approach used to derive the triple junction conditions can be applied to the setting in [9, 13].

3. **Numerical Computations.** We conclude with some numerical simulations for an approximation of the phase field system (3a–d) with Ω being a rectangle, $g = 0$ on the top and bottom boundaries, and $g = \pm 2$ on the right and left boundaries, respectively. The interested reader is referred to [1] for details on the approximation, the iterative solver as well as the exact discretization parameters used. The first experiment is for the scaling $\ell(\gamma) := \gamma^2$, and so corresponds to the sharp interface limit (4). The initial profile for the phase field (u, v) is chosen such that it approximates a situation where the material boundary $\Gamma^B \cup \Gamma^C$ is given by a circle, while the grain boundaries Γ^A consist of two straight line segments. In Figure 1 we show the evolution for $\alpha = 5\,\pi$ for a decreasing sequence of values for γ. In line with the asymptotic analysis, we see that as γ decreases the grain boundaries Γ^A get closer and closer to straight lines with a 90° contact angle with the external boundary. In the second experiment we use the same setup for a simulation with the scaling $\ell(\gamma) := \gamma$, i.e. for the sharp interface limit (5). We now obtain a dramatically different evolution, see Figure 2, with the void detaching from the

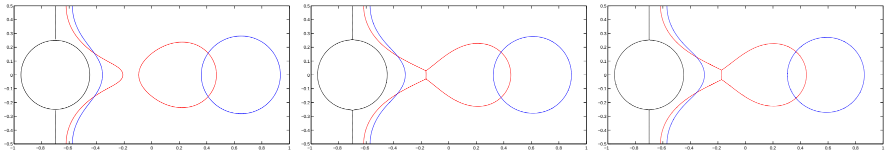

FIGURE 2. Results for the scaling $\ell(\gamma) := \gamma$ for $\gamma = \frac{1}{12\pi}$, $\frac{1}{24\pi}$ and $\frac{1}{48\pi}$.

grain boundary. It can also be seen that there is very good agreement between the results as γ is decreased, suggesting that the phase field computations are close to the actual sharp interface solution.

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