Correspondence between a phase-field theory and a sharp-interface theory for crystal growth

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Abstract

A matched asymptotic analysis is used to show that, under certain constitutive hypotheses and a particular scaling, a recently developed phase-field theory corresponds to a sharp-interface theory for crystal growth that accounts for orientation dependence in the crystalline surface energy density as well as orientation and surface normal velocity dependence in the crystalline surface mobility.

1 Introduction

In their recent survey of geometric theories for crystal growth, TAYLOR, CAHN & HANDWERKER [1] suggested the need for a phase-field theory that accounts for variations of crystalline surface energy and surface mobility with surface orientation. Here, we use a matched asymptotic analysis to show that, granted certain constitutive hypotheses and a particular scaling, a theory proposed by FRIED & GURTIN [2] encompasses not only those effects, but also allows the crystalline surface mobility to depend on the surface normal velocity.[1]

We begin with an overview, provided in Section 2, of the theory that serves as our point of reference in establishing the aforementioned result. In that theory, which is due to GURTIN,[2] an interface separating crystal from melt (or vapor[3])

[1] To account for nonlinear transition kinetics in theories for the evolution of solid-solid phase interfaces, HILLERT [3] and OWEN, SCHOEN & SRINIVASAN [4] incorporate interfacial normal velocity dependence in the interfacial mobility. That certain crystals may display nonlinear growth kinetics is evident from the work of CAHN, HILLIG & SEARS [5].

[2] A conscise presentation of the theory to which we refer appears in GURTIN [6] (see also GURTIN [7], in which attention is restricted to two spatial dimensions). That theory can be traced to GURTIN [8], where it arises as a specialization on neglecting thermal effects.

[3] While GURTIN'S theory is equally capable of describing the growth of a crystal from its vapor or from its melt, for simplicity, we refer, hereafter, only to crystal growth from the melt.

is treated as a sharp nonmaterial surface $\mathcal{S}$ that is endowed with energy and is capable of sustaining force; w denotes the crystalline surface energy density, which is determined by a response function $\hat{w}$ that, in general, depends on the orientation $\mathfrak{n}$ of $\mathcal{S}$; b denotes the kinetic coefficient,[4] which is determined by a response function $\hat{b}$ that, in general, depends on $\mathfrak{n}$ as well as the scalar normal velocity $V_{\mathcal{S}}$ describing the motion of $\mathcal{S}$; and, the bulk energy density W is taken to be piecewise constant—with values $W^{\mathfrak{a}}$ and $W^{\mathfrak{b}}$ in the crystal and melt, respectively.

Following our summary of GURTIN'S "sharp-interface theory," is a survey, appearing in Section 3, of the "phase-field theory" of FRIED & GURTIN. In that theory, material response is determined by constitutive functions $\hat{W}$ and $\hat{\beta}$ that deliver the energy density W and the damping modulus β:[5] in general, $\hat{W}$ may depend on the phase field φ and its spatial gradient $\nabla\varphi$, while $\hat{\beta}$ may depend on φ, $\nabla\varphi$, and also on the rate $\dot{\varphi}$ at which φ changes with respect to time.

In Section 4, we introduce assumptions that restrict the manner in which the response functions $\hat{W}$ and $\hat{\beta}$ of the phase-field theory may depend on the independent constitutive variables φ, $\nabla\varphi$, and $\dot{\varphi}$, leading to a description that associates the crystal phase $\mathfrak{a}$ and the melt phase $\mathfrak{b}$ of the sharp-interface theory with the values $\varphi = \varphi_{\mathfrak{a}}$ and $\varphi = \varphi_{\mathfrak{b}}$ of the phase field and models an interface separating crystal from melt by a narrow transition layer that connects regions with $\varphi \approx \varphi_{\mathfrak{a}}$ and $\varphi \approx \varphi_{\mathfrak{b}}$. Moreover, these assumptions imply a decomposition of $\hat{W}$ in the form

$$\hat{W}(\varphi, \nabla\varphi) = \hat{W}^{\mathrm{bu}}(\varphi) + \hat{W}^{\mathrm{xs}}(\varphi, \nabla\varphi), \tag{1.1}$$

where $W^{\mathrm{bu}} = \hat{W}^{\mathrm{bu}}(\varphi)$ determines the energy density of the bulk phases and $W^{\mathrm{xs}} = \hat{W}^{\mathrm{xs}}(\varphi, \nabla\varphi)$ determines the energy density of transition layers. In particular, we find that $\hat{W}^{\mathrm{xs}}$ admits a representation of the form

$$\hat{W}^{\mathrm{xs}}(\varphi, \nabla\varphi) = \Psi(\varphi) + \tfrac{1}{2}|\nabla\varphi|^2\lambda(\boldsymbol{n}), \tag{1.2}$$

with Ψ a double-well potential possessing equal minima at $\varphi = \varphi_{\mathfrak{a}}$ and $\varphi = \varphi_{\mathfrak{b}}$, and λ and even function of $\boldsymbol{n} = \nabla\varphi/|\nabla\varphi|$. A further consequence of the assumptions put forth in Section 4 is that

$$\hat{\beta}(\varphi, \nabla\varphi, \dot{\varphi}) = \tilde{\beta}(\boldsymbol{n}, V), \tag{1.3}$$

with $V = -\dot{\varphi}/|\nabla\varphi|$.

An outgrowth of the decompositions of Section 4 is to determine versions of the field equations of the phase-field theory that are specific to transition layers, equations that we present in Section 5.

[4] The kinetic coefficient is the reciprocal of the crystalline surface mobility.

[5] We rely on italic and sans-serif characters to distinguish between various fields that appear in both of the theories considered here. In particular, whereas W denotes the bulk energy density sharp-interface theory, W denotes the energy density of the phase-field theory.

Next, in Section 6, we perform a scaling of the independent and dependent variables of phase-field theory. That scaling, upon which our asymptotic results hinge, involves a small dimensionless parameter ϵ, with which the dimensionless transition layer thickness h tends to zero.

The remainder of the paper focuses on demonstrating the consonance of the two theories considered here, granted the constitutive restrictions of Section 4 and the scaling of Section 6. To simplify the presentation of our results, we suppose, in Section 7, that $\hat{W}^{\mathrm{bu}}$ is related to $W^{\mathfrak{a}}$ and $W^{\mathfrak{b}}$ through

$$\hat{W}^{\mathrm{bu}}(\varphi_{\mathfrak{a}}) = W^{\mathfrak{a}} \qquad \text{and} \qquad \hat{W}^{\mathrm{bu}}(\varphi_{\mathfrak{b}}) = W^{\mathfrak{b}}, \tag{1.4}$$

and also that λ and $\tilde{\beta}$ are related to $\hat{w}$ and $\hat{b}$ through

$$\sigma\sqrt{\lambda(\mathfrak{n})} = \hat{w}(\mathfrak{n}) \qquad \text{and} \qquad \sigma^2\tilde{\beta}(\mathfrak{n}, V_{\mathfrak{S}}) = \hat{w}(\mathfrak{n})\hat{b}(\mathfrak{n}, V_{\mathfrak{S}}), \tag{1.5}$$

where σ is the constant determined by

$$\sigma = \int_{\varphi_{\mathfrak{a}}}^{\varphi_{\mathfrak{b}}} \sqrt{2\Psi(\varphi)}\, d\varphi; \tag{1.6}$$

clearly, (1.4) and (1.5) do not represent a restriction of the constitutive generality possible in the sharp-interface theory.

Asymptotic expansions are introduced in Section 8, while certain useful preliminary results concerning those expansions are derived in Section 9. Among those results is the estimate

$$\Psi(\varphi) - \tfrac{1}{2}\epsilon^2|\nabla\varphi|^2\lambda(\boldsymbol{n}) = O(\epsilon), \tag{1.7}$$

which holds within transition layers and shows that, therein, the double-well and gradient terms that comprise the excess energy density W^{xs} are equal to most significant order in ϵ.[6] Aside from its physical significance, this result serves a pivotal role in our analysis: in particular, it implies an estimate

$$h(\epsilon) = \tfrac{1}{2}\epsilon\sqrt{\lambda(\boldsymbol{n})} \int_{\varphi_{\mathfrak{a}}+\epsilon}^{\varphi_{\mathfrak{b}}-\epsilon} \frac{d\varphi}{\sqrt{2\Psi(\varphi)}} + o(h(\epsilon)) \tag{1.8}$$

for the thickness of transition layers, and also allows us to evaluate certain key integrals across transition layers.

In Section 10, we show that the global integral laws of the phase-field theory tend, as ϵ and, hence, the transition layer thickness h approaches zero, toward

[6] The factor of ϵ^2 in the second term on the left-hand-side of (1.7) reflects the scaling of Section 6. In Section 9 we find that, within layers, $\epsilon|\nabla\varphi| = O(1)$, whereby, granted that Ψ and λ are of $O(1)$ in ϵ, both terms on the left-hand-side of (1.7) are of $O(1)$ in ϵ. Further, away from layers, the left-hand-side of (1.7) is of $o(1)$ in ϵ.

those of the sharp-interface theory. Furthermore, because the limits involved in integration over a region containing a layer and decreasing the thickness of that layer toward zero do not necessarily commute, we show, in Section 11, that the local balance laws of the phase-field theory tend, as ϵ approaches zero, toward those of the sharp-interface theory. In Section 12 we develop a power identity for the phase-field theory and demonstrate the asymptotic correspondence of this identity to a power identity for the sharp-interface theory.

Based on the results of Sections 10, 11, and 12 we conclude that, given bulk energies $W^{\mathfrak{a}}$ and $W^{\mathfrak{b}}$ and interfacial constitutive response functions $\hat{w}$ and $\hat{b}$ determining a particular sharp-interface theory, the class of phase-field theories determined by the constitutive relations[7]

$$\left.\begin{aligned} \hat{W}^{\mathrm{bu}}(\varphi) &= (1-z(\varphi))W^{\mathfrak{a}} + z(\varphi)W^{\mathfrak{b}}, \\ \hat{W}^{\mathrm{xs}}(\varphi,\boldsymbol{p}) &= \epsilon^{-1}\Psi(\varphi) + \frac{\epsilon}{2\sigma^2}|\boldsymbol{p}|^2\hat{w}^2(\boldsymbol{n}), \\ \hat{\beta}(\varphi,\boldsymbol{p},\dot{\varphi}) &= \frac{\epsilon}{\sigma^2}\hat{b}(\boldsymbol{n},V)\hat{w}(\boldsymbol{n}), \end{aligned}\right\} \tag{1.9}$$

with z a monotonic function from $\mathbb{R}$ into $[0,1]$ that satisfies $z(\varphi_{\mathfrak{a}}) = 0$ and $z(\varphi_{\mathfrak{b}}) = 1$ but is otherwise arbitrary, provides an asymptotically consistent regularization of that theory. This conclusion and related issues, including the correspondence of the partial differential equation of the phase-field theory to that of the sharp-interface theory, are discussed in Section 13.

2 Review of the sharp-interface theory

In this section we survey the theory of GURTIN. In so doing, bulk vectors and tensors are distinguished from scalars using bold-face type—lower case for vectors and upper case for tensors. Similarly, interfacial vectors and tensors are denoted using lower and upper case hollow type.

2.1 Kinematics

Consider a region $\mathcal{B}$ in $\mathbb{R}^3$ that, over the course of some time-interval, is separated by a smoothly evolving orientable surface $\mathcal{S}$ into subregions $\mathcal{B}^{\mathfrak{a}}$ and $\mathcal{B}^{\mathfrak{b}}$ occupied, respectively, by a crystalline solid and its melt. Let $\mathbb{n}$ denote the unit normal field for $\mathcal{S}$, directed outward from the region $\mathcal{B}^{\mathfrak{a}}$ occupied by the solid, whereby the tensor field

$$\mathbb{P} = \boldsymbol{1} - \mathbb{n}\otimes\mathbb{n}, \tag{2.1}$$

is the projector onto $\mathcal{S}$, and write $V_{\mathcal{S}}$ for the scalar normal velocity field of $\mathcal{S}$ in the direction of $\mathbb{n}$.

[7] The factors of ϵ^{-1} and ϵ appearing in the relations $(1.9)_{2,3}$ reflect the scaling of Section 6. All constitutive functions on the right-hand-side of (1.9) are of $O(1)$ in ϵ.

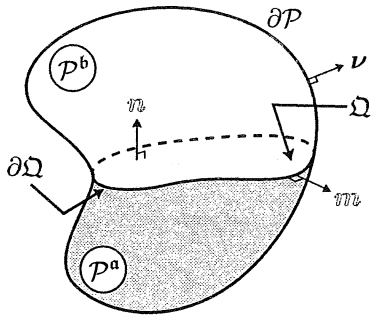

Figure 1. Subregion $\mathcal{P}$ of $\mathcal{B}$ composed of evolving parts $\mathcal{P}^{\mathfrak{a}}$ and $\mathcal{P}^{\mathfrak{b}}$ occupied by phases $\mathfrak{a}$ and $\mathfrak{b}$ and the portion $\mathfrak{Q}$ of the phase interface $\mathfrak{S}$.

Given an interfacial field g, let $\nabla_{\mathfrak{S}} g$ and $\mathring{g}$ denote its surface gradient and normal time-rate.[8] Then

$$\mathbb{L} = -\nabla_{\mathfrak{S}} \mathfrak{n} \qquad \text{and} \qquad K_{\mathfrak{S}} = \operatorname{tr} \mathbb{L} = -\operatorname{div}_{\mathfrak{S}} \mathfrak{n} \tag{2.2}$$

determine the curvature tensor and total curvature (i.e., twice the mean curvature) of $\mathfrak{S}$, and $\mathfrak{n}$ and $V_{\mathfrak{S}}$ are related by

$$\mathring{\mathfrak{n}} = -\nabla_{\mathfrak{S}} V_{\mathfrak{S}}. \tag{2.3}$$

The basic laws of the sharp-interface theory will be written for a subregion $\mathcal{P}$ of $\mathcal{B}$, with outward unit normal $\boldsymbol{\nu}$, chosen so that, over some subset of the time-interval at hand, the intersection

$$\mathfrak{Q} = \mathfrak{S} \cap \mathcal{P} \tag{2.4}$$

is nonempty and $\mathfrak{S}$ crosses $\partial\mathcal{P}$ transversely. Then, $\mathfrak{n}$ and $\boldsymbol{\nu}$ must comply with $0 \leq |\mathfrak{n} \cdot \boldsymbol{\nu}| < 1$,

$$\mathfrak{m} = \frac{\mathbb{P}\boldsymbol{\nu}}{\sqrt{1 - |\mathfrak{n} \cdot \boldsymbol{\nu}|^2}} \tag{2.5}$$

determines a unit vector field tangent to $\mathfrak{S}$ and directed outward from $\partial\mathfrak{Q}$ (cf. Fig. 1), and

$$U_{\partial\mathfrak{Q}} = -\frac{(\mathfrak{n} \cdot \boldsymbol{\nu}) V_{\mathfrak{S}}}{\sqrt{1 - |\mathfrak{n} \cdot \boldsymbol{\nu}|^2}} \tag{2.6}$$

represents the rate at which interfacial area enters or leaves $\mathcal{P}$ through $\partial\mathcal{P}$ as $\mathfrak{S}$ evolves.

[8] See GURTIN [9] for a definition of the normal time-rate.

2.2 Basic fields. Configurational force balance. Dissipation imbalance

On ignoring external forces, the basic variables of the sharp-interface theory consist of the bulk fields

W	*bulk energy density,*
$\boldsymbol{C}$	*bulk configurational stress,*
$\boldsymbol{f}$	*bulk internal configurational force density,*

and the interfacial fields[9]

w	*interfacial energy density,*
$\mathbb{C}$	*interfacial configurational stress,*
$\mathbb{f}$	*interfacial internal configurational force density.*

These fields are required, for each suitable subregion $\mathcal{P}$ of $\mathcal{B}$ and each time, to obey the configurational force balance

$$\int_{\partial\mathcal{P}} \boldsymbol{C}\boldsymbol{\nu}\, da + \int_{\mathcal{P}} \boldsymbol{f}\, dv + \int_{\partial\Omega} \mathbb{C}\mathbb{m}\, dl + \int_{\Omega} \mathbb{f}\, da = \boldsymbol{0}, \tag{2.7}$$

and the dissipation imbalance

$$\dot{\int_{\mathcal{P}} W\, dv + \int_{\Omega} w\, da} - \int_{\partial\Omega} w U_{\partial\Omega}\, dl \leq \int_{\partial\Omega} \mathbb{c}\cdot(V_{\mathfrak{S}}\mathbb{m})\, dl, \tag{2.8}$$

asserting the second law.[10] Here $\mathbb{c} = \mathbb{C}^T\mathbb{n}$ is the normal component of $\mathbb{C}$.[11]

The foregoing global configurational force balance has the local forms

$$\operatorname{div}\boldsymbol{C} + \boldsymbol{f} = \boldsymbol{0}, \tag{2.9}$$

valid in bulk, and

$$[\![\boldsymbol{C}\mathbb{n}]\!] + \operatorname{div}_{\mathfrak{S}}\mathbb{C} + \mathbb{f} = \boldsymbol{0} \tag{2.10}$$

valid on $\mathfrak{S}$. Further, the dissipation imbalance requires that

$$\dot{W} \leq 0 \tag{2.11}$$

[9] The field $\mathbb{C}$ obeys $\mathbb{C}\mathbb{n} = \boldsymbol{0}$ on $\mathfrak{S}$ and therefore is *superficial* in the sense of GURTIN [10].

[10] In writing (2.8), we have imposed the requirement (cf. GURTIN & STRUTHERS and GURTIN [10, 6]) that the power generated by the configurational stress be invariant under reparametrization of $\mathfrak{S}$. As the configurational forces $\boldsymbol{f}$ and $\mathbb{f}$ act *internally* to the bulk and interface, respectively, they do not contribute to the power.

[11] By virtue of the requirement that $\mathbb{C}$ be superficial (cf. Footnote 9), $\mathbb{c}$ obeys $\mathbb{c}\cdot\mathbb{n} = 0$ on $\mathfrak{S}$ and therefore is *tangential* on $\mathfrak{S}$.

hold in bulk, and that

$$\mathring{w} \leq \mathbb{n}\cdot[\![(W\mathbf{1}-\boldsymbol{C})\mathbb{n}]\!]V_{\mathfrak{G}} + \big((w\mathbb{P}-\mathbb{C})\cdot\mathbb{L}\big)V_{\mathfrak{G}} - \mathbb{c}\cdot\mathring{\mathbb{n}} - (\mathbb{f}\cdot\mathbb{n})V_{\mathfrak{G}} \tag{2.12}$$

hold on $\mathfrak{G}$.

An invariance argument originated recently by GURTIN [6] yields the representations

$$\boldsymbol{C} = W\mathbf{1} \qquad \text{and} \qquad \mathbb{C}_{\text{tan}} = w\mathbb{P} \tag{2.13}$$

for the bulk configurational stress $\boldsymbol{C}$ and the tangential component $\mathbb{C}_{\text{tan}} = \mathbb{P}\mathbb{C}$ of the interfacial configurational stress. Consequences of these representations are a reduced version

$$\mathring{w} + \mathbb{c}\cdot\mathring{\mathbb{n}} + (\mathbb{f}\cdot\mathbb{n})V_{\mathfrak{G}} \leq 0 \tag{2.14}$$

of the interfacial dissipation imbalance (2.12), and the power identity

$$\int_{\partial\Omega} \mathbb{c}\cdot(V_{\mathfrak{G}}\mathbb{n})\,dl = -\int_{\Omega}\big([\![W]\!] + \mathbb{f}\cdot\mathbb{n})V_{\mathfrak{G}} + wK_{\mathfrak{G}}V_{\mathfrak{G}} + \mathbb{c}\cdot\mathring{\mathbb{n}}\big)\,da. \tag{2.15}$$

2.3 Constitutive equations

In bulk, the energy density of each phase $\mathfrak{c} = \mathfrak{a}, \mathfrak{b}$ is taken to be constant:

$$W = W^{\mathfrak{c}}, \qquad \mathfrak{c} = \mathfrak{a}, \mathfrak{b}. \tag{2.16}$$

For the interfacial constitutive theory, it is assumed that w, $\mathbb{c}$, and $\mathbb{f}\cdot\mathbb{n}$ are given by response functions depending on $\mathbb{n}$ and $V_{\mathfrak{G}}$. Compatibility with the interfacial dissipation imbalance (2.14) then requires that

$$w = \hat{w}(\mathbb{n}), \quad \mathbb{c} = \hat{\mathbb{c}}(\mathbb{n}) = -\frac{\partial}{\partial\mathbb{n}}\hat{w}(\mathbb{n}), \quad \mathbb{f}\cdot\mathbb{n} = -\hat{b}(\mathbb{n}, V_{\mathfrak{G}})V_{\mathfrak{G}}, \tag{2.17}$$

where the *kinetic coefficient* $b = \hat{b}(\mathbb{n}, V_{\mathfrak{G}})$ is nonnegative.

On inserting the relations (2.17) in the inequality (2.14) and evaluating the normal time-rate of w through the response function $\hat{w}$, we obtain an *interfacial dissipation balance*

$$\mathring{w} + \mathbb{c}\cdot\mathring{\mathbb{n}} + (\mathbb{f}\cdot\mathbb{n})V_{\mathfrak{G}} = -bV_{\mathfrak{G}}^2 \leq 0, \tag{2.18}$$

that identifies accretion (through interface propagation) as the sole source of dissipation in the theory at hand. For future reference, we introduce the *dissipation density*

$$\delta = -(\mathbb{f}\cdot\mathbb{n})V_{\mathfrak{G}} = bV_{\mathfrak{G}}^2. \tag{2.19}$$

2.4 Internal configurational forces

Together with the expression (2.16) for W, the representation $(2.13)_1$ for $\boldsymbol{C}$ implies that

$$\operatorname{div} \boldsymbol{C} = \boldsymbol{0}, \tag{2.20}$$

so that the bulk internal configurational force $\boldsymbol{f}$ must vanish, viz.

$$\boldsymbol{f} = \boldsymbol{0}. \tag{2.21}$$

Further, the expression $(2.13)_2$ for $\mathbb{C}_{\tan}$ and the constitutive equations $(2.17)_1$ and $(2.17)_2$ for w and $\mathbb{c}$ imply that

$$\mathbb{P}\big(\llbracket \boldsymbol{C}\mathfrak{n} \rrbracket + \operatorname{div}_{\mathfrak{S}} \mathbb{C}\big) = \boldsymbol{0}, \tag{2.22}$$

so that, like the bulk internal configurational force, the tangential component $\mathfrak{f}_{\tan} = \mathbb{P}\mathfrak{f}$ of the interfacial internal configurational force must vanish, viz.

$$\mathfrak{f}_{\tan} = \boldsymbol{0}. \tag{2.23}$$

Hence, the relation $(2.17)_3$ determining $\mathfrak{f}\cdot\mathfrak{n}$ yields

$$\mathfrak{f} = -bV_{\mathfrak{S}}\mathfrak{n}, \tag{2.24}$$

and satisfaction of the interfacial configurational force balance (2.10) is equivalent to satisfaction of its normal component

$$\mathfrak{n}\cdot\llbracket \boldsymbol{C}\mathfrak{n} \rrbracket + \mathbb{C}\cdot\mathbb{L} + \operatorname{div}_{\mathfrak{S}} \mathbb{c} + \mathfrak{f}\cdot\mathfrak{n} = 0, \tag{2.25}$$

which, for brevity, we refer to as the *normal configurational balance.*

3 Review of the phase-field theory

Here we outline the theory of FRIED & GURTIN. In so doing, we distinguish vectors and tensors from scalars using bold-faced type—lower case for vectors and upper case for tensors. Further, fields possessing counterparts in the sharp-interface theory are distinguished with the aid of sans-serif type.

3.1 Basic fields. Balance laws. Dissipation inequality

The phase-field theory involves only bulk fields, that, ignoring external forces, are[12]

W	*energy density,*
$\boldsymbol{\xi}$	*microstress,*
π	*internal microforce density.*

[12] The microstructural fields $\boldsymbol{\xi}$ and π act in response to changes in the phase field, and are introduced under the precept that there should exist a force system that accounts for power expenditures associated with the evolution of the phase field. FRIED & GURTIN [2] referred to $\boldsymbol{\xi}$ and π as the *accretive stress* and *internal accretive force*, respectively.

For each $\mathcal{P}$ in $\mathcal{B}$ and each time, these fields are required to obey the microforce balance[13]

$$\int_{\partial\mathcal{P}} \boldsymbol{\xi}\cdot\boldsymbol{\nu}\, da + \int_{\mathcal{P}} \pi\, dv = 0, \tag{3.1}$$

and also the dissipation imbalance

$$\overline{\int_{\mathcal{P}} W\, dv}^{\cdot} \leq \int_{\partial\mathcal{P}} \boldsymbol{\xi}\cdot(\dot{\varphi}\boldsymbol{\nu})\, da, \tag{3.2}$$

enforcing the second law.[14]

The foregoing global laws have the local forms

$$\left.\begin{aligned} \operatorname{div}\boldsymbol{\xi} + \pi &= 0, \\ \dot{W} &\leq \boldsymbol{\xi}\cdot(\nabla\dot{\varphi}) - \pi\dot{\varphi}. \end{aligned}\right\} \tag{3.3}$$

3.2 Constitutive equations

In the phase-field theory, W, $\boldsymbol{\xi}$, and π are given by response functions depending on the phase field φ, phase-field gradient $\nabla\varphi$, and phase-field rate $\dot{\varphi}$. Consistency with the local dissipation inequality $(3.3)_2$ then requires that

$$\left.\begin{aligned} W = \hat{W}(\varphi,\nabla\varphi), \quad \boldsymbol{\xi} &= \frac{\partial}{\partial(\nabla\varphi)}\hat{W}(\varphi,\nabla\varphi), \\ \pi &= -\frac{\partial}{\partial\varphi}\hat{W}(\varphi,\nabla\varphi) - \hat{\beta}(\varphi,\nabla\varphi,\dot{\varphi})\dot{\varphi}, \end{aligned}\right\} \tag{3.4}$$

where the *damping modulus* $\beta = \hat{\beta}(\varphi,\nabla\varphi,\dot{\varphi})$ must be non-negative.[15]

On inserting the relations (3.4) into the inequality $(3.3)_2$, we deduce a dissipation balance

$$\dot{W} - \boldsymbol{\xi}\cdot(\nabla\dot{\varphi}) + \pi\dot{\varphi} = -\beta\dot{\varphi}^2 \leq 0, \tag{3.5}$$

which isolates the microforce $-\beta\dot{\varphi}$ as the sole source of dissipation in the theory and, hence, motivates our choice to refer to β as the *damping modulus*. For future reference, we introduce the dissipation density

$$\Delta = \beta\dot{\varphi}^2 \tag{3.6}$$

for the phase-field theory.

[13] Motivated by work of OSEEN [11], ERICKSEN [12, 13] included a microforce balance in his early theories of anisotropic fluids and liquid crystals. CAPRIZ [14] provides a comprehensive discussion of the notion of microforce balance and a systematic overview of applications where such a balance is relevant.

[14] Because it acts internally to $\mathcal{P}$, π does not contribute to the working in (3.2).

[15] FRIED & GURTIN [15] refer to β as the *kinetic modulus*.

3.3 Configurational force balance

On introducing the fields

$$\boldsymbol{C} = W\boldsymbol{1} - (\nabla\varphi)\otimes\boldsymbol{\xi} \qquad \text{and} \qquad \boldsymbol{f} = \beta\dot{\varphi}\nabla\varphi, \tag{3.7}$$

a simple calculation shows that, granted the constitutive equations (3.4),

$$\operatorname{div}\boldsymbol{C} + \boldsymbol{f} = -(\operatorname{div}\boldsymbol{\xi} + \pi)\nabla\varphi, \tag{3.8}$$

so that, drawing on the microforce balance $(3.3)_1$, we have

$$\operatorname{div}\boldsymbol{C} + \boldsymbol{f} = \boldsymbol{0}. \tag{3.9}$$

We recognize (3.9) as the the local statement of configurational force balance for the phase-field theory, with $\boldsymbol{C}$ and $\boldsymbol{f}$ the configurational stress and the internal configurational force relevant to that theory. Considering (3.8), we see that the microforce balance $(3.3)_3$ implies the configurational force balance (3.9); conversely, granted that $\nabla\varphi$ does not vanish, the configurational force balance (3.9) implies the microforce balance $(3.3)_1$. Hence, on any subregion $\mathcal{R}$ of $\mathcal{B}$ where $\nabla\varphi$ is nonvanishing, we may impose—in place of the microforce balance $(3.3)_1$—the configurational force balance (3.9) or the equivalent requirement that

$$\int_{\partial\mathcal{P}} \boldsymbol{C}\boldsymbol{\nu}\, da + \int_{\mathcal{P}} \boldsymbol{f}\, dv = \boldsymbol{0} \tag{3.10}$$

holds for all $\mathcal{P}$ in $\mathcal{R}$.

3.4 Uniformity surfaces

Consider a subregion $\mathcal{P}$ of $\mathcal{B}$ where, over the course of some time-interval, $\nabla\varphi$ is nonvanishing. Then, the level sets

$$\mathcal{S}_q = \{\boldsymbol{x} \in \mathcal{P} : \varphi(\boldsymbol{x}, \cdot) = q\} \tag{3.11}$$

are actually surfaces, which, following FRIED & GURTIN [15], we refer to as *uniformity surfaces*. Now, within $\mathcal{P}$: the field

$$V = -\frac{\dot{\varphi}}{|\nabla\varphi|} \tag{3.12}$$

determines the scalar normal velocity of uniformity surfaces in the direction of the unit vector field

$$\boldsymbol{n} = \frac{\nabla\varphi}{|\nabla\varphi|}; \tag{3.13}$$

the tensor field

$$\boldsymbol{P} = \boldsymbol{1} - \boldsymbol{n}\otimes\boldsymbol{n} \tag{3.14}$$

projects vectors onto their components tangent to uniformity surfaces; the fields

$$\boldsymbol{L} = -(\nabla\boldsymbol{n})\boldsymbol{P} \qquad \text{and} \qquad K = -\operatorname{tr}\boldsymbol{L} \tag{3.15}$$

are the curvature tensor and total curvature of uniformity surfaces; and

$$\mathring{g} = \dot{g} + (\nabla g)\cdot(V\boldsymbol{n}), \tag{3.16}$$

represents the rate, along the normal trajectories of uniformity surfaces, at which a scalar field g changes with respect to time.

Useful consequences of the foregoing definitions are the identities

$$\boldsymbol{L} = -|\nabla\varphi|^{-1}\boldsymbol{P}(\nabla\nabla\varphi)\boldsymbol{P} \qquad \text{and} \qquad \mathring{\boldsymbol{n}} + (\overline{\ln|\nabla\varphi|})\boldsymbol{n} = -\nabla V. \tag{3.17}$$

4 Constitutive specialization within the phase-field theory

Here our goal is to identify choices of the constitutive response functions $\hat{W}$ and $\hat{\beta}$ (cf. (3.4)) for which the phase-field theory presented in Section 3 becomes a regularization of the sharp-interface theory introduced in Section 2. In particular, this regularization should account for

i. the ability of the bulk phases of the sharp-interface theory to coexist,

ii. orientation dependence in the response function $\hat{w}$ for the interfacial energy density w of the sharp-interface theory, and

iii. orientation and interfacial normal velocity dependence in the response function $\hat{b}$ for the kinetic coefficient b of the sharp-interface theory,

and, in so doing, encompass properly the range of bulk and interfacial structure present in the sharp-interface theory.

4.1 Exchange energy

To model the bulk phases of the sharp-interface theory we assume that:

A1. $\hat{W}(\cdot,\boldsymbol{0})$ *is a double-well potential with minima at* $\varphi = \varphi_{\mathfrak{a}}$ *and* $\varphi = \varphi_{\mathfrak{b}}$, *where, without loss of generality,* $\varphi_{\mathfrak{a}} < \varphi_{\mathfrak{b}}$.

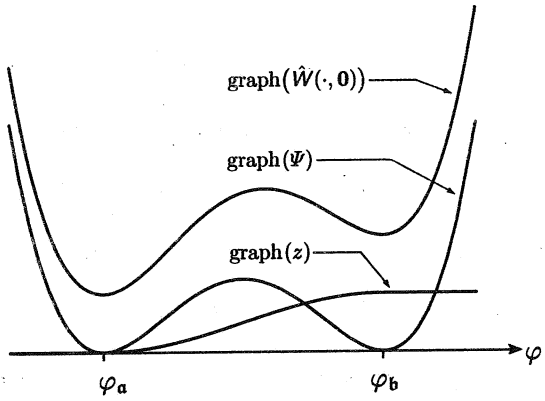

Figure 2. Graphs depicting the qualitative properties of $\hat{W}(\cdot,\mathbf{0})$, Ψ, and z.

As a consequence of *A1*, $\hat{W}(\varphi,\mathbf{0})$ can be expressed in the form

$$\hat{W}(\varphi,\mathbf{0}) = \Psi(\varphi) + \big(1 - z(\varphi)\big)\hat{W}(\varphi_a,\mathbf{0}) + z(\varphi)\hat{W}(\varphi_b,\mathbf{0}), \tag{4.1}$$

where the *exchange energy* Ψ is a double-well potential with equal minima at $\varphi = \varphi_a$ and $\varphi = \varphi_b$ and z is a monotonic function z that takes $\mathbb{R}$ onto $[0,1]$ and satisfies $z(\varphi_a) = 0$ and $z(\varphi_b) = 1$ (cf. Fig. 2).

The set

$$\{\varphi : \frac{\partial}{\partial\varphi}\Psi(\varphi) < 0\} \tag{4.2}$$

is the *spinodal* of Ψ; roughly speaking, the phase-field values $\varphi \approx \varphi_a$ and $\varphi \approx \varphi_b$ characterize the bulk material of phases $\mathfrak{a}$ and $\mathfrak{b}$, respectively, while an interval (q_a, q_b), with

$$\{\varphi : \frac{\partial}{\partial\varphi}\Psi(\varphi) < 0\} \subsetneq (q_a, q_b) \subsetneq (\varphi_a, \varphi_b) \tag{4.3}$$

defines layers that serve as interfaces separating crystalline solid from melt. Anticipating a result established in Section 9.2, we assume that $\nabla\varphi$ does not vanish within such transition layers, whereby the level sets $\mathcal{S}_q$, with $q_a < q < q_b$, will actually be uniformity surfaces (cf. Section 3.4).

4.2 Gradient energy

While the exchange energy establishes a preference for equilibrium states in which φ is homogeneously equal to either φ_a or φ_b, it is constitutive dependence

on $\nabla\varphi$ through the *gradient energy density* $\gamma = \hat{\gamma}(\varphi, \nabla\varphi)$, determined by

$$\gamma = \hat{\gamma}(\varphi, \nabla\varphi) = \hat{W}(\varphi, \nabla\varphi) - \hat{W}(\varphi, \mathbf{0}), \tag{4.4}$$

that allows for these preferred values of the phase field to coexist and be connected by smooth layers. To account for orientation dependence in the crystalline surface energy density, we express dependence on $\nabla\varphi = |\nabla\varphi|\boldsymbol{n}$ in terms of separate dependencies on the variables $|\nabla\varphi|$ and $\boldsymbol{n}$, and, in particular, take the gradient energy quadratic in $|\nabla\varphi|$ but an arbitrary function of $\boldsymbol{n}$.[16] Further, we require that the gradient energy density be independent of φ. Precisely, we assume that:

A2. $\hat{\gamma}$ satisfies the functional equation

$$\hat{\gamma}(\varphi_1, \alpha\boldsymbol{p}) = \alpha^2\hat{\gamma}(\varphi_2, \boldsymbol{p}) \tag{4.5}$$

for all φ_1 and φ_2, for all $\boldsymbol{p}$, and for all α.

As a straightforward consequence of *A2*, we find that

$$\gamma = \tfrac{1}{2}|\nabla\varphi|^2\lambda(\boldsymbol{n}), \tag{4.6}$$

with λ an even function of $\boldsymbol{n}$.

4.3 Damping modulus

Our assumptions concerning the response function $\hat{\beta}$ determining the damping modulus are guided by those imposed on the gradient energy density γ. To account for dependence of the crystalline surface mobility on orientation and interfacial normal velocity, $\hat{\beta}$ should depend on $(\nabla\varphi, -\dot{\varphi}) = |\nabla\varphi|(\boldsymbol{n}, V)$ through $(\boldsymbol{n}, V)$; we do not, however, allow for a dependence of $\hat{\beta}$ on $|\nabla\varphi|$.[17] Further, we require that $\hat{\beta}$, like $\hat{\gamma}$, be independent of φ. Precisely, we assume that:

A3. $\hat{\beta}$ satisfies the functional equation

$$\hat{\beta}(\varphi_1, \alpha\boldsymbol{p}, \alpha s) = \hat{\beta}(\varphi_2, \boldsymbol{p}, s) \tag{4.7}$$

for all φ_1 and φ_2, for all $\boldsymbol{p}$, for all s, and for all positive α.

Employing *A3*, we find readily that

$$\beta = \tilde{\beta}(\boldsymbol{n}, V), \tag{4.8}$$

where $\tilde{\beta}(\boldsymbol{n}, V)$ must be nonnegative for $(\boldsymbol{n}, V)$ (cf. the remark following (3.4)).

[16] Bases for this and the other assumptions put forth here are discussed in Section 7.

[17] Together with the constitutive equation $\beta = \hat{\beta}(\varphi, \nabla\varphi, \dot{\varphi})$, the definition $(3.7)_2$ of the internal configurational force determines a constitutive relation $\boldsymbol{f} = \hat{\boldsymbol{f}}(\varphi, \nabla\varphi, \dot{\varphi}) = \hat{\beta}(\varphi, \nabla\varphi, \dot{\varphi})\dot{\varphi}\nabla\varphi$ for that force (provided $\hat{\boldsymbol{f}}$ is consistent with $\boldsymbol{P}\hat{\boldsymbol{f}}(\varphi, \nabla\varphi, \dot{\varphi}) = \mathbf{0}$). The assumption that $\hat{\beta}$ be independent of $\nabla\varphi$ is equivalent to requiring that $\hat{\beta}$, like the gradient energy $\hat{\gamma}$, be *quadratic* in $|\boldsymbol{p}|$. An analogous remark holds for the dissipation density $\Delta = \hat{\beta}(\varphi, \nabla\varphi, \dot{\varphi})\dot{\varphi}^2$.

4.4 Decomposition of fields into bulk and excess components

Since $\Psi(\varphi_a) = \Psi(\varphi_b) = 0$, we expect that the exchange energy should contribute only to the energy of transition layers, wherein φ varies between q_a and q_b. Thus, in light of the expressions (4.1) and (4.4) defining $\hat{W}(\cdot, \mathbf{0})$ and $\hat{\gamma}$, we are motivated to decompose the energy density as a sum

$$W = W^{\mathrm{bu}} + W^{\mathrm{xs}} \tag{4.9}$$

consisting of *bulk* (bu) and *excess* (xs) terms, defined by

$$\begin{aligned} W^{\mathrm{bu}} &= \hat{W}^{\mathrm{bu}}(\varphi) \\ &= \hat{W}(\varphi, \mathbf{0}) - \Psi(\varphi) \end{aligned} \tag{4.10}$$

and

$$\begin{aligned} W^{\mathrm{xs}} &= \hat{W}^{\mathrm{xs}}(\varphi, \nabla\varphi) \\ &= \hat{W}(\varphi, \nabla\varphi) - \hat{W}^{\mathrm{bu}}(\varphi) \\ &= \Psi(\varphi) + \tfrac{1}{2}|\nabla\varphi|^2\lambda(\boldsymbol{n}), \end{aligned} \tag{4.11}$$

respectively.

Together with the constitutive equations $(3.4)_2$ and $(3.4)_3$, the decomposition (4.9)–(4.11) of W leads immediately to natural decompositions of the microstress $\boldsymbol{\xi}$ into bulk and excess components. Specifically, we find that[18]

$$\boldsymbol{\xi} = \boldsymbol{\xi}^{\mathrm{xs}}, \tag{4.12}$$

where

$$\boldsymbol{\xi}^{\mathrm{xs}} = |\nabla\varphi|\big(\lambda(\boldsymbol{n})\boldsymbol{n} + \tfrac{1}{2}\frac{\partial}{\partial \boldsymbol{n}}\lambda(\boldsymbol{n})\big), \tag{4.13}$$

Further, the decompositions (4.9) and (4.12) of W and $\boldsymbol{\xi}$ yield, bearing in mind the definition (3.7) of $\boldsymbol{C}$, a decomposition

$$\boldsymbol{C} = \boldsymbol{C}^{\mathrm{bu}} + \boldsymbol{C}^{\mathrm{xs}} \tag{4.14}$$

of the configurational stress $\boldsymbol{C}$ into bulk and excess components, with

$$\boldsymbol{C}^{\mathrm{bu}} = W^{\mathrm{bu}}\boldsymbol{1} \qquad \text{and} \qquad \boldsymbol{C}^{\mathrm{xs}} = W^{\mathrm{xs}}\boldsymbol{1} - (\nabla\varphi)\otimes\boldsymbol{\xi}^{\mathrm{xs}}. \tag{4.15}$$

A useful alternative to the expression $(4.15)_2$ for the excess configurational stress $\boldsymbol{C}^{\mathrm{xs}}$ is

$$\boldsymbol{C}^{\mathrm{xs}} = W^{\mathrm{xs}}\boldsymbol{P} + \boldsymbol{n}\otimes\boldsymbol{c}^{\mathrm{xs}} + \jmath^{\mathrm{xs}}\boldsymbol{n}\otimes\boldsymbol{n}, \tag{4.16}$$

[18] Although it would cause no confusion to drop "xs" superscripts from the symbols denoting the excess components of fields, such as the microstress, that do not possess bulk components, we retain these for emphasis.

with

$$\boldsymbol{c}^{\mathrm{xs}} = \boldsymbol{P}(\boldsymbol{C}^{\mathrm{xs}})^{T}\boldsymbol{n} = -|\nabla\varphi|\boldsymbol{P}\boldsymbol{\xi}^{\mathrm{xs}}, \tag{4.17}$$

and

$$\jmath^{\mathrm{xs}} = \boldsymbol{n}\cdot(\boldsymbol{C}^{\mathrm{xs}}\boldsymbol{n}) = \Psi(\varphi) - \tfrac{1}{2}|\nabla\varphi|^{2}\lambda(\boldsymbol{n}). \tag{4.18}$$

Further, using the expressions (4.13) for $\boldsymbol{\xi}^{\mathrm{xs}}$ in (4.17), we determine a more convenient representation,

$$\boldsymbol{c}^{\mathrm{xs}} = -\tfrac{1}{2}|\nabla\varphi|^{2}\frac{\partial}{\partial\boldsymbol{n}}\lambda(\boldsymbol{n}), \tag{4.19}$$

for $\boldsymbol{c}^{\mathrm{xs}}$.

Next, guided by the foregoing decompositions, wherein the gradient energy density γ contributes only to excess terms, we designate the damping modulus β as an excess quantity, and hence, arrive at decompositions

$$\pi = \pi^{\mathrm{bu}} + \pi^{\mathrm{xs}}, \qquad \boldsymbol{f} = \boldsymbol{f}^{\mathrm{xs}}, \qquad \Delta = \Delta^{\mathrm{xs}}, \tag{4.20}$$

with

$$\left.\begin{aligned} \pi^{\mathrm{bu}} &= -\frac{\partial}{\partial\varphi}\hat{W}^{\mathrm{bu}}(\varphi), & \pi^{\mathrm{xs}} &= -\frac{\partial}{\partial\varphi}\Psi(\varphi) + |\nabla\varphi|\tilde{\beta}(\boldsymbol{n},V)V, \\ \boldsymbol{f}^{\mathrm{xs}} &= -|\nabla\varphi|^{2}\tilde{\beta}(\boldsymbol{n},V)V\boldsymbol{n}, & \Delta^{\mathrm{xs}} &= |\nabla\varphi|^{2}\beta(\boldsymbol{n},V)V^{2}. \end{aligned}\right\} \tag{4.21}$$

Finally, using the expressions (4.11), (4.18), (4.19), and $(4.21)_4$ for W^{xs}, $\jmath^{\mathrm{xs}}$, $\boldsymbol{c}^{\mathrm{xs}}$, and $\boldsymbol{f}^{\mathrm{xs}}$ in the relations $(4.13)_3$ and $(4.21)_{2,3}$ for the excess components of the microstress and internal microforce, we find that

$$|\nabla\varphi|\boldsymbol{\xi}^{\mathrm{xs}} = (W^{\mathrm{xs}} - \jmath^{\mathrm{xs}})\boldsymbol{n} - \boldsymbol{c}^{\mathrm{xs}}, \tag{4.22}$$

and that

$$|\nabla\varphi|\pi^{\mathrm{xs}} = -\tfrac{1}{2}\big(\nabla(W^{\mathrm{xs}} + \jmath^{\mathrm{xs}})\big)\cdot\boldsymbol{n} - \boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n}. \tag{4.23}$$

5 Versions of normal configurational force balance and dissipation imbalance specific to transition layers

In regions where $\nabla\varphi$ does not vanish, the local configurational force balance (3.9) is, bearing in mind the expression $(4.21)_3$ for $\boldsymbol{f}^{\mathrm{xs}}$, equivalent to a scalar equation

$$(\mathrm{div}(\boldsymbol{C}^{\mathrm{bu}} + \boldsymbol{C}^{\mathrm{xs}}) + \boldsymbol{f}^{\mathrm{xs}})\cdot\boldsymbol{n} = 0 \tag{5.1}$$

that enforces the balance of configurational force normal to uniformity surfaces. On appeal to (4.16), (5.1) becomes

$$(\operatorname{div} \boldsymbol{C}^{\mathrm{bu}})\cdot\boldsymbol{n} + \boldsymbol{C}^{\mathrm{xs}}\cdot\boldsymbol{L} + \operatorname{div}\boldsymbol{c}^{\mathrm{xs}} + \boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n} + \operatorname{div}(j^{\mathrm{xs}}\boldsymbol{n}) = 0, \tag{5.2}$$

which bears a striking resemblence to the normal configurational force balance (2.25) of the sharp-interface theory.

Similarly, in regions where $\nabla\varphi$ does not vanish, the local dissipation balance (3.5) can—by appeal to the local microforce balance $(3.3)_1$, the relation $(3.17)_2$ determining ∇V, the identity $\boldsymbol{C}^{\mathrm{xs}}\cdot\boldsymbol{L} = W^{\mathrm{xs}}K$ (which is a consequence of the expression (4.16) for $\boldsymbol{C}^{\mathrm{xs}}$ and the result $\boldsymbol{L}^T\boldsymbol{n} = \boldsymbol{0}$ arising from the requirement that $\boldsymbol{n}$ is a unit vector field), the expression (4.22) for $\boldsymbol{\xi}^{\mathrm{xs}}$—be written in the alternate form

$$\mathring{W}^{\mathrm{bu}} + \mathring{W}^{\mathrm{xs}} + \boldsymbol{c}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{n}} + (\boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n})V - (W^{\mathrm{xs}} - j^{\mathrm{xs}})\overset{\diamond}{\ln|\nabla\varphi|} = -\Delta^{\mathrm{xs}}. \tag{5.3}$$

6 Scaling

In this section we scale the dependent and independent variables of the phase-field theory. In doing so, we assume, without loss of generality, that the balance laws and constitutive equations of the sharp-interface theory, as presented in Section 2, are in dimensionless form—having been rendered so with the aid of a characteristic length L, a characteristic time T, a characteristic measure μ of bulk energy per unit volume, and a characteristic measure κ of interfacial energy per unit area.

6.1 Preliminaries

We begin by assuming that L, μ, and κ yield a dimensionless modulus

$$0 < \epsilon = \frac{\kappa}{\mu L} \ll 1, \tag{6.1}$$

and, labeling the dimensional (unscaled) fields with asterisks, introduce the dimensionless independent and dependent variables

$$\boldsymbol{x} = \frac{\boldsymbol{x}^*}{L}, \qquad t = \frac{t^*}{T}, \qquad \varphi(\boldsymbol{x},t) = \varphi^*(\boldsymbol{x}^*,t^*), \tag{6.2}$$

and constitutive functions

$$\left.\begin{aligned} \hat{W}^{\mathrm{bu}}(\varphi) &= \frac{1}{\mu}\hat{W}^{\mathrm{bu}*}(\varphi^*), \qquad \Psi(\varphi) = \frac{\kappa}{\mu^2 L}\Psi^*(\varphi^*), \\ \lambda(\boldsymbol{n}) &= \frac{1}{\kappa L}\lambda^*(\boldsymbol{n}^*), \qquad \tilde{\beta}(\boldsymbol{n},V) = \frac{L}{\kappa T}\tilde{\beta}^*(\boldsymbol{n}^*,V^*), \end{aligned}\right\} \tag{6.3}$$

where the quantities without asterisks in (6.2) and (6.3) are assumed to be of $O(1)$ in ϵ.

This scaling yields

$$W^{\mathrm{bu}*} = \mu W^{\mathrm{bu}}, \qquad \boldsymbol{C}^{\mathrm{bu}*} = \mu \boldsymbol{C}^{\mathrm{bu}}, \qquad \pi^{\mathrm{bu}*} = \mu \pi^{\mathrm{bu}}, \tag{6.4}$$

with W^{bu}, $\boldsymbol{C}^{\mathrm{bu}}$, and π^{bu} of $O(1)$ in ϵ and given by

$$W^{\mathrm{bu}} = \hat{W}^{\mathrm{bu}}(\varphi), \qquad \boldsymbol{C}^{\mathrm{bu}} = W^{\mathrm{bu}}(\varphi)\boldsymbol{1}, \qquad \pi^{\mathrm{bu}} = -\frac{\partial}{\partial \varphi}\hat{W}^{\mathrm{bu}}(\varphi), \tag{6.5}$$

as well as

$$\left.\begin{aligned} W^{\mathrm{xs}*} &= \epsilon\mu W^{\mathrm{xs}}, \qquad \boldsymbol{C}^{\mathrm{xs}*} = \epsilon\mu \boldsymbol{C}^{\mathrm{xs}}, \qquad \boldsymbol{\xi}^{\mathrm{xs}*} = \epsilon\mu L \boldsymbol{\xi}^{\mathrm{xs}}, \\ \pi^{\mathrm{xs}*} &= \epsilon\mu\pi^{\mathrm{xs}}, \qquad \boldsymbol{f}^{\mathrm{xs}*} = \epsilon\frac{\mu}{L}\boldsymbol{f}^{\mathrm{xs}}, \qquad \Delta^{\mathrm{xs}*} = \epsilon\frac{\mu}{T}\Delta^{\mathrm{xs}}, \end{aligned}\right\} \tag{6.6}$$

with

$$\left.\begin{aligned} W^{\mathrm{xs}} &= |\nabla\varphi|^2\lambda(\boldsymbol{n}) + \jmath^{\mathrm{xs}}, \\ \boldsymbol{C}^{\mathrm{xs}} &= W^{\mathrm{xs}}\boldsymbol{P} + \boldsymbol{n}\otimes\boldsymbol{c}^{\mathrm{xs}} + \jmath^{\mathrm{xs}}\boldsymbol{n}\otimes\boldsymbol{n}, \\ \boldsymbol{\xi}^{\mathrm{xs}} &= |\nabla\varphi|^{-1}\big((W^{\mathrm{xs}} - \jmath^{\mathrm{xs}})\boldsymbol{n} - \boldsymbol{c}^{\mathrm{xs}}\big), \\ \pi^{\mathrm{xs}} &= -\epsilon^{-2}\frac{\partial}{\partial\varphi}\Psi(\varphi) + |\nabla\varphi|\tilde{\beta}(\boldsymbol{n}, V)V, \\ \boldsymbol{f}^{\mathrm{xs}} &= -|\nabla\varphi|^2\tilde{\beta}(\boldsymbol{n}, V)V\boldsymbol{n}, \\ \Delta^{\mathrm{xs}} &= |\nabla\varphi|^2\tilde{\beta}(\boldsymbol{n}, V)V^2, \end{aligned}\right\} \tag{6.7}$$

where $\boldsymbol{c}^{\mathrm{xs}}$ and $\jmath^{\mathrm{xs}}$ are determined through

$$\boldsymbol{c}^{\mathrm{xs}} = -\tfrac{1}{2}|\nabla\varphi|^2\frac{\partial}{\partial\nabla\varphi}\lambda(\boldsymbol{n}) \quad \text{and} \quad \jmath^{\mathrm{xs}} = \epsilon^{-2}\Psi(\varphi) - \tfrac{1}{2}|\nabla\varphi|^2\lambda(\boldsymbol{n}) \tag{6.8}$$

(whereby $\boldsymbol{c}^{\mathrm{xs}*} = \epsilon\mu\boldsymbol{c}^{\mathrm{xs}}$ and $\jmath^{\mathrm{xs}*} = \epsilon\mu\jmath^{\mathrm{xs}}$).

Finally, we denote the region associated with the dimensional coordinate $\boldsymbol{x}^*$ by $\mathcal{B}^*$, so that $\mathcal{B}$ is the region associated with the dimensionless coordinate $\boldsymbol{x}$, and we write

$$dv = \frac{1}{L^3}dv^* \qquad \text{and} \qquad da = \frac{1}{L^2}da^* \tag{6.9}$$

for the volume and surface area measures associated with a subregion $\mathcal{P}$ of $\mathcal{B}$ and its boundary $\partial\mathcal{P}$.

6.2 Scaled integral laws

The integral statements (3.1), (3.10), and (3.2) expressing microforce balance, configurational force balance, and dissipation imbalance for the phase-field theory were written for the unscaled fields. Hence, we think of the terms appearing in these as carrying asterisks. If we use the scaling relations (6.2), (6.4), (6.6), and (6.9) to convert these statements to nondimensional form, we arrive at dimensionless statements,

$$\left.\begin{aligned} &\int_{\partial\mathcal{P}} \epsilon\boldsymbol{\xi}\cdot\boldsymbol{\nu}\,da + \int_{\mathcal{P}} (\epsilon\pi^{\mathrm{xs}} + \pi^{\mathrm{bu}})\,dv = 0,\\ &\int_{\partial\mathcal{P}} (\boldsymbol{C}^{\mathrm{bu}} + \epsilon\boldsymbol{C}^{\mathrm{xs}})\boldsymbol{\nu}\,da + \int_{\mathcal{P}} \epsilon\boldsymbol{f}^{\mathrm{xs}}\,dv = \boldsymbol{0},\\ &\overline{\int_{\mathcal{P}} (W^{\mathrm{bu}} + \epsilon W^{\mathrm{xs}})\,dv} \le \int_{\partial\mathcal{P}} \epsilon\boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\,da, \end{aligned}\right\} \tag{6.10}$$

of microforce balance, configurational force balance, and dissipation imbalance for $\mathcal{P}$.

6.3 Scaled local laws

Proceeding as above, we may use the scaling relations (6.2), (6.4), and (6.6) to obtain dimensionless versions,

$$\left.\begin{aligned} \epsilon(\operatorname{div}\boldsymbol{\xi}^{\mathrm{xs}} + \pi^{\mathrm{xs}}) + \pi^{\mathrm{bu}} &= 0,\\ \operatorname{div}(\boldsymbol{C}^{\mathrm{bu}} + \epsilon\boldsymbol{C}^{\mathrm{xs}}) + \epsilon\boldsymbol{f}^{\mathrm{xs}} &= \boldsymbol{0},\\ \dot{W}^{\mathrm{bu}} + \epsilon\dot{W}^{\mathrm{xs}} - \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\nabla\dot{\varphi}) + (\pi^{\mathrm{bu}} + \epsilon\pi^{\mathrm{xs}})\dot{\varphi} &= -\epsilon\Delta^{\mathrm{xs}}, \end{aligned}\right\} \tag{6.11}$$

of the local balances for microforce, configurational force, and dissipation.

Further, the version (5.3) of the dissipation balance for regions in which $\nabla\varphi$ is nonvanishing can be written in the dimensionless form

$$\hat{W}^{\mathrm{bu}} + \epsilon\hat{W}^{\mathrm{xs}} + \epsilon\boldsymbol{c}^{\mathrm{xs}}\cdot\hat{\boldsymbol{n}} + \epsilon(\boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n})V - \epsilon(W^{\mathrm{xs}} - \jmath^{\mathrm{xs}})\overset{\diamond}{\overline{\ln|\nabla\varphi|}} = -\epsilon\Delta^{\mathrm{xs}}. \tag{6.12}$$

7 A constitutive connection

To simplify the presentation of results that we will obtain in the sequel, we now posit that the bulk energy densities W^{a} and W^{b} of the sharp-interface theory are related to the response function $\hat{W}^{\mathrm{bu}}$ of the phase-field theory through

$$W^{\mathrm{a}} = \hat{W}^{\mathrm{bu}}(\varphi_{\mathrm{a}}) \qquad \text{and} \qquad W^{\mathrm{b}} = \hat{W}^{\mathrm{bu}}(\varphi_{\mathrm{b}}), \tag{7.1}$$

and that the interfacial response functions $\hat{w}$ $\hat{c}$, and $\hat{b}$ of the sharp-interface theory are related the response functions λ and $\tilde{\beta}$ of the phase-field theory through

$$\hat{w}(\mathbb{n}) = \sigma\sqrt{\lambda(\mathbb{n})}, \quad \hat{c}(\mathbb{n}) = -\sigma\frac{\partial}{\partial\mathbb{n}}\sqrt{\lambda(\mathbb{n})}, \quad \hat{b}(\mathbb{n}, V_{\mathfrak{S}}) = \frac{\sigma\tilde{\beta}(\mathbb{n}, V_{\mathfrak{S}})}{\sqrt{\lambda(\mathbb{n})}}, \tag{7.2}$$

with the *conversion modulus*[19] σ a constant determined by

$$\sigma = \int_{\varphi_{\mathfrak{a}}}^{\varphi_{\mathfrak{b}}} \sqrt{2\Psi(\varphi)}\, d\varphi. \tag{7.3}$$

We emphasize that the connections (7.1) and (7.2) allow for the full level of constitutive generality encompassed by the sharp-interface theory. While not at all obvious, the choices $(7.2)_{1,4}$ of interfacial free-energy $\hat{w}$ and kinetic coefficient $\hat{b}$ will be justified from the ensuing asymptotic analysis; given $\hat{w}$, the choices $(7.2)_{2,3}$ are predicated upon the relation $(2.17)_2$ determining $\hat{c}$.

On examining $(7.2)_1$ and $(7.2)_3$, we find that assumptions *A2* and *A3* suffice to ensure that the homogeneous extensions $\tilde{w}$ and $\tilde{b}$ of $\hat{w}$ and $\hat{b}$ obey

$$\tilde{w}(\boldsymbol{p}) = |\boldsymbol{p}|\hat{w}\big(\frac{\boldsymbol{p}}{|\boldsymbol{p}|}\big) \qquad \text{and} \qquad \tilde{b}(\boldsymbol{p}, s) = |\boldsymbol{p}|^{-1}\hat{b}\big(\frac{\boldsymbol{p}}{|\boldsymbol{p}|}, -\frac{s}{|\boldsymbol{p}|}\big) \tag{7.4}$$

for all nonzero vectors $\boldsymbol{p}$. We observe that (7.4) are consistent with the standard belief that the extensions, to the set of all nonzero vectors, of the response functions delivering the surface energy density and surface mobility[20] of a cystalline solid should be homogeneous of degree one.[21]

8 Decomposition of the reference region. Expansions

Hereafter, we focus on a situation wherein $\mathcal{B}$ is the union of three evolving subregions: $\mathcal{R}^{\mathfrak{a}}$, $\mathcal{L}$, and $\mathcal{R}^{\mathfrak{b}}$. At each time t, $\mathcal{L}(t,\epsilon)$ is a transition layer comprised by those points $\boldsymbol{x}$ in $\mathcal{B}$ for which $q_{\mathfrak{a}} < \varphi(\boldsymbol{x}, t, \epsilon) < q_{\mathfrak{b}}$, while $\mathcal{R}^{\mathfrak{a}}(t,\epsilon)$ and $\mathcal{R}^{\mathfrak{b}}(t,\epsilon)$ consist of those points $\boldsymbol{x}$ in $\mathcal{B}$ where $\varphi(\boldsymbol{x}, t, \epsilon) \approx \varphi_{\mathfrak{a}}$ and $\varphi(\boldsymbol{x}, t, \epsilon) \approx \varphi_{\mathfrak{b}}$, respectively. We assume that the thickness $h(\epsilon)$ of $\mathcal{L}(\cdot, \epsilon)$ tends to zero with ϵ, but at slightly slower rate, viz.

$$\lim_{\epsilon\to 0+} h(\epsilon) = 0 \qquad \text{and} \qquad \lim_{\epsilon\to 0+} \epsilon^{-1}h(\epsilon) = +\infty, \tag{8.1}$$

[19] We borrow the term *conversion modulus* from FRIED & GURTIN [15]—who introduce such a modulus in their study of the asymptotic limit of a generalized phase-field theory for solidification. However, the right-hand-side of (7.3) would require a factor of $1/\sqrt{\lambda(\boldsymbol{n})}$ for σ to be completely analogous to the conversion modulus of FRIED & GURTIN [15].

[20] We recall that the surface mobility is the reciprocal of the kinetic coefficient.

[21] See, for example, the discussion of TAYLOR, CAHN & HANDWERKER [1].

and that the limit

$$\mathcal{S} = \lim_{\epsilon \to 0+} \mathcal{L}(\cdot, \epsilon) \tag{8.2}$$

exists, with $\mathcal{S}$ a smoothly evolving surface surface contained in $\mathcal{L}(\cdot, \epsilon)$ for each $\epsilon > 0$. Granted that $\mathcal{B} = \mathcal{R}^{\mathfrak{a}}(t, \epsilon) \cup \mathcal{L}(t, \epsilon) \cup \mathcal{R}^{\mathfrak{b}}(t, \epsilon)$ for all t, a direct consequence of (8.2) is that

$$\mathcal{B} = \mathcal{B}^{\mathfrak{a}}(t) \cup \mathcal{S}(t) \cup \mathcal{B}^{\mathfrak{b}}(t), \tag{8.3}$$

where

$$\mathcal{B}^{\mathfrak{c}}(t) = \lim_{\epsilon \to 0+} \mathcal{R}^{\mathfrak{c}}(t, \epsilon) \tag{8.4}$$

for $\mathfrak{c} = \mathfrak{a}, \mathfrak{b}$.

We suppose that, within $\mathcal{R}^{\mathfrak{c}}(\cdot, \epsilon)$, $\mathfrak{c} = \mathfrak{a}, \mathfrak{b}$, φ possesses an *outer expansion*

$$\varphi(\boldsymbol{x}, t, \epsilon) = \varphi_0^{\text{out}}(\boldsymbol{x}, t) + \epsilon \varphi_1^{\text{out}}(\boldsymbol{x}, t) + O(\epsilon^2), \tag{8.5}$$

and that, within $\mathcal{L}(\cdot, \epsilon)$, φ possesses an *inner expansion*

$$\varphi(\boldsymbol{x}, t, \epsilon) = \varphi_0^{\text{in}}\big(r(\boldsymbol{x}, t), z(\boldsymbol{x}, t), t\big) + \epsilon \varphi_1^{\text{in}}\big(r(\boldsymbol{x}, t), z(\boldsymbol{x}, t), t\big) + O(\epsilon^2), \tag{8.6}$$

where (ℓ, z) defines a coordinate system corresponding to the surface $\mathcal{S}$,[22] and the stretched coordinate r, defined for each $\boldsymbol{x}$ in $\mathcal{L}(t)$ by

$$r(\boldsymbol{x}, t) = \epsilon^{-1} \ell(\boldsymbol{x}, t), \tag{8.7}$$

varies from $-\infty$ to $+\infty$ as $\epsilon \to 0+$.

A definitive boundary between the layer and bulk regions is precluded by the manner by which interfaces are described—as layers of finite thickness—within the phase-field theory. Hence, $\mathcal{L}(t, \epsilon)$ is not presumed to be disjoint from $\mathcal{R}^{\mathfrak{c}}(t, \epsilon)$. Further, the regions $\mathcal{L}(t, \epsilon) \cap \big(\mathcal{R}^{\mathfrak{a}}(t, \epsilon) \cup \mathcal{R}^{\mathfrak{b}}(t, \epsilon)\big)$ of overlap represent sets in which the outer and inner expansions agree. In particular, we have the matching condition

$$\lim_{\ell(\boldsymbol{x}, t) \to 0\pm} \varphi_0^{\text{out}}(\boldsymbol{x}, t) = \lim_{r \to \pm\infty} \varphi_0^{\text{in}}(r, z, t) \tag{8.8}$$

relating the inner and outer expansions of φ within the overlap region.

[22] We assume that, within the region $\mathcal{L}(\cdot, \epsilon)$, the mapping $\boldsymbol{x} \mapsto (\ell, z)$ is one-to-one. Further details concerning the coordinate system (ℓ, z) can be found in Appendix A.

9 Basic estimates

9.1 Estimates in bulk

Using the outer expansion of φ in the scaled local microforce balance $(6.11)_1$ and neglecting terms of $O(1)$ and smaller in ϵ, we find that φ_0^{out} must satisfy

$$\frac{\partial}{\partial\varphi}\Psi(\varphi)\big|_{\varphi=\varphi_0^{\text{out}}} = 0 \qquad \text{on} \qquad \mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}, \tag{9.1}$$

and hence, be constant in $\mathcal{R}^{\mathfrak{a}}$ and $\mathcal{R}^{\mathfrak{b}}$. By hypothesis, the constant values of φ_0^{out} on either side of $\mathcal{L}$ are required to lie outside of the spinodal. Recalling that Ψ is a double-well potential with minima at $\varphi = \varphi_{\mathfrak{a}}$ and $\varphi = \varphi_{\mathfrak{b}}$, we therefore conclude that

$$\varphi = \begin{cases} \varphi_{\mathfrak{a}} + O(\epsilon) & \text{on} \quad \mathcal{R}^{\mathfrak{a}}, \\ \varphi_{\mathfrak{b}} + O(\epsilon) & \text{on} \quad \mathcal{R}^{\mathfrak{b}}, \end{cases} \tag{9.2}$$

that

$$\frac{\partial}{\partial\varphi}\Psi(\varphi) = o(1) \qquad \text{on} \qquad \mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}, \tag{9.3}$$

that

$$\Psi(\varphi) = o(\epsilon) \qquad \text{on} \qquad \mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}, \tag{9.4}$$

and, further, that

$$\dot{\varphi}, \nabla\varphi, \nabla\dot{\varphi} = O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}. \tag{9.5}$$

Together with the relations (7.1) connecting $W^{\mathfrak{c}}$ to $\hat{W}^{\text{bu}}$ and the expressions $(6.5)_1$ and $(6.5)_2$ for W^{bu} and $\boldsymbol{C}^{\text{bu}}$, the bulk estimates (9.2) for φ yield

$$\left.\begin{aligned} W^{\text{bu}} &= W + O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}, \\ \boldsymbol{C}^{\text{bu}} &= \boldsymbol{C} + O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}. \end{aligned}\right\} \tag{9.6}$$

Similarly, on appeal to (9.2), the expression $(6.5)_4$ for π^{bu} implies that

$$\pi^{\text{bu}} = O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}. \tag{9.7}$$

Further, drawing on the estimates (9.3), (9.4), and $(9.5)_2$, and the expressions (6.7) and (6.8) for the excess fields, we conclude that

$$W^{\text{xs}}, \boldsymbol{C}^{\text{xs}}, \boldsymbol{\xi}^{\text{xs}}, \pi^{\text{xs}}, \boldsymbol{f}^{\text{xs}}, \Delta^{\text{xs}}, c^{\text{xs}}, \jmath^{\text{xs}} = o(1) \quad \text{on} \quad \mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}, \tag{9.8}$$

whereby each of those fields is negligible in bulk.

9.2 Estimates within the transition layer

The estimates obtained in this section rest on a decomposition of the gradient operator, valid within the transition layer, into components associated with the stretched coordinate r normal to $\mathcal{S}$ and the coordinate z on $\mathcal{S}$. Specifically, given a scalar field g, the identity (A.2) and the relation (8.7) between ℓ and r imply that

$$\nabla g = \epsilon^{-1}\acute{g}\mathfrak{n} + \nabla_{\mathcal{S}} g, \tag{9.9}$$

where the value of $\acute{g}$ at (r, z) in $\mathcal{L}(t)$ is determined by

$$\acute{g}(r, z, t) = \frac{\partial}{\partial r} g(r, z, t). \tag{9.10}$$

9.2.1 Partition of energy

The stipulated form of inner expansion for φ and the expressions for $(6.5)_1$, $(6.5)_2$, and $(6.5)_3$ for W^{bu}, $\boldsymbol{C}^{\mathrm{bu}}$, and π^{bu} imply that

$$W^{\mathrm{bu}}, \boldsymbol{C}^{\mathrm{bu}}, \pi^{\mathrm{bu}} = O(1) \qquad \text{on} \qquad \mathcal{L}, \tag{9.11}$$

so that all bulk fields are of $O(1)$ within the layer.

Now, we use the inner expansion of φ and (9.9) to obtain

$$\nabla\varphi = \epsilon^{-1}\acute{\varphi}_0^{\mathrm{in}}\mathfrak{n} + \nabla_{\mathcal{S}}\varphi_0^{\mathrm{in}} + \acute{\varphi}_1^{\mathrm{in}}\mathfrak{n} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}, \tag{9.12}$$

whereby

$$|\nabla\varphi|^2 = \epsilon^{-2}|\acute{\varphi}_0^{\mathrm{in}}|^2 + 2\epsilon^{-1}\acute{\varphi}_0^{\mathrm{in}}\acute{\varphi}_1^{\mathrm{in}} + O(1) \qquad \text{on} \qquad \mathcal{L} \tag{9.13}$$

and

$$|\nabla\varphi| = \epsilon^{-1}|\acute{\varphi}_0^{\mathrm{in}}| + \big(\mathrm{sgn}(\acute{\varphi}_0^{\mathrm{in}})\big)\acute{\varphi}_1^{\mathrm{in}} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{9.14}$$

Together, (9.12) and (9.14) yield

$$\boldsymbol{n} = \frac{\nabla\varphi}{|\nabla\varphi|} = \big(\mathrm{sgn}(\acute{\varphi}_0^{\mathrm{in}})\big)\mathfrak{n} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}, \tag{9.15}$$

so that

$$\boldsymbol{P} = \boldsymbol{1} - \boldsymbol{n}\otimes\boldsymbol{n} = \mathbb{P} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{9.16}$$

Next, appealing to the identity $\dot{r} = -\epsilon^{-1}V_{\mathcal{S}}$, we have

$$\dot{\varphi} = -\epsilon^{-1}V_{\mathcal{S}}\acute{\varphi}_0^{\mathrm{in}} + O(1) \qquad \text{on} \qquad \mathcal{L}, \tag{9.17}$$

which, in combination with (9.12), leads to

$$V = -\frac{\dot{\varphi}}{|\nabla\varphi|} = \big(\mathrm{sgn}(\acute{\varphi}_0^{\mathrm{in}})\big)V_{\mathfrak{S}} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{9.18}$$

Further, from (9.12) and (A.6), we deduce that

$$\begin{aligned}\nabla\nabla\varphi = \epsilon^{-2}\acute{\varphi}_0^{\mathrm{in}}\mathfrak{n}\otimes\mathfrak{n} + \epsilon^{-1}\big((\nabla_{\mathfrak{S}}\acute{\varphi}_0^{\mathrm{in}})\otimes\mathfrak{n} + \mathfrak{n}\otimes(\nabla_{\mathfrak{S}}\acute{\varphi}_0^{\mathrm{in}})\big)\\ - \epsilon^{-1}\acute{\varphi}_0^{\mathrm{in}}\mathbb{L} + \epsilon^{-1}\acute{\varphi}_1^{\mathrm{in}}\mathfrak{n}\otimes\mathfrak{n} + O(1) \quad \text{on} \quad \mathcal{L},\end{aligned} \tag{9.19}$$

which, granted $(3.17)_1$ and (9.16), yields

$$\boldsymbol{L} = -(\nabla\boldsymbol{n})\boldsymbol{P} = \big(\mathrm{sgn}(\acute{\varphi}_0^{\mathrm{in}})\big)\mathbb{L} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{9.20}$$

Now, using the estimates (9.12), (9.19), and (9.17) in the scaled local microforce balance $(6.11)_1$ and recalling that λ is an even function of $\boldsymbol{n}$ (cf. the remark following (4.6)), we find, on neglecting terms of $O(\epsilon^{-1})$ and smaller, that φ_0^{in} must satisfy the differential equation

$$\acute{\Psi}(\varphi_0^{\mathrm{in}}) - \tfrac{1}{2}\acute{\lambda}(\mathfrak{n})|\acute{\varphi}_0^{\mathrm{in}}|^2 = 0 \tag{9.21}$$

on $\mathbb{R}$; moreover, the result (9.2) concerning the outer expansion of φ and the matching condition (8.8) imply that φ_0^{in} must also obey the boundary conditions

$$\lim_{r\to-\infty}\varphi_0^{\mathrm{in}}(r,\cdot,\cdot) = \varphi_{\mathfrak{a}} \qquad \text{and} \qquad \lim_{r\to+\infty}\varphi_0^{\mathrm{in}}(r,\cdot,\cdot) = \varphi_{\mathfrak{b}}. \tag{9.22}$$

Since double-well potential Ψ has equal minima at $\varphi = \varphi_{\mathfrak{a}}$ and $\varphi = \varphi_{\mathfrak{b}}$, the boundary-value problem comprised by (9.21) and (9.22) has a unique solution. Further, that solution satisfies the *energy-partition relation*

$$\Psi(\varphi_0^{\mathrm{in}}) = \tfrac{1}{2}\lambda(\mathfrak{n})|\acute{\varphi}_0^{\mathrm{in}}|^2 \tag{9.23}$$

and is therefore of the form

$$\varphi_0^{\mathrm{in}}(r,z,t) = \phi\big(\eta(r,z,t)\big), \tag{9.24}$$

with ϕ the solution of the boundary value problem

$$\left.\begin{aligned}&\frac{d}{d\eta}\phi(\eta) = \sqrt{2\Psi\big(\phi(\eta)\big)} \qquad \forall\eta\in\mathbb{R},\\ &\lim_{\eta\to-\infty}\phi(\eta) = \varphi_{\mathfrak{a}}, \qquad \lim_{\eta\to+\infty}\phi(\eta) = \varphi_{\mathfrak{b}},\end{aligned}\right\} \tag{9.25}$$

and η determined through

$$\eta(r,z,t) = \frac{r}{\sqrt{\lambda\big(\mathfrak{n}(z,t)\big)}}. \tag{9.26}$$

An important consequence of (9.24)–(9.25) is that

$$\dot{\varphi}_0^{\text{in}} > 0 \tag{9.27}$$

on $\mathbb{R}$, whereby our assumption that $\nabla\varphi$ does not vanish within transition layers is justified—to most significant order in ϵ and the estimates (9.15), (9.18), and (9.20) for $\boldsymbol{n}$, V, and $\boldsymbol{L}$ simplify to

$$\left.\begin{array}{lll} \boldsymbol{n} = \mathbb{n} + O(\epsilon) & \text{on} & \mathcal{L}, \\ V = V_{\mathfrak{S}} + O(\epsilon) & \text{on} & \mathcal{L}, \\ \boldsymbol{L} = \mathbb{L} + O(\epsilon) & \text{on} & \mathcal{L}. \end{array}\right\} \tag{9.28}$$

Next, (9.24), (9.25), and fact that both Ψ and its derivative vanish at $\varphi = \varphi_{\mathfrak{a}}$ and $\varphi = \varphi_{\mathfrak{b}}$ imply that there is a constant $\alpha > 0$ such that

$$\dot{\varphi}_0^{\text{in}}(r, \cdot, \cdot) = O(e^{-\alpha|r|}) \qquad \text{as} \quad |r| \to \infty; \tag{9.29}$$

$\dot{\varphi}_0^{\text{in}}$ is therefore, as a function of r, square integrable on $\mathbb{R}$; in fact, using (9.24) and (9.25), we find that

$$\int_{-\infty}^{+\infty} \sqrt{\lambda(\mathbb{n})}\,|\dot{\varphi}_0^{\text{in}}|^2\,dr = \int_{\varphi_{\mathfrak{a}}}^{\varphi_{\mathfrak{b}}} \sqrt{2\Psi(\varphi)}\,d\varphi. \tag{9.30}$$

9.2.2 Interfacial thickness

Drawing on (9.27) to solve the energy-partition relation (9.23) for $\dot{\varphi}_0^{\text{in}}$, separating variables, integrating over r from $-\epsilon^{-1}h(\epsilon)$ to $\epsilon^{-1}h(\epsilon)$, and appealing to the connection (7.2) between λ and $\hat{w}$, we obtain an estimate

$$h(\epsilon) = \tfrac{1}{2}\epsilon\hat{w}(\mathbb{n})\Big(\int_{\varphi_{\mathfrak{a}}}^{\varphi_{\mathfrak{b}}} \sqrt{2\Psi(\varphi)}\,d\varphi\Big)^{-1}\Big(\int_{\varphi_{\mathfrak{a}}+\epsilon}^{\varphi_{\mathfrak{b}}-\epsilon} \frac{d\varphi}{\sqrt{2\Psi(\varphi)}}\Big) + o(h(\epsilon)), \tag{9.31}$$

showing that the thickness of the transition layer is determined by the orders of the zeros of Ψ and may vary with the orientation $\mathbb{n}$ of $\mathfrak{S}$. On selecting, in particular, the quartic exchange energy $\Psi(\varphi) = \frac{1}{2}\nu(\varphi_{\mathfrak{a}} - \varphi)^2(\varphi_{\mathfrak{b}} - \varphi)^2$, a straightforward integration shows that $h(\epsilon) = O(\epsilon \ln \epsilon)$.

9.2.3 Further results

Bearing in mind $(9.28)_{1,2}$ and using the definition (3.16) of the time derivative following uniformity surfaces, we deduce an estimate

$$\mathring{\boldsymbol{n}} = \dot{\boldsymbol{n}} + (\nabla\boldsymbol{n})(V\boldsymbol{n}) = \mathring{\mathbb{n}} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L} \tag{9.32}$$

that relates the rate at which $\boldsymbol{n}$ changes following uniformity surfaces to the normal time derivative $\mathring{m}$ of the orientation m of $\mathfrak{S}$. Further, by the estimate (9.14) for $|\nabla\varphi|$, we have that

$$\overset{\circ}{\overline{\ln|\nabla\varphi|}} = O(1) \qquad \text{on} \qquad \mathcal{L}. \tag{9.33}$$

Next, recalling the expression $(6.8)_2$ for $\jmath^{\mathrm{xs}}$, the energy-partition relation (9.23) implies, together with the estimates (9.13) and $(9.28)_1$ for $|\nabla\varphi|^2$ and $\boldsymbol{n}$, that

$$\epsilon\jmath^{\mathrm{xs}} = \epsilon^{-1}\Psi(\varphi) - \tfrac{1}{2}\epsilon|\nabla\varphi|^2\lambda(\boldsymbol{n}) = O(1) \qquad \text{on} \qquad \mathcal{L}, \tag{9.34}$$

so that, by appealing to (9.13), $(9.28)_1$, and the expression $(6.7)_1$ for W^{xs}, we obtain

$$\epsilon W^{\mathrm{xs}} = \epsilon^{-1}\big(\sqrt{\lambda(m)}|\acute{\varphi}_0^{\mathrm{in}}|^2\big)\sqrt{\lambda(m)} + O(1) \quad \text{on} \quad \mathcal{L}. \tag{9.35}$$

Thus, the connection $(7.2)_1$ between $\hat{w}$ and λ allows the estimate

$$\epsilon W^{\mathrm{xs}} = \epsilon^{-1}\varsigma w + O(1) \qquad \text{on} \qquad \mathcal{L}, \tag{9.36}$$

with ς defined by

$$\varsigma = \sigma^{-1}\sqrt{\lambda(m)}|\acute{\varphi}_0^{\mathrm{in}}|^2. \tag{9.37}$$

Similarly, drawing on the expressions $(6.7)_2$, $(6.8)_1$, $(6.7)_5$, and $(6.7)_6$ for $\boldsymbol{C}^{\mathrm{xs}}$, $\boldsymbol{c}^{\mathrm{xs}}$, $\boldsymbol{f}^{\mathrm{xs}}$, and Δ^{xs}, the relations (7.2) connecting $\hat{w}$, $\hat{\mathbb{c}}$, and $\hat{b}$ with λ and $\tilde{\beta}$, and the equations (2.24) and (2.19) determining $\mathbb{f}$ and δ, we extract the estimates

$$\left.\begin{aligned} \epsilon\boldsymbol{C}^{\mathrm{xs}} &= \epsilon^{-1}\varsigma\mathbb{C} + O(1) \qquad \text{on} \qquad \mathcal{L}, \\ \epsilon\boldsymbol{c}^{\mathrm{xs}} &= \epsilon^{-1}\varsigma\mathbb{c} + O(1) \qquad \text{on} \qquad \mathcal{L}, \\ \epsilon\boldsymbol{f}^{\mathrm{xs}} &= \epsilon^{-1}\varsigma\mathbb{f} + O(1) \qquad \text{on} \qquad \mathcal{L}, \\ \epsilon\Delta^{\mathrm{xs}} &= \epsilon^{-1}\varsigma\delta + O(1) \qquad \text{on} \qquad \mathcal{L}. \end{aligned}\right\} \tag{9.38}$$

Finally, for later reference, we note that ς as defined in (9.37) obeys the relation

$$\epsilon^{-1}\int_{-h(\epsilon)}^{h(\epsilon)} \varsigma\, d(\epsilon r) = 1 + o(1), \tag{9.39}$$

which follows from the definition (7.3) of σ, the limit $(8.1)_2$ whereby the interfacial thickness h approaches zero more slowly than ϵ, the far-field estimate (9.29) for $\acute{\varphi}_0^{\mathrm{in}}$, and the integral relation (9.30).

10 Asymptotic limit of the integral statements of configurational force balance and dissipation imbalance for the phase-field theory

Our purpose in this section is to demonstrate the consonance of the integral laws enforcing configurational force balance and dissipation imbalance in the theories considered here. Toward this, we focus attention on a subregion $\mathcal{P}$ of $\mathcal{B}$, with outward unit normal $\boldsymbol{\nu}$, chosen so that, at each instant t during the course of some time interval, portions of the regions $\mathcal{R}^{\mathrm{a}}(t,\epsilon)$ and $\mathcal{R}^{\mathrm{b}}(t,\epsilon)$ are contained in $\mathcal{P}$ and each uniformity surface within $\mathcal{L}(t,\epsilon)$ intersects $\partial\mathcal{P}$ transversely. We write $\mathfrak{Q}(t)=\mathcal{P}\cap\mathcal{G}(t)$ for the portion of $\mathcal{G}$ within $\mathcal{P}$ at time t.

Granted (7.1) and (7.2), we find that

i. the terms comprising the scaled configurational force balance $(6.10)_2$ of the phase-field theory admits the estimates

$$\left.\begin{aligned}
&\int_{\partial\mathcal{P}} \mathbf{C}^{\mathrm{bu}}\boldsymbol{\nu}\,da=\int_{\partial\mathcal{P}}\mathbf{C}\boldsymbol{\nu}\,da+o(1),\\
&\epsilon\int_{\partial\mathcal{P}} \mathbf{C}^{\mathrm{xs}}\boldsymbol{\nu}\,da=\int_{\partial\mathfrak{Q}}\mathbb{C}\mathbb{m}\,dl+o(1),\\
&\epsilon\int_{\mathcal{P}} \mathbf{f}^{\mathrm{xs}}\,dv=\int_{\mathfrak{Q}}\mathbb{f}\,da+o(1),
\end{aligned}\right\}\tag{10.1}$$

and hence, as the thickness of the layer vanishes, that balance corresponds to the configurational force balance (2.7) of the sharp-interface theory;[23]

ii. the terms comprising the scaled dissipation imbalance $(6.10)_3$ of the phase-field theory admit the estimates

$$\left.\begin{aligned}
&\epsilon\int_{\partial\mathcal{P}} \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\boldsymbol{\varphi}}\boldsymbol{\nu})\,da=\int_{\partial\mathfrak{Q}}(\mathbb{C}\mathbb{m}\cdot(V_{\mathcal{G}}\mathbb{m})+wU_{\partial\mathfrak{Q}})\,dl+o(1),\\
&\int_{\mathcal{P}} W^{\mathrm{bu}}\,dv=\int_{\mathcal{P}} W\,dv+o(1),\\
&\epsilon\int_{\mathcal{P}} W^{\mathrm{xs}}\,dv=\int_{\mathfrak{Q}} w\,da+o(1),
\end{aligned}\right\}\tag{10.2}$$

and hence, as the thickness of the layer vanishes, that imbalance corresponds to the dissipation imbalance (2.8) of the sharp-interface theory.

[23] We recall that the bulk configurational force $\boldsymbol{f}$ of the sharp-interface theory vanishes (cf. (2.21)).

We consider only the estimates (10.2) associated with the dissipation imbalance $(6.10)_3$, since to establish these we will call upon all ingredients necessary to verify (10.1). First, inasmuch as the area of $\partial\mathcal{P}\cap\mathcal{L}(t;\epsilon)$ and the volume of $\mathcal{P}\cap\mathcal{L}(t;\epsilon)$ are bounded by $h(\epsilon)$ at each t in the time interval under consideration, we see that

$$\int\limits_{\partial\mathcal{P}} g\,da = \int\limits_{\partial\mathcal{P}\setminus\mathcal{L}} g\,da + o(1) \qquad \text{and} \qquad \int\limits_{\mathcal{P}} g\,dv = \int\limits_{\mathcal{P}\setminus\mathcal{L}} g\,dv + o(1) \tag{10.3}$$

for any field g that is of $O(1)$ in ϵ on $\mathcal{P}$. Hence, $(10.2)_1$, $(10.2)_3$, and $(10.2)_4$ follow directly from the results $(9.11)_1$ showing that $W^{\rm bu}$ is of $O(1)$ on $\mathcal{L}$ and $(9.6)_1$ determining the specific form for the expansion of $W^{\rm bu}$ on $\mathcal{R}^{\rm a}\cup\mathcal{R}^{\rm b}$.

Next, we attend to $(10.2)_2$. Since each uniformity surface crosses $\partial\mathcal{P}$ transversely, $\boldsymbol{n}$ and $\boldsymbol{\nu}$ satisfy $0\le|\boldsymbol{n}\cdot\boldsymbol{\nu}|<1$ on $\partial\mathcal{P}\cap\mathcal{L}$. Hence, the restriction to $\partial\mathcal{P}\cap\mathcal{L}$ of the outward normal $\boldsymbol{\nu}$ to $\partial\mathcal{P}$ admits the representation

$$\boldsymbol{\nu} = (\boldsymbol{n}\cdot\boldsymbol{\nu})\boldsymbol{n} + (\boldsymbol{m}\cdot\boldsymbol{\nu})\boldsymbol{m}, \tag{10.4}$$

where

$$\boldsymbol{m} = \frac{\boldsymbol{P}\boldsymbol{\nu}}{\sqrt{1-|\boldsymbol{n}\cdot\boldsymbol{\nu}|^2}} \tag{10.5}$$

defines a unit vector field tangent to uniformity surfaces and directed outward from $\mathcal{P}\cap\mathcal{L}$. Thus, given a vector field $\boldsymbol{g}$, we have the identity

$$\int\limits_{\mathcal{P}} \boldsymbol{g}\cdot\boldsymbol{\nu}\,da = \int\limits_{\partial\mathcal{P}\setminus(\partial\mathcal{P}\cap\mathcal{L})} \boldsymbol{g}\cdot\boldsymbol{\nu}\,da + \int\limits_{\partial\mathcal{P}\cap\mathcal{L}} \big((\boldsymbol{n}\otimes\boldsymbol{n})\boldsymbol{g}\big)\cdot\boldsymbol{\nu}\,da + \int\limits_{\partial\mathcal{P}\cap\mathcal{L}} \boldsymbol{g}\cdot\boldsymbol{m}\,dA, \tag{10.6}$$

where the measure

$$dA = \boldsymbol{m}\cdot\boldsymbol{\nu}\,da \tag{10.7}$$

determines the projection, onto a plane perpendicular to uniformity surfaces, of the area on $\partial\mathcal{P}\cap\mathcal{L}$.

In particular, bearing in mind the identities

$$\boldsymbol{\xi}^{\rm xs}\cdot(\dot{\boldsymbol{\varphi}}\boldsymbol{n}) = -(W^{\rm xs}-\jmath^{\rm xs})V \qquad \text{and} \qquad \boldsymbol{\xi}^{\rm xs}\cdot(\dot{\boldsymbol{\varphi}}\boldsymbol{m}) = \boldsymbol{C}^{\rm xs}\boldsymbol{m}\cdot(V\boldsymbol{n}), \tag{10.8}$$

the first of which follows from the expression $(6.7)_3$ for $\boldsymbol{\xi}^{\rm xs}$ and the second of which issues from $(6.7)_3$, the definition (10.5) of $\boldsymbol{m}$, and the expression $(6.7)_3$ for $\boldsymbol{C}^{\rm xs}$, the identity (10.6) allows us to write the left-hand-side of $(10.2)_2$ as

$$\int\limits_{\partial\mathcal{P}} \boldsymbol{\xi}^{\rm xs}\cdot(\dot{\boldsymbol{\varphi}}\boldsymbol{\nu})\,da = \int\limits_{\partial\mathcal{P}\setminus(\mathcal{P}\cap\mathcal{L})} \boldsymbol{\xi}^{\rm xs}\cdot(\dot{\boldsymbol{\varphi}}\boldsymbol{\nu})\,da + \int\limits_{\partial\mathcal{P}\cap\mathcal{L}} \big(\boldsymbol{C}^{\rm xs}\boldsymbol{m}\cdot(V\boldsymbol{n}) + (W^{\rm xs}-\jmath^{\rm xs})U\big)\,dA, \tag{10.9}$$

where

$$U = -\frac{(\boldsymbol{n}\cdot\boldsymbol{\nu})V}{\sqrt{1-|\boldsymbol{n}\cdot\boldsymbol{\nu}|^2}} \tag{10.10}$$

represents the rate at which uniformity surface area enters or leaves $\mathcal{P}$ through $\partial\mathcal{P}\cap\mathcal{L}$ as $\mathcal{L}$ evolves.

An immediate consequence of the results $(9.5)_1$ and $(9.8)_3$ concerning the orders of $\dot{\varphi}$ and $\boldsymbol{\xi}^{\mathrm{xs}}$ is the estimate

$$\int\limits_{\partial\mathcal{P}\setminus(\mathcal{P}\cap\mathcal{L})} \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\,da = o(1). \tag{10.11}$$

Hence, it remains to show that the second term on the right-hand-side of (10.9) actually yields the right-hand-side of $(10.2)_2$. Toward this, we first record the estimates

$$\boldsymbol{m} = \mathbb{m} + O(\epsilon) \qquad \text{and} \qquad U = U_{\partial\Omega} + O(\epsilon), \tag{10.12}$$

that follow from the definitions (10.5) and (10.10) of $\boldsymbol{m}$ and U, the estimates $(9.28)_1$, $(9.28)_2$, and (9.16) for $\boldsymbol{n}$, V, and $\boldsymbol{P}$, and the definitions (2.5) and (2.6) for $\boldsymbol{m}$ and $U_{\partial\Omega}$. Proceeding, we observe that, given a field g independent of the coordinate r normal to $\mathfrak{S}$ that satisfies

$$g = \epsilon^{-1}\varsigma g + O(1) \quad \text{on} \quad \mathcal{L}, \tag{10.13}$$

the identity (9.39) for ς implies that

$$\int\limits_{\partial\mathcal{P}} g\,dA = \int\limits_{\partial\Omega}\Big(\int\limits_{-h(\epsilon)}^{h(\epsilon)} g\,d(\epsilon r)\Big)\,dl = \int\limits_{\partial\Omega} g\,dl + o(1). \tag{10.14}$$

Thus, along with $(9.28)_1$, $(9.28)_2$, and (10.12), the estimates $(9.38)_1$, (9.36), and (9.34) for $\boldsymbol{C}^{\mathrm{xs}}$, W^{xs}, and $\jmath^{\mathrm{xs}}$ yield

$$\left.\begin{aligned} &\epsilon\int\limits_{\partial\mathcal{P}\cap\mathcal{L}} \boldsymbol{C}^{\mathrm{xs}}\boldsymbol{m}\cdot(V\boldsymbol{n})\,dA = \int\limits_{\partial\Omega} \mathbb{C}\mathbb{m}\cdot(V_{\mathfrak{S}}\mathbb{m})\,dl + o(1),\\ &\epsilon\int\limits_{\partial\mathcal{P}\cap\mathcal{L}} W^{\mathrm{xs}}U\,dA = \int\limits_{\partial\Omega} wU_{\partial\Omega}\,dl + o(1),\\ &\epsilon\int\limits_{\partial\mathcal{P}\cap\mathcal{L}} \jmath^{\mathrm{xs}}U\,dA = o(1), \end{aligned}\right\} \tag{10.15}$$

whereby $(10.2)_2$ holds.

Finally, bearing in mind the estimates $(9.8)_1$ and (9.36) for W^{xs}, $(10.2)_5$ follows from the identity

$$\int_{\mathcal{P}} g\,dv = \int_{\Omega}\Big(\int_{-h(\epsilon)}^{h(\epsilon)} g\,d(\epsilon r)\Big)\,da = \int_{\Omega} g\,da + o(1), \tag{10.16}$$

which, by virtue of (9.39), holds for any field g independent of the coordinate r normal to $\mathfrak{S}$ that satisfies (10.13) and is of $o(1)$ on $\mathcal{R}^{\mathrm{a}} \cap \mathcal{R}^{\mathrm{b}}$.

11 Asymptotic limit of the local statements for configurational force balance and dissipation balance of the phase-field theory

In this section we aim to demonstrate the consonance of the local laws expressing configurational force balance and dissipation balance in the theories considered here. Granted (7.1) and (7.2), we find that

i. on $\mathcal{R}^{\mathrm{a}} \cup \mathcal{R}^{\mathrm{b}}$ the terms comprising scaled field equation $(6.11)_2$ imposing configurational force balance for the phase-field theory admit the estimates

$$\operatorname{div} \boldsymbol{C}^{\mathrm{bu}} = \operatorname{div} \boldsymbol{C} + o(1), \quad \epsilon \operatorname{div} \boldsymbol{C}^{\mathrm{xs}} = o(1), \quad \epsilon \boldsymbol{f}^{\mathrm{xs}} = o(1), \tag{11.1}$$

so that, as the thickness of the layer vanishes, that balance yields the bulk configurational force balance (2.9) of the sharp-interface theory; further, the terms of $(6.11)_2$ obey the relations

$$\left.\begin{aligned} &\int_{-h(\epsilon)}^{h(\epsilon)} \operatorname{div} \boldsymbol{C}^{\mathrm{bu}}\, d(\epsilon r) = [\![\boldsymbol{C}\boldsymbol{n}]\!] + o(1), \\ &\epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \operatorname{div} \boldsymbol{C}^{\mathrm{xs}}\, d(\epsilon r) = \operatorname{div}_{\mathfrak{S}} \mathbb{C} + o(1), \\ &\epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{f}^{\mathrm{xs}} d(\epsilon r) = \mathbb{f} + o(1), \end{aligned}\right\} \tag{11.2}$$

and the integral across the layer of the scaled field equation imposing configurational force balance for the phase-field theory equation yields, as the thickness of that layer vanishes, the interfacial configurational force balance (2.10) of the sharp-interface theory;

ii. on $\mathcal{R}^a \cup \mathcal{R}^b$ the terms comprising the scaled dissipation balance $(6.11)_3$ of the phase-field theory admit the estimates

$$\dot{W}^{\mathrm{bu}} = \dot{W} + o(1) \tag{11.3}$$

and

$$\epsilon \boldsymbol{\xi}^{\mathrm{xs}} \cdot (\nabla \dot{\varphi}), \pi^{\mathrm{bu}} \dot{\varphi}, \epsilon \pi^{\mathrm{xs}} \dot{\varphi}, \epsilon \dot{W}^{\mathrm{xs}}, \epsilon \Delta^{\mathrm{xs}} = o(1), \tag{11.4}$$

so that, as the thickness of the layer vanishes, that balance yields the bulk dissipation balance of the sharp-interface theory (cf. (2.11) and (2.16)); further, the terms comprising the alternate form (6.12) of the scaled dissipation balance obey the relations

$$\left.\begin{aligned}
&\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{c}^{\mathrm{xs}} \cdot \hat{\boldsymbol{n}}\, d(\epsilon r) = \mathring{\boldsymbol{c}} \cdot \mathring{\boldsymbol{n}} + o(1), \\
&\epsilon \int_{-h(\epsilon)}^{h(\epsilon)} (\boldsymbol{f}^{\mathrm{xs}} \cdot \boldsymbol{n}) V\, d(\epsilon r) = (\mathring{f} \cdot \mathring{n}) V_{\mathfrak{S}} + o(1), \\
&\epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \left(\hat{W}^{\mathrm{xs}} - \left(W^{\mathrm{xs}} - \jmath^{\mathrm{xs}}\right) \overset{\diamond}{\overline{\ln |\nabla \varphi|}}\right) d(\epsilon r) = \mathring{w} + o(1), \\
&\epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \Delta^{\mathrm{xs}}\, d(\epsilon r) = \delta + o(1),
\end{aligned}\right\} \tag{11.5}$$

and the integral across the layer of that balance yields, as the thickness of that layer vanishes, the interfacial dissipation balance (2.18) of the sharp-interface theory.

We establish only the estimates (11.1) and (11.2) associated with the configurational force balance $(6.11)_2$. The remaining estimates, (11.3), (11.4), and (11.5), follow similarly.

To begin, we observe that the bulk results (11.1) are direct consequences of the estimates $(9.6)_2$, $(9.8)_2$, and $(9.8)_5$, for $\boldsymbol{C}^{\mathrm{bu}}$, $\boldsymbol{C}^{\mathrm{xs}}$, and $\boldsymbol{f}^{\mathrm{xs}}$ on $\mathcal{R}^a \cup \mathcal{R}^b$.

Next, we consider the results (11.2). First, bearing in mind $(9.6)_2$, whereby $\boldsymbol{C}^{\mathrm{bu}}$ is of $O(1)$ on $\mathcal{L}$, we obtain

$$\operatorname{div} \boldsymbol{C}^{\mathrm{bu}} = \epsilon^{-1} \acute{\boldsymbol{C}}^{\mathrm{bu}} \mathring{n} + O(1) \tag{11.6}$$

on $\mathcal{L}$. Thus, $(11.2)_1$ follows from the estimate (9.16) for $\boldsymbol{P}$ on $\mathcal{L}$, the estimate $(9.6)_3$ for $\boldsymbol{C}^{\mathrm{bu}}$ on $\mathcal{R}^a \cup \mathcal{R}^b$, and the matching condition (8.8).

Next, in light of the identity

$$\operatorname{div} \boldsymbol{C}^{\mathrm{xs}} = \boldsymbol{P} \operatorname{div} \boldsymbol{C}^{\mathrm{xs}} + \big(\boldsymbol{C}^{\mathrm{xs}} \cdot \boldsymbol{L} + \operatorname{div} \boldsymbol{c}^{\mathrm{xs}} + \operatorname{div}(j^{\mathrm{xs}} \boldsymbol{n})\big)\boldsymbol{n} \tag{11.7}$$

and the estimate $(9.28)_1$ for $\boldsymbol{n}$, we observe that to verify $(11.2)_2$ it is sufficient to establish

$$\left.\begin{aligned} \epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{P} \operatorname{div} \boldsymbol{C}^{\mathrm{xs}}\, d(\epsilon r) &= \mathbb{P} \operatorname{div}_{\mathfrak{S}} \mathbb{C} + o(1), \\ \epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{C}^{\mathrm{xs}} \cdot \boldsymbol{L}\, d(\epsilon r) &= \mathbb{C} \cdot \mathbb{L} + o(1), \\ \epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \operatorname{div} \boldsymbol{c}^{\mathrm{xs}}\, d(\epsilon r) &= \operatorname{div}_{\mathfrak{S}} \mathbb{c} + o(1), \end{aligned}\right\} \tag{11.8}$$

and

$$\epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \operatorname{div}(j^{\mathrm{xs}} \boldsymbol{n})\, d(\epsilon r) = o(1). \tag{11.9}$$

Now, the estimates (9.16), $(9.28)_3$, $(9.38)_2$, and $(9.38)_3$ for $\boldsymbol{P}$, $\boldsymbol{L}$, $\boldsymbol{C}^{\mathrm{xs}}$, and $\boldsymbol{c}^{\mathrm{xs}}$, imply that

$$\left.\begin{aligned} \epsilon \operatorname{div} \boldsymbol{C}^{\mathrm{xs}} &= \epsilon^{-1} \operatorname{div}_{\mathfrak{S}} (\varsigma \mathbb{C}) + O(1) \\ \epsilon \boldsymbol{C}^{\mathrm{xs}} \cdot \boldsymbol{L} &= \epsilon^{-1} \varsigma \mathbb{C} \cdot \mathbb{L} + O(1), \\ \epsilon \operatorname{div} \boldsymbol{c}^{\mathrm{xs}} &= \epsilon^{-1} \operatorname{div}_{\mathfrak{S}} (\varsigma \mathbb{c}) + O(1), \end{aligned}\right\} \tag{11.10}$$

whereby (11.8) follow from the integral identity (9.39) involving ς. Next, since

$$\epsilon \operatorname{div}(j^{\mathrm{xs}} \boldsymbol{n}) = (\hat{j}^{\mathrm{xs}}) \boldsymbol{m} \cdot \boldsymbol{n} + \epsilon (\nabla_{\mathfrak{S}} j^{\mathrm{xs}}) \cdot \boldsymbol{n} = \hat{j}^{\mathrm{xs}} + O(1) \tag{11.11}$$

on $\mathcal{L}$, and

$$\epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \operatorname{div}(j^{\mathrm{xs}} \boldsymbol{n})\, d(\epsilon r) = \epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \hat{j}^{\mathrm{xs}}\, dr + o(1) \tag{11.12}$$

(11.9) holds provided that, as $\epsilon \to 0$,

$$\epsilon j^{\mathrm{xs}}(\pm \epsilon^{-1} h(\epsilon), \cdot, \cdot) = o(1). \tag{11.13}$$

To demonstrate (11.13), we expand $\jmath^{\mathrm{xs}}$ to yield

$$\epsilon^2\jmath^{\mathrm{xs}} = \Psi(\varphi_0^{\mathrm{in}}) + \epsilon\Psi'(\varphi_0^{\mathrm{in}})\varphi_1^{\mathrm{in}} - \acute{\varphi}_0^{\mathrm{in}}(\acute{\varphi}_0^{\mathrm{in}} + 2\epsilon\acute{\varphi}_1^{\mathrm{in}})\big(\tfrac{1}{2}\lambda(\mathbb{m}) + O(\epsilon)\big) + O(\epsilon^2) \tag{11.14}$$

on $\mathcal{L}$, whereby, on recalling the assumption $(8.1)_2$, the requirements

$$\frac{\partial}{\partial\varphi}\Psi(\varphi)\big|_{\varphi=\varphi_{\mathfrak{a}}} = \frac{\partial}{\partial\varphi}\Psi(\varphi)\big|_{\varphi=\varphi_{\mathfrak{b}}} = 0, \tag{11.15}$$

and the far-field bound (9.29) on $\acute{\varphi}_0^{\mathrm{in}}$, (11.13) follows.

Finally, the estimate $(9.38)_3$ for $\boldsymbol{f}^{\mathrm{xs}}$ and the integral identity (9.39) involving ς imply $(11.2)_3$.

12 Asymptotic limit of a power identity for the phase-field theory

Here, we derive a power identity relevant to the phase-field theory and then demonstrate the correspondence between that identity and the power identity (2.15) of the sharp-interface theory.

A simple consequence of the results $(10.2)_1$, $(10.2)_2$, and $(10.15)_3$ established in determining the asymptotic limit of the scaled dissipation imbalance $(6.10)_3$ of the phase-field theory is that, as $\epsilon \to 0$,

$$\epsilon\int\limits_{\partial\mathcal{P}} \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\,da - \epsilon\int\limits_{\partial\mathcal{P}\cap\mathcal{L}} W^{\mathrm{xs}}U\,dA = \int\limits_{\partial\Omega} \mathbb{c}\cdot(V_{\mathfrak{S}}\mathbb{m})\,dl + o(1), \tag{12.1}$$

whereby the surfeit of the total power expended on $\partial\mathcal{P}$ (by the tractions associated with the microstress $\boldsymbol{\xi}^{\mathrm{xs}}$) over the efflux of excess energy W^{xs} through $\partial\mathcal{P}\cap\mathcal{L}$ corresponds asymptotically to the net power expended on $\partial\Omega$ (by the tractions associated with the normal component $\mathbb{c} = \mathbb{C}^{\mathrm{T}}\mathbb{n}$ of the interfacial configurational stress). Thus, bearing in mind the form of the power identity (2.15) for the sharp-interface theory, we develop a power identity for the left-hand-side of (12.1).

Toward this identity, we first apply the divergence theorem to the left-hand-side of (12.1) and decompose the resulting integral over $\mathcal{P}$ into components over $\mathcal{P}\setminus\mathcal{L}$ and $\mathcal{P}\cap\mathcal{L}$. In the integral over $\mathcal{P}\setminus\mathcal{L}$, we expand the integrand and use the scaled local microforce balance $(6.11)_1$ to give

$$\epsilon\int\limits_{\mathcal{P}\setminus\mathcal{L}} \mathrm{div}(\dot{\varphi}\boldsymbol{\xi}^{\mathrm{xs}})\,dv = \int\limits_{\mathcal{P}\setminus\mathcal{L}} \big(\epsilon\boldsymbol{\xi}^{\mathrm{xs}}\cdot\nabla\dot{\varphi} - (\pi^{\mathrm{bu}} + \epsilon\pi^{\mathrm{xs}})\dot{\varphi}\big)\,dv, \tag{12.2}$$

while we use the expression $(6.7)_3$ for $\boldsymbol{\xi}^{\mathrm{xs}}$ and the dimensionless counterpart of $(3.17)_2$ in the integral over $\mathcal{P}\cap\mathcal{L}$ to obtain

$$\epsilon\int\limits_{\mathcal{P}\cap\mathcal{L}}\operatorname{div}(\dot\varphi\boldsymbol{\xi}^{\mathrm{xs}})\,dv=-\epsilon\int\limits_{\mathcal{P}\cap\mathcal{L}}\big(\varpi+\operatorname{div}(W^{\mathrm{xs}}V\boldsymbol{n})\big)\,dv, \tag{12.3}$$

with ϖ given by

$$\varpi=(\epsilon^{-1}\nabla W^{\mathrm{bu}}+\boldsymbol{f}^{\mathrm{xs}})\cdot(V\boldsymbol{n})+W^{\mathrm{xs}}KV+\boldsymbol{c}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{n}}+\jmath^{\mathrm{xs}}\overset{\diamond}{\ln|\nabla\varphi|}. \tag{12.4}$$

Thus, consolidating (12.2) and (12.3), and using the result

$$\int\limits_{\mathcal{P}\cap\mathcal{L}}\operatorname{div}(W^{\mathrm{xs}}V\boldsymbol{n})\,dv=-\int\limits_{\partial\mathcal{P}\cap\mathcal{L}}W^{\mathrm{xs}}U\,dA+\int\limits_{\mathcal{P}\cap\partial\mathcal{L}}W^{\mathrm{xs}}V\boldsymbol{n}\cdot\boldsymbol{\nu}\,da, \tag{12.5}$$

which follows from the divergence theorem and the definitions (10.7) and (10.10) of dA and U, we arrive at a power identity,

$$\begin{aligned}\epsilon\int\limits_{\partial\mathcal{P}}\boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot\varphi\boldsymbol{\nu})\,da-\epsilon\int\limits_{\partial\mathcal{P}\cap\mathcal{L}}W^{\mathrm{xs}}U\,dA&\\ =\int\limits_{\mathcal{P}\setminus\mathcal{L}}\big(\epsilon\boldsymbol{\xi}^{\mathrm{xs}}\cdot(\nabla\dot\varphi)-(\pi^{\mathrm{bu}}+\epsilon\pi^{\mathrm{xs}})\dot\varphi\big)\,dv&\\ -\epsilon\int\limits_{\mathcal{P}\cap\mathcal{L}}\varpi\,dv-\epsilon\int\limits_{\mathcal{P}\cap\partial\mathcal{L}}W^{\mathrm{xs}}(V\boldsymbol{n})\cdot\boldsymbol{\nu}\,da,&\end{aligned} \tag{12.6}$$

for the phase-field theory.

Now, from $(10.2)_4$ and (12.1), the left-hand-side of the power identity (12.6) differs, in the limit of decreasing transition layer thickness, from the left-hand-side of the power identity (2.15) of the sharp-interface theory by terms of at most $o(1)$ in ϵ. Further, granted that the constitutive equations of the sharp-interface theory are given by (7.1) and (7.2), we find that

i. the term of (12.6) involving integration over $\mathcal{P}\cap\mathcal{L}$ obeys

$$\epsilon\int\limits_{\mathcal{P}\cap\mathcal{L}}\varpi\,dv=\int\limits_{\mathfrak{Q}}\big((\llbracket W\rrbracket+\mathfrak{f}\cdot\mathfrak{m})V_{\mathfrak{S}}+wK_{\mathfrak{S}}V_{\mathfrak{S}}+\mathfrak{c}\cdot\mathring{\mathfrak{m}}\big)\,da+o(1) \tag{12.7}$$

and, hence, as the thickness of the layer vanishes, that term reckons the power expended on $\mathfrak{Q}$ by: the exchange of material between phases due to the action of $\llbracket W\rrbracket+\mathfrak{f}\cdot\mathfrak{m}$ over $V_{\mathfrak{S}}$, altering the interfacial area through the action of $wK_{\mathfrak{S}}$ over $V_{\mathfrak{S}}$, and altering the orientation of the interface resulting from the action of the configurational shear $\mathfrak{c}$ over $\mathring{\mathfrak{m}}$;[24]

[24] This delineation of the manner in which power is expended by the evolution of $\mathfrak{Q}$ through $\mathcal{P}$ is due to GURTIN [6].

ii. the terms of (12.6) involving integration over $\mathcal{P} \setminus \mathcal{L}$ and over $\mathcal{P} \cap \partial\mathcal{L}$ obey

$$\left.\begin{aligned} &\int\limits_{\mathcal{P}\setminus\mathcal{L}} \left(\epsilon \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\nabla\dot{\varphi}) - (\pi^{\mathrm{bu}} + \epsilon\pi^{\mathrm{xs}})\dot{\varphi}\right) dv = o(1), \\ &\epsilon \int\limits_{\mathcal{P}\cap\partial\mathcal{L}} W^{\mathrm{xs}}(V\boldsymbol{n})\cdot\boldsymbol{\nu}\, da = o(1), \end{aligned}\right\} \tag{12.8}$$

and, hence, as the thickness of the layer vanishes, those terms contribute nothing to the power.

To establish (12.7), we actually show that

$$\left.\begin{aligned} &\int\limits_{\mathcal{P}\cap\mathcal{L}} (\nabla W^{\mathrm{bu}})\cdot\boldsymbol{n}\, dv = \int\limits_{\mathfrak{Q}} [\![W]\!] V_{\mathfrak{S}}\, da + o(1), \\ &\epsilon \int\limits_{\mathcal{P}\cap\mathcal{L}} (\boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n}) V\, dv = \int\limits_{\mathfrak{Q}} (\mathfrak{f}\cdot\mathfrak{n}) V_{\mathfrak{S}}\, da + o(1), \\ &\epsilon \int\limits_{\mathcal{P}\cap\mathcal{L}} W^{\mathrm{xs}} K V\, dA = \int\limits_{\mathfrak{Q}} w K_{\mathfrak{S}} V_{\mathfrak{S}}\, da + o(1), \\ &\epsilon \int\limits_{\mathcal{P}\cap\mathcal{L}} \boldsymbol{c}^{\mathrm{xs}}\cdot\hat{\boldsymbol{n}}\, dv = \int\limits_{\mathfrak{Q}} \mathfrak{c}\cdot\mathring{\mathfrak{n}}\, da + o(1), \end{aligned}\right\} \tag{12.9}$$

and that

$$\epsilon \int\limits_{\mathcal{P}\cap\mathcal{L}} \jmath^{\mathrm{xs}} \overset{\circ}{\overline{\ln|\nabla\varphi|}}\, dv = o(1). \tag{12.10}$$

Toward (12.9), we first record the identity

$$\int\limits_{\mathcal{P}\cap\mathcal{L}} g\, dv = \int\limits_{\mathfrak{Q}} \Big(\int\limits_{-h(\epsilon)}^{h(\epsilon)} g\, d(\epsilon r) \Big)\, da, \tag{12.11}$$

whereby integration over $\mathcal{P} \cap \mathcal{L}$ is achieved by an integration across the layer in the direction normal to $\mathfrak{S}$ followed by integration on $\mathfrak{S}$. Bearing in mind (12.11), the expansion

$$(\nabla W^{\mathrm{bu}})\cdot\boldsymbol{n} = \epsilon^{-1}\dot{W}^{\mathrm{bu}} + O(1), \tag{12.12}$$

the matching condition (8.8), and the estimate $(9.6)_1$ for W^{bu} on $\mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}$, we obtain $(12.9)_1$. Similarly, $(12.9)_{2\text{–}4}$ follow from (12.11), the estimates $(9.28)_1$,

$(9.28)_2$, $(9.28)_3$, (9.32), (9.36), $(9.38)_1$, $(9.38)_3$, and $(9.38)_4$ for $\boldsymbol{n}$, V, $\boldsymbol{L}$, $\mathring{\boldsymbol{n}}$, $W^{\rm xs}$, $c^{\rm xs}$, and $f^{\rm xs}$, and the integral identity (9.30) involving ς. Next, on recalling that the volume of $\mathcal{P}\cap\mathcal{L}$ is bounded by $h(\epsilon)$ (cf. the argument used to justify (10.3)), the results (12.10) follow from the estimate (9.34) for $\jmath^{\rm xs}$ in tandem with the result (9.33), whereby the time rate, following uniformity surfaces, of $\ln|\nabla\varphi|$ is of $O(1)$ on $\mathcal{L}$.

Next, to verify $(12.8)_1$, we employ the estimates $(9.8)_3$, (9.7), $(9.8)_4$, $(9.5)_3$, and $(9.5)_1$ for $\boldsymbol{\xi}^{\rm xs}$, $\pi^{\rm bu}$, $\pi^{\rm xs}$, $\nabla\dot\varphi$, and $\dot\varphi$ on $\mathcal{R}^{\rm a}\cup\mathcal{R}^{\rm b}$, whereby, as $\epsilon\to 0$,

$$\epsilon\int\limits_{\mathcal{P}\setminus\mathcal{L}}\boldsymbol{\xi}^{\rm xs}\cdot(\nabla\dot\varphi)\,dv=o(1),\quad\int\limits_{\mathcal{P}\setminus\mathcal{L}}\pi^{\rm bu}\dot\varphi\,dv=o(1),\quad\epsilon\int\limits_{\mathcal{P}\setminus\mathcal{L}}\pi^{\rm xs}\dot\varphi\,dv=o(1).\tag{12.13}$$

Finally, concerning $(12.8)_3$, we observe first that $\mathcal{P}\cap\partial\mathcal{L}$ belongs to the overlap region $\mathcal{L}\cap(\mathcal{R}^{\rm a}\cup\mathcal{R}^{\rm b})$ where the outer and inner expansions agree. Thus, the bulk estimate $(9.8)_1$ for $W^{\rm xs}$ and the estimates $(9.28)_1$ and $(9.28)_2$ for $\boldsymbol{n}$, and V on $\mathcal{L}$ imply that $W^{\rm xs}(V\boldsymbol{n})\cdot\boldsymbol{\nu}=o(1)$ on $\mathcal{P}\cap\partial\mathcal{L}$, and $(12.8)_3$ follows immediately.

13 Discussion

Our analysis shows that a phase-field regularization that is asymptotically consistent with the sharp-interface theory determined by the bulk energies $W^{\rm a}$ and $W^{\rm b}$ and the interfacial constitutive response functions $\hat w$ and $\hat b$ is obtained on selecting $\hat W^{\rm bu}$, $\hat W^{\rm xs}$, and $\hat\beta$ to be of the form

$$\left.\begin{aligned}\hat W^{\rm bu}(\varphi)&=(1-z(\varphi))W^{\rm a}+z(\varphi)W^{\rm b},\\ \hat W^{\rm xs}(\varphi,\nabla\varphi)&=\epsilon^{-1}\Psi(\varphi)+\frac{\epsilon}{2\sigma^2}|\nabla\varphi|^2\hat w^2(\boldsymbol{n}),\\ \hat\beta(\varphi,\nabla\varphi,\dot\varphi)&=\frac{\epsilon}{\sigma^2}\hat b(\boldsymbol{n},V)\hat w(\boldsymbol{n}),\end{aligned}\right\}\tag{13.1}$$

with Ψ a double-well potential possessing equal minima at $\varphi=\varphi_{\rm a}$ and $\varphi=\varphi_{\rm a}$, and with z a monotonic function taking $\mathbb{R}$ into the interval $[0,1]$ and obeying $z(\varphi_{\rm a})=0$ and $z(\varphi_{\rm b})=1$ (cf. Fig. 2). In particular, on using the homogeneous extensions $\tilde w$ and $\tilde b$ of $\hat w$ and $\hat b$ as defined in (7.4), our results allow lead us to conclude that, as $\epsilon\to 0$, the equation[25]

$$\begin{aligned}\epsilon\tilde b(\nabla\varphi,\dot\varphi)\tilde w(\nabla\varphi)\dot\varphi=\epsilon\,\mathrm{div}\big(\tilde w(\nabla\varphi)\frac{\partial}{\partial(\nabla\varphi)}\tilde w(\nabla\varphi)\big)\\ -\sigma^2\epsilon^{-1}\frac{\partial}{\partial\varphi}\Psi(\varphi)-\sigma^2[\![W]\!]\frac{\partial}{\partial\varphi}z(\varphi),\end{aligned}\tag{13.2}$$

[25] Equation (13.2) arises on using the constitutive equations (13.1) in $(6.5)_3$, $(6.7)_3$, $(6.7)_4$, $(6.8)_1$, and $(6.8)_2$ for $\pi^{\rm bu}$, $\boldsymbol{\xi}^{\rm xs}$, $\pi^{\rm xs}$, $c^{\rm xs}$, and $\jmath^{\rm xs}$ and inserting the results in the microforce balance (6.11).

which holds on $\mathcal{B}$ and expresses microforce balance in the phase-field theory, can be imposed in lieu of the parital differential equation[26]

$$\hat{b}(\mathbb{n}, V_{\mathfrak{S}})V_{\mathfrak{S}} = \big(\hat{w}(\mathbb{n})\mathbb{P} + \frac{\partial^2}{\partial \mathbb{n}^2}\hat{w}(\mathbb{n})\big)\cdot\mathbb{L} + [\![W]\!], \tag{13.3}$$

enforcing normal configurational force balance in the the sharp-interface theory.

Since the asymptotic validity of the phase-field regularization is insensitive to the particular features of z and Ψ, those features may be selected to facilitate analysis and/or computation.[27] We, therefore, view this latitude not as an undesirable lack of uniqueness, but, rather, as a strength of the phase-field regularization of the sharp-interface theory.

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A Appendix

Assume that the layer $\mathcal{L}$ of the phase-field theory contains the interface $\mathfrak{S}$ of the sharp-interface theory. At each instant t, let $\ell(\boldsymbol{x}, t)$ denote the signed distance between $\boldsymbol{x} \in \mathcal{L}(t)$ and $\mathfrak{S}(t)$, with $\ell(\boldsymbol{x}, t) < 0$ when $\boldsymbol{x} \in \mathcal{B}^{\mathfrak{a}}$ and $\ell(\boldsymbol{x}, t) > 0$ when $\boldsymbol{x} \in \mathcal{B}^{\mathfrak{b}}$. Also, let $\mathbb{z}$ denote an interfacial vector field defined so that

$$\nabla \mathbb{z} = \mathbb{P}, \tag{A.1}$$

with $\mathbb{P} = \boldsymbol{1} - \mathbb{n}\otimes\mathbb{n}$ the projector onto $\mathfrak{S}$.

Assume, further, that the region $\mathcal{L}$ is sufficiently thin so that within it the mapping $\boldsymbol{x} \mapsto (\ell, \mathbb{z})$ is one-to-one. Hence, within $\mathcal{L}$, the gradient of a scalar field g can be written as

$$\nabla g = \big((\nabla g)\cdot\mathbb{n}\big)\mathbb{n} + \nabla_{\mathfrak{S}} g, \tag{A.2}$$

[26] Equation (13.3) arises on inserting the representation $(2.13)_1$ for the bulk configurational stress and the interfacial constitutive equations (2.17) in the normal configurational force balance (2.25).

[27] For instance, in studying the Ginzburg-Landau-Allen-Cahn equation (which results from (13.3) on taking both $\tilde{w}$ and $\tilde{\beta}$ to be constant), NOCHETTO, PAOLINI, ROVINDA & VERDI [16] find that taking Ψ to be a double-obstacle potential renders more straightforward the proof of certain results concerning the convergence of that equation to the sharp-interface equation describing motion by mean curvature and also leads naturally to highly efficient numerical methods for approximating solutions.

with $(\nabla_{\mathcal{S}} g)\cdot n = 0$, and the values of $(\nabla g)\cdot n$ and $\nabla_{\mathcal{S}} g$ at (ℓ, z, t) determined by

$$\big(\nabla g(\ell, z, t)\big)\cdot n(z, t) = \frac{\partial}{\partial \ell} g(\ell, z, t), \tag{A.3}$$

and

$$\nabla_{\mathcal{S}} g(\ell, z, t) = \frac{\partial}{\partial z} g(\ell, z, t), \tag{A.4}$$

respectively.

In terms of the surface-related coordinate system (ℓ, z), fields intrinsic to $\mathcal{S}$ may be thought as a fields defined throughout $\mathcal{L}$ but independent of ℓ. In this sense, $\nabla\ell$ and $\dot{\ell}$ are intrinsic and satisfy

$$\nabla\ell = n \qquad \text{and} \qquad \dot{\ell} = -V_{\mathcal{S}}. \tag{A.5}$$

Further, since n is independent of ℓ, the curvature tensor $\mathbb{L} = -\nabla_{\mathcal{S}} n$ associated with $\mathcal{S}$ is given by

$$\mathbb{L} = -\nabla n. \tag{A.6}$$

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