An order-parameter based theory as a regularization of a sharp-interface theory for solid-solid phase transitions

ELIOT FRIED & GERMAN GRACH

Department of Theoretical and Applied Mechanics
University of Illinois at Urbana-Champaign
Urbana, IL 61801, USA

1 Introduction

Recently, FRIED & GURTIN [1] developed an extension of nonlinear elasticity theory in which an order parameter joins the deformation as an additional independent kinematic variable. While the most natural application of that theory is to coupled ordering and deformation in crystalline solids, in which case the order parameter describes atomic arrangements within unit cells of a crystal lattice and the deformation accounts for distortions of that lattice, an analysis due to FRIED & GURTIN suggests that their theory may also pertain to other types of solid-state phenomena, phenomena where atomic ordering is of negligible importance and, hence, for which the physical status of the order parameter is, at best, obscure.

Specifically, FRIED & GURTIN showed that, granted certain constitutive assumptions and an appropriate scaling, their governing equations are asymptotic to governing equations that arise in a theory for displacive solid-solid transitions advanced by GURTIN & STRUTHERS [2]. In that theory, bulk phases are modeled as nonlinearly hyperelastic and phase interfaces are treated as sharp nonmaterial surfaces across which, consistent with the requirement of coherency, the deformation is continuous but the deformation gradient may jump. Further, these surfaces are endowed with energy and are assumed capable of sustaining force. Interfacial fields that are central to the theory include the energy density w and the kinetic coefficient b.[1] The interfacial energy density is determined by a constitutive response function $\hat{w}$ that, in appreciation of influences that coherent lattice mismatch and interfacial orientation may exert on the morphology of

[1] The kinetic coefficient corresponds to the reciprocal of the interfacial mobility.

equilibrated microstructures,[2] depends on the tangential deformation-gradient $\mathbb{F}$ and the interfacial unit normal $\mathbb{n}$. The kinetic coefficient, which governs transition kinetics, is determined by a constitutive response function $\hat{b}$ that may vary with $\mathbb{F}$, $\mathbb{n}$, and also the interfacial scalar normal velocity $V_{\mathbb{S}}$. The latter dependence accounts for nonlinear transition kinetics,[3] while the former dependencies allow coherent lattice mismatch and interfacial orientation to influence transition kinetics.[4] Within this theory, a complete constitutive description entails, in addition to giving $\hat{w}$ and $\hat{b}$, provision of a response function $\hat{W}^{\mathfrak{c}}$, depending on the deformation gradient $\boldsymbol{F}$, determining the strain-energy density W of each bulk phase $\mathfrak{c} = \mathfrak{a}, \mathfrak{b}$.

The correspondence demonstrated by FRIED & GURTIN applies only to a narrowing of the theory of GURTIN & STRUTHERS wherein $\hat{w}$ and $\hat{b}$ are both material constants, so that interfaces may support only surface tension and transition kinetics must be linear. Here, our purpose is to extend the result of FRIED & GURTIN—showing that their theory embraces the full range of interfacial structure present in the sharp-interface theory of GURTIN & STRUTHERS.

We begin, in Section 2, with a synopsis of the theory of GURTIN & STRUTHERS, which, hereafter, we will often refer to as the "sharp-interface theory." This is followed, in Section 3, by a summary of the theory of FRIED & GURTIN, which we refer to as the "order-parameter based theory." In that theory, a material is characterized by response functions $\hat{W}$ and $\hat{\beta}$ that deliver the energy density W and the damping modulus β: in general, $\hat{W}$ may depend on the deformation gradient $\boldsymbol{F}$,[5] the order parameter φ, and the order-parameter gradient $\nabla\varphi$, while $\hat{\beta}$ may depend on $\boldsymbol{F}$, φ, $\nabla\varphi$, and on the order-parameter rate $\dot{\varphi}$ as well.

In Section 4, we introduce a series of assumptions that restrict the manner in which the response functions $\hat{W}$ and $\hat{\beta}$ may depend on the independent constitutive variables $\boldsymbol{F}$, φ, $\nabla\varphi$, and $\dot{\varphi}$,[6] leading to a description that associates the bulk phases $\mathfrak{a}$ and $\mathfrak{b}$ of the sharp-interface theory with the order-parameter values $\varphi = 0$ and $\varphi = 1$ and models phase interfaces by narrow transition layers

[2] BROOKS [3], MULLINS [4], LARCHÉ & CAHN [5, 6], and LEO & SEKERKA [7] treat applications where lattice mismatch impacts the morphology of equilibrated microstructures, while HERRING [8], MULLINS [4], SHEWMON & ROBERTSON [9], CAHN & HOFFMAN [10], and CAHN & LARCHÉ [11] consider applications where orientation dependence is significant.

[3] HILLERT [12] and OWEN, SCHOEN & SRINIVASAN [13] discuss applications where the dependence of interfacial mobility on interfacial velocity is important.

[4] The inclusion of orientation dependence in the kinetic coefficient is motivated by analogy to theories of crystal growth, where the prominence of such dependence effect is well-recognized (cf., e.g., TAYLOR, CAHN & HANDWERKER [14] and CAHN & CARTER [15]). Although it seems to us entirely reasonable that the velocity of an evolving interface may, in general, vary with the distribution of coherent mismatch along that interface, we are unaware of experiments that test such a hypothesis.

[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, W and $\boldsymbol{F}$ denote the bulk energy density and deformation gradient of the sharp-interface theory, whereas W and $\boldsymbol{F}$ denote the energy density and deformation gradient of the order-parameter based theory.

[6] In framing these assumptions, we follow closely considerations put forth by FRIED & GURTIN [16] in their generalized phase-field theory for solidification.

within which the order-parameter gradient is large in magnitude. Moreover, these assumptions imply a decomposition of $\hat{W}$ in the form

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

where $\hat{W}^{\mathrm{bu}}$ determines the energy density of the bulk phases and $\hat{W}^{\mathrm{xs}}$ determines the energy density of transition layers. In particular, $\hat{W}^{\mathrm{xs}}$ admits the representation

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

where Ψ is a double-well potential with equal minima at $\varphi = 0$ and $\varphi = 1$, $\boldsymbol{P} = \boldsymbol{1} - \boldsymbol{n}\otimes\boldsymbol{n}$, and $\boldsymbol{n} = \nabla\varphi/|\nabla\varphi|$. A further consequence of the assumptions put forth in Section 4 is that

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

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

Next, in Section 5, we perform a scaling of the independent and dependent variables of order-parameter based theory. That scaling, upon which our asymptotic results hinges, 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 5. To simplify the presentation of our results, we suppose, in Section 6, that $\hat{W}^{\mathrm{a}}$ and $\hat{W}^{\mathrm{b}}$ are related to $\hat{W}^{\mathrm{bu}}$ through

$$\hat{W}^{\mathrm{a}}(\boldsymbol{F}) = \hat{W}^{\mathrm{bu}}(\boldsymbol{F},0) \qquad \text{and} \qquad \hat{W}^{\mathrm{b}}(\boldsymbol{F}) = \hat{W}^{\mathrm{bu}}(\boldsymbol{F},1), \tag{1.4}$$

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

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

where σ is the constant determined by

$$\sigma = \int_0^1 \sqrt{2\Psi(\varphi)}\,d\varphi; \tag{1.6}$$

clearly, (1.4) and (1.5) do not restrict, in any manner, the breadth of constitutive generality possible in the sharp-interface theory.

Asymptotic expansions are introduced in Section 7 and attendant preliminary results concerning those expansions are derived in Section 8. Among the latter is the estimate

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

that 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.[7] Aside from its physical significance, this result serves an important role in our analysis: in particular, it implies an estimate

$$h(\epsilon) = \tfrac{1}{2}\epsilon\sqrt{\lambda(\boldsymbol{F}\boldsymbol{P},\boldsymbol{n})}\int_{\epsilon}^{1-\epsilon}\frac{d\varphi}{\sqrt{2\Psi(\varphi)}} + o(h(\epsilon)) \tag{1.8}$$

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

In Section 9, we show that the global integral laws of the order-parameter based theory tend, as ϵ and, hence, the thickness h of interfacial layers approaches zero, toward 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 10, that the local balance laws of the order-parameter based theory tend, as ϵ approaches zero, toward those of the sharp-interface theory. In Section 11 we develop a power identity for the order-parameter based theory and demonstrate the asymptotic correspondence of this identity to a power identity for the sharp-interface theory.

The results of Sections 9, 10, and 11 show that, given constitutive response functions $\hat{W}^{\mathrm{a}}$, $\hat{W}^{\mathrm{b}}$, $\hat{w}$, and $\hat{b}$ determining a particular sharp-interface theory, the class of order-parameter based theories determined by the constitutive relations[8]

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

provides a regularization of that theory. Here z is an arbitrary monotonic function taking $\mathbb{R}$ into $[0,1]$ and consistent with $z(0) = 0$ and $z(1) = 1$. Since that asymptotic correspondence holds regardless of the particular features of z and Ψ (except for those that have been mentioned above), those features may be selected to facilitate analysis and/or computation. This latitude is to be viewed not as an undesirable lack of uniqueness, but, rather, as a strength of the order-parameter based regularization of the sharp-interface theory.

The paper concludes, in Section 12, with a discussion of the recipe (1.9) and related issues.

[7] The factor of ϵ^2 in the second term on the left-hand-side of (1.7) reflects the scaling of Section 5. In Section 8 we find that, within layers, $\epsilon|\nabla\varphi| = O(1)$, so that, 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.

[8] The factors of ϵ^{-1} and ϵ appearing in the relations $(1.9)_{2,3}$ reflect the scaling of Section 5. All constitutive functions on the right-hand-side of (1.9) are of $O(1)$ in ϵ.

2 Review of the sharp-interface theory

In this section we survey the theory of GURTIN & STRUTHERS.[9] In doing so, we take advantage of recent results due to GURTIN [20, 21, 22] concerning the role of configurational forces within that theory.[10]

2.1 Kinematics

Consider a coherent motion $\boldsymbol{y}$ of a two-phase body that occupies a region $\mathcal{B}$ in a fixed reference configuration with uniform mass density ϱ. Suppose that, at each instant of the motion, $\mathcal{B}$ is separated by a phase interface, represented by a smoothly evolving orientable surface $\mathcal{S}$, into regions $\mathcal{B}^{\mathfrak{a}}$ and $\mathcal{B}^{\mathfrak{b}}$ associated with its phases $\mathfrak{a}$ and $\mathfrak{b}$. Let $\boldsymbol{n}$ denote the unit normal field, directed outward from $\mathcal{B}^{\mathfrak{a}}$, for $\mathcal{S}$, so that the tensor field

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

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

Let $\nabla_{\mathcal{S}} g$ and $\mathring{g}$ denote the surface gradient and normal time-rate of a field g defined on $\mathcal{S}$.[11] Then

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

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

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

The coherence of the motion implies that $\boldsymbol{y}$ must be continuous across $\mathcal{S}$, so that, writing $[\![g]\!]$ for the jump ($\mathfrak{b}$-side minus $\mathfrak{a}$-side) across $\mathcal{S}$ of a bulk field g, and

$$\boldsymbol{F} = \nabla\boldsymbol{y} \tag{2.4}$$

for the deformation gradient, we have

$$[\![\boldsymbol{y}]\!] = \boldsymbol{0}, \qquad [\![\boldsymbol{F}]\!]\mathbb{P} = \boldsymbol{0}, \qquad \text{and} \qquad [\![\dot{\boldsymbol{y}}]\!] + [\![\boldsymbol{F}\boldsymbol{n}]\!]V_{\mathcal{S}} = \boldsymbol{0} \tag{2.5}$$

[9] Concurrent with GURTIN & STRUTHERS, LEO & SEKERKA [7] derived, from a variational perspective, versions of the governing equations of GURTIN & STRUTHERS appropriate to equilibrium (see also PITTERI [17]). PFENNING & WILLIAMS [18] derived, working within the context of geometric measure theory, equations resembling those of GURTIN & STRUTHERS. Following an approach taken ABEYARATNE & KNOWLES [28] in work that neglects interfacial structure, LUSK [19] provided an independent derivation of the equations of GURTIN & STRUTHERS.

[10] GURTIN & STRUTHERS used the adjective *accretive* in place of *configurational* when referring to these forces.

[11] See GURTIN & STRUTHERS and Appendix A.1 for a definition of the normal time-rate.

on $\mathcal{S}$. By virtue of $(2.5)_2$ we can introduce the *tangential deformation-gradient*

$$\mathbb{F} = \langle\!\langle \boldsymbol{F} \rangle\!\rangle \mathbb{P}, \tag{2.6}$$

with $\langle\!\langle g \rangle\!\rangle$ the average across $\mathcal{S}$ of a bulk field g. Further, on writing y for the restriction to $\mathcal{S}$ of the deformation $\boldsymbol{y}$, viz.

$$y = \boldsymbol{y}|_{\mathcal{S}}, \tag{2.7}$$

we have the identities[12]

$$\nabla_{\mathcal{S}} y = \langle\!\langle \boldsymbol{F} \rangle\!\rangle \mathbb{P} = \mathbb{F} \qquad \text{and} \qquad \mathring{y} = \langle\!\langle \dot{\boldsymbol{y}} \rangle\!\rangle + \langle\!\langle \boldsymbol{F} n \rangle\!\rangle V_{\mathcal{S}}. \tag{2.8}$$

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, at each instant during the course of some time interval, portions of the regions $\mathcal{B}^{\mathfrak{a}}$ and $\mathcal{B}^{\mathfrak{b}}$ are contained in $\mathcal{P}$ and $\mathcal{S}$ crosses $\partial\mathcal{P}$ transversely to yield a nonempty intersection

$$\Omega = \mathcal{S} \cap \mathcal{P}. \tag{2.9}$$

Then, n and $\boldsymbol{\nu}$ must satisfy $0 \leq |n \cdot \boldsymbol{\nu}| < 1$,

$$m = \frac{\mathbb{P}\boldsymbol{\nu}}{\sqrt{1 - |n \cdot \boldsymbol{\nu}|^2}} \tag{2.10}$$

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

$$U_{\partial\Omega} = -\frac{(n \cdot \boldsymbol{\nu}) V_{\mathcal{S}}}{\sqrt{1 - |n \cdot \boldsymbol{\nu}|^2}} \tag{2.11}$$

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

2.2 Basic fields. Balance laws. Dissipation imbalance

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

W	*strain energy density,*
$\boldsymbol{S}$	*deformational stress,*
$\boldsymbol{C}$	*configurational stress,*
$\boldsymbol{f}$	*internal configurational force density,*
$\boldsymbol{q}$	*configurational momentum density,*

[12] These identities are special cases of results discussed in Appendix A.1.

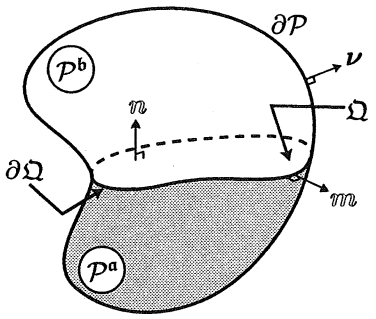

Figure 1. Subregion $\mathcal{P}$ of $\mathcal{B}$ composed of evolving parts $\mathcal{P}^{\mathfrak{a}}$ and $\mathcal{P}^{\mathfrak{b}}$ occupied by phases $\mathfrak{a}$ and $\mathfrak{b}$ and the portion $\mathfrak{Q}$ of the phase interface $\mathfrak{S}$.

and the interfacial fields[13]

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

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

$$\left.\begin{aligned}
\int_{\partial\mathcal{P}} \boldsymbol{S}\boldsymbol{\nu}\,da + \int_{\partial\mathfrak{Q}} \mathbb{S}\boldsymbol{m}\,dl &= \overset{\cdot}{\int_{\mathcal{P}}} \varrho\dot{\boldsymbol{y}}\,dv,\\
\int_{\partial\mathcal{P}} \boldsymbol{y}\times\boldsymbol{S}\boldsymbol{\nu}\,da + \int_{\partial\mathfrak{Q}} \boldsymbol{y}\times\mathbb{S}\boldsymbol{m}\,dl &= \overset{\cdot}{\int_{\mathcal{P}}} \boldsymbol{y}\times\varrho\dot{\boldsymbol{y}}\,dv,\\
\int_{\partial\mathcal{P}} \boldsymbol{C}\boldsymbol{\nu}\,da + \int_{\mathcal{P}} \boldsymbol{f}\,dv + \int_{\partial\mathfrak{Q}} \mathbb{C}\boldsymbol{m}\,dl + \int_{\mathfrak{Q}} \mathbb{f}\,da &= \overset{\cdot}{\int_{\mathcal{P}}} \boldsymbol{q}\,dv,
\end{aligned}\right\} \tag{2.12}$$

enforcing linear momentum balance, angular momentum balance, and configurational force balance, as well as the dissipation imbalance

$$\int_{\partial\mathcal{P}} \boldsymbol{S}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}\,da + \int_{\partial\mathfrak{Q}} \left(\mathbb{S}\boldsymbol{m}\cdot\mathring{\dot{y}} + \mathbb{C}\boldsymbol{m}\cdot(V_{\mathfrak{S}}\boldsymbol{m})\right) dl$$

$$\geq \overset{\cdot}{\int_{\mathcal{P}}} (W + \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2)\,dv + \int_{\mathfrak{Q}} w\,da - \int_{\partial\mathfrak{Q}} wU_{\partial\mathfrak{Q}}\,dl, \tag{2.13}$$

[13] The fields $\mathbb{S}$ and $\mathbb{C}$ obey $\mathbb{S}\boldsymbol{n} = \boldsymbol{0}$ and $\mathbb{C}\boldsymbol{n} = \boldsymbol{0}$ on $\mathfrak{S}$ and therefore are *superficial* in the sense of GURTIN [20].

asserting the second law.[14]

The foregoing global balances have the local forms

$$\left.\begin{aligned} \operatorname{div} \boldsymbol{S} &= \varrho \ddot{\boldsymbol{y}}, \\ \boldsymbol{F}\boldsymbol{S}^T &= \boldsymbol{S}\boldsymbol{F}^T, \\ \operatorname{div} \boldsymbol{C} + \boldsymbol{f} &= \dot{\boldsymbol{q}}, \end{aligned}\right\} \tag{2.14}$$

valid in bulk, and

$$\left.\begin{aligned} [\![\boldsymbol{S}\boldsymbol{n}]\!] + \varrho [\![\dot{\boldsymbol{y}}]\!] V_{\mathfrak{S}} + \operatorname{div}_{\mathfrak{S}} \mathbb{S} &= \boldsymbol{0}, \\ \mathbb{F}\mathbb{S}^T &= \mathbb{S}\mathbb{F}^T, \\ [\![\boldsymbol{C}\boldsymbol{n}]\!] + [\![\boldsymbol{q}]\!] V_{\mathfrak{S}} + \operatorname{div}_{\mathfrak{S}} \mathbb{C} + \mathbb{f} &= \boldsymbol{0}, \end{aligned}\right\} \tag{2.15}$$

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

$$\boldsymbol{S}\cdot\dot{\boldsymbol{F}} \geq \dot{W} \tag{2.16}$$

in bulk, and that

$$\begin{aligned} &\boldsymbol{n}\cdot[\![\big((W - \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2)\boldsymbol{1} - \boldsymbol{F}^T\boldsymbol{S} - \boldsymbol{C}\big)\boldsymbol{n}]\!] V_{\mathfrak{S}} - [\![(\varrho \boldsymbol{F}^T\dot{\boldsymbol{y}} + \boldsymbol{q})\cdot\boldsymbol{n}]\!] V_{\mathfrak{S}}^2 \\ &\quad + \big((w\mathbb{P} - \mathbb{F}^T\mathbb{S} - \mathbb{C})\cdot\mathbb{L}\big) V_{\mathfrak{S}} + \mathbb{S}\cdot\mathring{\mathbb{F}} - (\mathbb{C}^T\boldsymbol{n})\cdot\mathring{\boldsymbol{n}} - (\mathbb{f}\cdot\boldsymbol{n}) V_{\mathfrak{S}} \geq \mathring{w} \end{aligned} \tag{2.17}$$

on $\mathfrak{S}$.

A slight extension of an invariance argument originated recently by GURTIN [21, 22] yields the representations[15]

$$\boldsymbol{C} = (W - \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2)\boldsymbol{1} - \boldsymbol{F}^T\boldsymbol{S} \qquad \text{and} \qquad \boldsymbol{q} = -\varrho \boldsymbol{F}^T\dot{\boldsymbol{y}} \tag{2.18}$$

for the bulk configurational stress $\boldsymbol{C}$ and the configurational momentum density $\boldsymbol{q}$, and also the representation

$$\mathbb{C}_{\text{tan}} = w\mathbb{P} - \mathbb{F}^T\mathbb{S} \tag{2.19}$$

for the tangential component $\mathbb{C}_{\text{tan}} = \mathbb{P}\mathbb{C}$ of the interfacial configurational stress. An immediate consequence of these representations is that the interfacial dissipation imbalance (2.17) reduces to

$$\mathbb{S}\cdot\mathring{\mathbb{F}} - \mathbb{c}\cdot\mathring{\boldsymbol{n}} - (\mathbb{f}\cdot\boldsymbol{n}) V_{\mathfrak{S}} \geq \mathring{w}, \tag{2.20}$$

[14] In writing (2.13), we have imposed the requirement (cf. GURTIN & STRUTHERS and GURTIN [20, 22]) that the power generated by the net effects of the deformational and configurational forces 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.

[15] The expressions for $\boldsymbol{C}$ and $\boldsymbol{q}$ in (2.18) coincide, respectively, with the *dynamic energy-momentum tensor* introduced by ESHELBY [24, equation (53)] in his study of material inhomogeneities, defects, and interfaces and the *pseudomomentum* of MAUGIN, EPSTEIN & TRIMARCO [25, equation (16)]. Derivations of (2.18) and (2.19) are given by CERMELLI, FRIED & GRACH [23].

with $\mathbb{c} = \mathbb{C}^T n$ the normal component of $\mathbb{C}$.[16] Further, in combination with the local bulk and interfacial balances (2.14) and (2.15), the representations (2.18) and (2.19) imply the power identity[17]

$$\int_{\partial\mathcal{P}} \boldsymbol{S}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}\,da + \int_{\partial\Omega} \big(\mathbb{S}n\cdot\mathring{y} + \mathbb{c}\cdot(V_{\mathfrak{S}}n)\big)\,dl - \overline{\int_{\mathcal{P}} \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2\,dv}$$

$$= \int_{\mathcal{P}\setminus\Omega} \boldsymbol{S}\cdot\dot{\boldsymbol{F}}\,dv - \int_{\Omega} \big((\llbracket W\rrbracket + \mathbb{f}\cdot n)V_{\mathfrak{S}} + wK_{\mathfrak{S}}V_{\mathfrak{S}} - \mathbb{S}\cdot\mathring{\mathbb{F}} + \mathbb{c}\cdot\mathring{n}\big)\,da. \quad (2.21)$$

2.3 Constitutive equations

In bulk, the material of each phase $\mathfrak{c} = \mathfrak{a}, \mathfrak{b}$ is taken to be nonlinearly hyperelastic and homogeneous, so that

$$W = \hat{W}^{\mathfrak{c}}(\boldsymbol{F}) \qquad \text{and} \qquad \boldsymbol{S} = \hat{\boldsymbol{S}}^{\mathfrak{c}}(\boldsymbol{F}) = \frac{d}{d\boldsymbol{F}}\hat{W}^{\mathfrak{c}}(\boldsymbol{F}), \quad (2.22)$$

and the inequality (2.16) reduces to an equality.

For the interfacial constitutive theory, it is assumed that w, $\mathbb{S}$, $\mathbb{c}$, and $\mathbb{f}\cdot n$ are given by response functions depending on $\mathbb{F}$, n, and $V_{\mathfrak{S}}$. Compatibility with the interfacial dissipation imbalance (2.20) then requires that

$$\left.\begin{aligned} w = \hat{w}(\mathbb{F}, n), \qquad \mathbb{S} = \hat{\mathbb{S}}(\mathbb{F}, n) = \frac{\partial}{\partial\mathbb{F}}\hat{w}(\mathbb{F}, n), \\ \mathbb{c} = \hat{\mathbb{c}}(\mathbb{F}, n) = -\frac{D}{Dn}\hat{w}(\mathbb{F}, n), \qquad \mathbb{f}\cdot n = -\hat{b}(\mathbb{F}, n, V_{\mathfrak{S}})V_{\mathfrak{S}}, \end{aligned}\right\} \quad (2.23)$$

where $(D/Dn)\hat{w}(\mathbb{F}, n)$ represents the value at $(\mathbb{F}, n)$ of the derivative of $\hat{w}$ with respect to n following $\mathfrak{S}$,[18] and the *kinetic coefficient* $b = \hat{b}(\mathbb{F}, n, V_{\mathfrak{S}})$ is nonnegative.

On inserting the relations (2.23) in the inequality (2.20) and using the identity (A.15) to evaluate the normal time-rate of w through the response function $\hat{w}$, we obtain an *interfacial dissipation balance*

$$\mathbb{S}\cdot\mathring{\mathbb{F}} - \mathbb{c}\cdot\mathring{n} - (\mathbb{f}\cdot n)V_{\mathfrak{S}} - \mathring{w} = bV_{\mathfrak{S}}^2 \geq 0, \quad (2.24)$$

that identifies propagating phase interfaces as the sole source of dissipation in the theory at hand.[19] For future reference, we introduce the *interfacial dissipation density*

$$\delta = -(\mathbb{f}\cdot n)V_{\mathfrak{S}} = bV_{\mathfrak{S}}^2. \quad (2.25)$$

[16] By virtue of the requirement that $\mathbb{C}$ be superficial (cf. Footnote 13), $\mathbb{c}$ obeys $\mathbb{c}\cdot n = 0$ on $\mathfrak{S}$ and therefore is *tangential* on $\mathfrak{S}$.

[17] A brief derivation of (2.21) appears in Appendix A.2.

[18] See GURTIN & STRUTHERS and Appendix A.1 for definitions of this derivative.

[19] Shock waves, which are generally dissipative, are excluded from our discussion.

Both the bulk and interfacial response functions are required to be invariant with respect to superposed rigid motions. Hence, the bulk response functions may depend on $\boldsymbol{F}$ through at most the *right stretch-tensor* $\boldsymbol{U} = \sqrt{\boldsymbol{F}^T\boldsymbol{F}}$, while the interfacial response functions may depend on $\mathbb{F}$ through at most the *interfacial right stretch-tensor* $\mathbb{U} = \sqrt{\mathbb{F}^T\mathbb{F}}$. Together with the relations $(2.22)_2$ and $(2.23)_2$ defining the deformational stresses $\boldsymbol{S}$ and $\mathbb{S}$, these requirements ensure that the local balances $(2.14)_2$ and $(2.15)_2$ for bulk and interfacial angular momentum are satisfied.

Associated with each bulk phase $\mathfrak{c}$, we assume that there exists a *natural stretch* $\boldsymbol{U}_\mathfrak{c}$, whereby $\hat{\boldsymbol{S}}^\mathfrak{c}(\boldsymbol{U}_\mathfrak{c}) = \boldsymbol{0}$ for each phase $\mathfrak{c} = \mathfrak{a}, \mathfrak{b}$. Further, we assume that, for each $\boldsymbol{n}$ in some open connected subset $\mathcal{K}$ of the set of unit vectors, there exists a *natural interfacial stretch* $\mathbb{U}_\mathfrak{S}(\boldsymbol{n})$ such that $\hat{\mathbb{S}}(\mathbb{U}_\mathfrak{S}(\boldsymbol{n}), \boldsymbol{n}) = \boldsymbol{0}$.

2.4 Internal configurational forces

Together with the constitutive equations (2.22), the representations (2.18) for $\boldsymbol{C}$ and $\boldsymbol{q}$ imply that

$$\operatorname{div}\boldsymbol{C} - \dot{\boldsymbol{q}} = -\boldsymbol{F}^T(\operatorname{div}\boldsymbol{S} - \varrho\ddot{\boldsymbol{y}}), \tag{2.26}$$

so that, granted the equations $(2.14)_1$ and $(2.14)_3$ enforcing the linear momentum balance and configurational momentum balance in bulk, the bulk internal configurational force must vanish, viz.

$$\boldsymbol{f} = \boldsymbol{0}. \tag{2.27}$$

Further, the expression (2.19) for $\mathbb{C}_{\text{tan}}$, the constitutive equations $(2.23)_1$, $(2.23)_2$, and $(2.23)_3$ for w, $\mathbb{S}$, and $\mathbb{c}$, and the identity (A.16) of Appendix A.1 imply that

$$\mathbb{P}\big(\llbracket\boldsymbol{C}\boldsymbol{n}\rrbracket + \llbracket\boldsymbol{q}\rrbracket V_\mathfrak{S} + \operatorname{div}_\mathfrak{S}\mathbb{C}\big) = \boldsymbol{0}, \tag{2.28}$$

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

$$\mathbb{f}_{\text{tan}} = \boldsymbol{0}. \tag{2.29}$$

Hence, the relation $(2.23)_4$ determining $\mathbb{f}\cdot\boldsymbol{n}$ yields

$$\mathbb{f} = -bV_\mathfrak{S}\boldsymbol{n}, \tag{2.30}$$

and satisfaction of the interfacial configurational momentum balance $(2.15)_3$ is equivalent to satisfaction of its normal component

$$\boldsymbol{n}\cdot\llbracket\boldsymbol{C}\boldsymbol{n}\rrbracket + \llbracket\boldsymbol{q}\cdot\boldsymbol{n}\rrbracket V_\mathfrak{S} + \mathbb{C}\cdot\mathbb{L} + \operatorname{div}_\mathfrak{S}\mathbb{c} + \mathbb{f}\cdot\boldsymbol{n} = 0, \tag{2.31}$$

which, for brevity, we refer to as the *normal configurational balance*.[20]

[20] The normal configurational balance (2.31) of GURTIN & STRUTHERS reduces, on ignoring interfacial energy, to a relation proposed by HEIDUG & LEHNER [26], TRUSKINOVSKY [27], and ABEYARATNE & KNOWLES [28] to determine the kinetics of coherent solid-solid phase transitions.

3 Review of the order-parameter based theory

Here we outline the theory of FRIED & GURTIN, focusing on the special case where the order parameter is unconstrained and scalar-valued.[21] Consistent with our aim, which is to show how this theory has the capacity to serve as a regularization of the sharp-interface theory, we do not provide a specific physical interpretation of the order parameter.

3.1 Kinematics

Setting aside the sharp-interface theory, consider a body the kinematical description of which involves a smooth motion $\boldsymbol{y}$ and a scalar order parameter φ. Suppose that the body possesses a reference state in which it occupies the region $\mathcal{B}$ with uniform density ϱ,[22] and let

$$\boldsymbol{F} = \nabla \boldsymbol{y} \qquad \text{and} \qquad \boldsymbol{p} = \nabla \varphi \tag{3.1}$$

denote the deformation and order-parameter gradients.

3.2 Basic fields. Balance laws. Dissipation imbalance

The order-parameter based theory involves only bulk fields, that, ignoring external forces, are[23]

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

[21] FRIED & GURTIN treat the more general case where the order parameter is vector-valued and is constrained to lie on an affine manifold.

[22] While the region $\mathcal{B}$ and density ϱ considered here are intended to be identical to those considered in connection with the sharp-interface theory, the motion $\boldsymbol{y}$, energy density W, and deformational stress $\boldsymbol{S}$ are distinct from the fields $\boldsymbol{y}$, W, and $\boldsymbol{S}$ of the sharp-interface theory.

[23] The microstructural fields $\boldsymbol{\xi}$ and π act in response to changes in the order parameter, and are introduced under the precept that with each kinematic process there should exist a corresponding force system that accounts for power expenditures associated with the evolution of the variable underlying that process. FRIED & GURTIN referred to $\boldsymbol{\xi}$ and π as the *configurational stress* and *internal configurational force*, respectively. The inappropriateness of such a choice of terms will become clear in Section 3.4, where we will discuss the actual configurational fields of the order-parameter based theory.

For each $\mathcal{P}$ in $\mathcal{B}$ and each time, these fields are required to obey the integral laws[24]

$$\left.\begin{aligned} \int_{\partial\mathcal{P}} \boldsymbol{S}\boldsymbol{\nu}\,da &= \overline{\int_{\mathcal{P}} \varrho\dot{\boldsymbol{y}}\,dv}^{\cdot}, \\ \int_{\partial\mathcal{P}} \boldsymbol{y}\times\boldsymbol{S}\boldsymbol{\nu}\,da &= \overline{\int_{\mathcal{P}} \boldsymbol{y}\times\varrho\dot{\boldsymbol{y}}\,dv}^{\cdot}, \\ \int_{\partial\mathcal{P}} \boldsymbol{\xi}\cdot\boldsymbol{\nu}\,da + \int_{\mathcal{P}} \pi\,dv &= 0, \end{aligned}\right\} \tag{3.2}$$

imposing linear momentum balance, angular momentum balance, and microforce balance, and also the dissipation imbalance

$$\int_{\partial\mathcal{P}} \left(\boldsymbol{S}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}} + \boldsymbol{\xi}\cdot(\dot{\varphi}\boldsymbol{\nu})\right) da \geq \overline{\int_{\mathcal{P}} (W + \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2)\,dv}^{\cdot}, \tag{3.3}$$

bringing to bear the second law.[25]

The foregoing global laws have the local forms

$$\left.\begin{aligned} \operatorname{div}\boldsymbol{S} &= \varrho\ddot{\boldsymbol{y}}, \\ \boldsymbol{S}\boldsymbol{F}^T &= \boldsymbol{F}\boldsymbol{S}^T, \\ \operatorname{div}\boldsymbol{\xi} + \pi &= 0, \\ \boldsymbol{S}\cdot\dot{\boldsymbol{F}} + \boldsymbol{\xi}\cdot\dot{\boldsymbol{p}} - \pi\dot{\varphi} &\geq \dot{W}. \end{aligned}\right\} \tag{3.4}$$

3.3 Constitutive equations

In the order-parameter based theory, W, $\boldsymbol{S}$, $\boldsymbol{\xi}$, and π are given by response functions depending on the deformation gradient $\boldsymbol{F}$, order parameter φ, order-parameter gradient $\boldsymbol{p}$, and order-parameter rate $\dot{\varphi}$. Consistency with the local dissipation inequality $(3.4)_4$ then requires that

$$\left.\begin{aligned} W = \hat{W}(\boldsymbol{F},\varphi,\boldsymbol{p}), \quad \boldsymbol{S} = \frac{\partial}{\partial\boldsymbol{F}}\hat{W}(\boldsymbol{F},\varphi,\boldsymbol{p}), \quad \boldsymbol{\xi} = \frac{\partial}{\partial\boldsymbol{p}}\hat{W}(\boldsymbol{F},\varphi,\boldsymbol{p}), \\ \pi = -\frac{\partial}{\partial\varphi}\hat{W}(\boldsymbol{F},\varphi,\boldsymbol{p}) - \hat{\beta}(\boldsymbol{F},\varphi,\boldsymbol{p},\dot{\varphi})\dot{\varphi}, \end{aligned}\right\} \tag{3.5}$$

where the *damping modulus* $\beta = \hat{\beta}(\boldsymbol{F},\varphi,\boldsymbol{p},\dot{\varphi})$ must be non-negative.

[24] The idea of a microforce balance was, to our knowledge, first introduced by CAPRIZ [29] in a framework that accounts also for microstructural inertia, an effect that is ignored in $(3.2)_3$.

[25] Because it acts internally to $\mathcal{P}$, π does not contribute to the working in (3.3).

On inserting the relations (3.5) into the inequality $(3.4)_4$, we deduce a dissipation balance

$$\boldsymbol{S}\cdot\dot{\boldsymbol{F}} + \boldsymbol{\xi}\cdot\dot{\boldsymbol{p}} - \pi\dot{\varphi} - \dot{W} = \beta\dot{\varphi}^2 \geq 0, \tag{3.6}$$

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.*[26] For future reference, we introduce the dissipation density

$$\Delta = \beta\dot{\varphi}^2 \tag{3.7}$$

for the order-parameter based theory.

As in the sharp-interface theory, the constitutive response functions are required to be properly invariant under superposed rigid motions. Hence, those functions may depend on $\boldsymbol{F}$ only through the right stretch tensor $\boldsymbol{U} = \sqrt{\boldsymbol{F}^T\boldsymbol{F}}$ and, by virtue of the relation $(3.5)_2$ determining $\boldsymbol{S}$, the local angular momentum balance $(3.4)_2$ is satisfied automatically.

3.4 Configurational momentum balance

On introducing the fields

$$\left.\begin{aligned} \boldsymbol{C} &= (W - \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2)\boldsymbol{1} - \boldsymbol{F}^T\boldsymbol{S} - \boldsymbol{p}\otimes\boldsymbol{\xi}, \\ \boldsymbol{q} &= -\varrho\boldsymbol{F}^T\dot{\boldsymbol{y}}, \qquad \boldsymbol{f} = \beta\dot{\varphi}\boldsymbol{p}, \end{aligned}\right\} \tag{3.8}$$

a simple calculation shows that, granted the constitutive equations (3.5),

$$\operatorname{div}\boldsymbol{C} + \boldsymbol{f} - \dot{\boldsymbol{q}} = -\boldsymbol{F}^T(\operatorname{div}\boldsymbol{S} - \varrho\ddot{\boldsymbol{y}}) - (\operatorname{div}\boldsymbol{\xi} + \pi)\boldsymbol{p}, \tag{3.9}$$

so that, drawing on the linear momentum balance $(3.4)_1$ and the microforce balance $(3.4)_3$, we have

$$\operatorname{div}\boldsymbol{C} + \boldsymbol{f} = \dot{\boldsymbol{q}}. \tag{3.10}$$

Thus, taking note of the formal similarity between the definitions $(3.8)_{1,2}$ and those in (2.18) for the bulk configurational stress $\boldsymbol{C}$ and configurational momentum density $\boldsymbol{q}$ of the sharp-interface theory, we recognize $\boldsymbol{C}$ and $\boldsymbol{q}$ as the configurational stress and configurational momentum density relevant to the order-parameter based theory. Moreover, bearing in mind these identifications and the balance (3.10), we recognize $\boldsymbol{f}$ as the internal configurational force of the order-parameter based theory.[27] Further, equation (3.10) is the local statement of configurational momentum balance for that theory.

[26] FRIED & GURTIN refer to β as the *kinetic modulus.* If the theory incorporated an inelastic functional dependence on the deformation and, thus, a dissipative contribution to the deformational stress, it might be more suitable to refer to β the *micro*damping modulus.

[27] The representations (3.8) for the fields $\boldsymbol{C}$, $\boldsymbol{q}$, and $\boldsymbol{f}$ can be derived from the perspective of GURTIN [21, 22] (see also CERMELLI, FRIED & GRACH [23]).

Considering the identity

$$\operatorname{div} \boldsymbol{C} + \boldsymbol{f} - \dot{\boldsymbol{q}} = -(\operatorname{div} \boldsymbol{\xi} + \pi)\boldsymbol{p} \tag{3.11}$$

that results from (3.9) under the assumption that the linear momentum balance $(3.4)_1$ holds, we see that the microforce balance $(3.4)_3$ implies the configurational momentum balance (3.10);[28] conversely, granted that $\boldsymbol{p}$ does not vanish, (3.11) shows that the configurational momentum balance (3.10) implies the microforce balance $(3.4)_3$. Hence, on any subregion $\mathcal{R}$ of $\mathcal{B}$ where $\boldsymbol{p}$ is nonvanishing, we may impose—in place of the microforce balance $(3.4)_3$—the configurational momentum balance (3.10) or the equivalent requirement that

$$\int_{\partial\mathcal{P}} \boldsymbol{C}\boldsymbol{\nu}\, da + \int_{\mathcal{P}} \boldsymbol{f}\, dv = \overline{\int_{\mathcal{P}} \boldsymbol{q}\, dv} \tag{3.12}$$

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

4 Constitutive specialization

Here our goal is to identify a subclass of the constitutive equations (3.5) for which the order-parameter based 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 in equilibrium,

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

iii. orientation, deformation-gradient, and interfacial 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 ranges 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. there exist connected sets $\mathcal{U}_a$ and $\mathcal{U}_b$ of positive-definite symmetric tensors whose intersection $\mathcal{U}_a \cap \mathcal{U}_b$ is a single tensor $\boldsymbol{U}_*$, such that:

[28] Hence, just as the *bulk* configurational momentum balance of the sharp-interface theory is redundant within that theory (cf. the discussion at the outset of Section 2.4), the configurational momentum balance (3.10) is redundant within the order-parameter based theory.

a. *the natural stretches* $\boldsymbol{U}_\mathfrak{a}$ *and* $\boldsymbol{U}_\mathfrak{b}$ *associated with the bulk phases* $\mathfrak{a}$ *and* $\mathfrak{b}$ *of the sharp-interface theory are contained in* $\mathcal{U}_\mathfrak{a} \setminus \{\boldsymbol{U}_*\}$ *and* $\mathcal{U}_\mathfrak{b} \setminus \{\boldsymbol{U}_*\}$, *respectively;*

b. *for each* $\boldsymbol{U}$ *in the union* $\mathcal{U}_\mathfrak{a} \cup \mathcal{U}_\mathfrak{b}$ *of the sets* $\mathcal{U}_\mathfrak{a}$ *and* $\mathcal{U}_\mathfrak{b}$, $\hat{W}(\boldsymbol{U}, \cdot, \boldsymbol{0})$ *possesses exactly two minima, which are attained at* $\varphi = \varphi_\mathfrak{a}(\boldsymbol{U})$ *and* $\varphi = \varphi_\mathfrak{b}(\boldsymbol{U})$, *where, without loss of generality,* $\varphi_\mathfrak{a}(\boldsymbol{U}) < \varphi_\mathfrak{b}(\boldsymbol{U})$;

c. *the minima of* $\hat{W}(\boldsymbol{U}, \cdot, \boldsymbol{0})$ *obey*

$$\hat{W}(\boldsymbol{U}, \varphi_\mathfrak{a}(\boldsymbol{U}), \boldsymbol{0}) < \hat{W}(\boldsymbol{U}, \varphi_\mathfrak{b}(\boldsymbol{U}), \boldsymbol{0})$$

when $\boldsymbol{U}$ *is an element of* $\mathcal{U}_\mathfrak{a} \setminus \{\boldsymbol{U}_*\}$, *and*

$$\hat{W}(\boldsymbol{U}, \varphi_\mathfrak{a}(\boldsymbol{U}), \boldsymbol{0}) > \hat{W}(\boldsymbol{U}, \varphi_\mathfrak{b}(\boldsymbol{U}), \boldsymbol{0})$$

when $\boldsymbol{U}$ *is an element of* $\mathcal{U}_\mathfrak{b} \setminus \{\boldsymbol{U}_*\}$.

An immediate consequence of *A1* is that the values $\hat{W}(\boldsymbol{U}_*, \varphi_\mathfrak{a}(\boldsymbol{U}_*), \boldsymbol{0})$ and $\hat{W}(\boldsymbol{U}_*, \varphi_\mathfrak{b}(\boldsymbol{U}_*), \boldsymbol{0})$ of the energy density must be equal; hence, without loss of generality, we require that

$$\hat{W}(\boldsymbol{U}_*, \varphi_\mathfrak{a}(\boldsymbol{U}_*), \boldsymbol{0}) = \hat{W}(\boldsymbol{U}_*, \varphi_\mathfrak{b}(\boldsymbol{U}_*), \boldsymbol{0}) = 0. \tag{4.1}$$

Now, by virtue of *A1* and (4.1), the energy density Ψ determined by

$$\Psi(\varphi) = \hat{W}(\boldsymbol{U}_*, \varphi, \boldsymbol{0}) \tag{4.2}$$

is a double-well potential whose minima coincide. We refer to Ψ as the *exchange energy density* and assume, again without loss in generality, that

$$\varphi_\mathfrak{a}(\boldsymbol{U}_*) = 0 \qquad \text{and} \qquad \varphi_\mathfrak{b}(\boldsymbol{U}_*) = 1, \tag{4.3}$$

so that, by (4.1), the exchange energy density obeys (cf. Fig. 2)

$$\Psi(0) = \Psi(1) = 0 \qquad \text{and} \qquad \Psi(\varphi) > 0 \qquad \text{for} \qquad \varphi \neq 0, 1. \tag{4.4}$$

The set $\{\varphi : \Psi'(\varphi) < 0\}$ is the *spinodal* of Ψ; roughly speaking, the order-parameter values $\varphi \approx 0$ and $\varphi \approx 1$ characterize the bulk material of phases $\mathfrak{a}$ and $\mathfrak{b}$, respectively, while an interval $(q_\mathfrak{a}, q_\mathfrak{b})$, with $\{\varphi : \Psi'(\varphi) < 0\} \subsetneq (q_\mathfrak{a}, q_\mathfrak{b}) \subsetneq (0, 1)$, defines layers that serve as phase interfaces. Anticipating a result established in Section 8.2, we assume that $|\boldsymbol{p}|$ does not vanish within such transition layers, whereby the level sets $\{\boldsymbol{x} : \varphi(\boldsymbol{x}, \cdot) = q, q_\mathfrak{a} < q < q_\mathfrak{b}\}$ will actually be *surfaces* that propagate with scalar normal velocity field

$$V = -\frac{\dot{\varphi}}{|\boldsymbol{p}|} \tag{4.5}$$

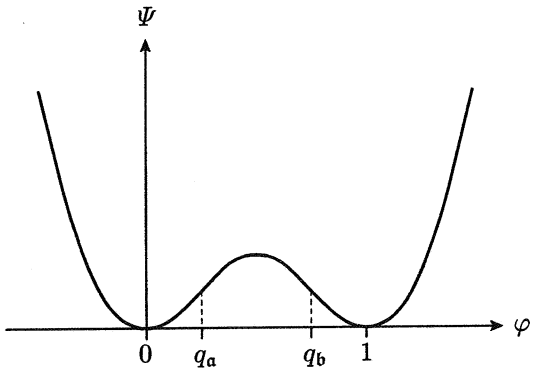

Figure 2. Graph depicting the qualitative properties of Ψ.

in the direction of the unit vector field

$$\boldsymbol{n} = \frac{\boldsymbol{p}}{|\boldsymbol{p}|}. \tag{4.6}$$

Following FRIED & GURTIN [16], we refer these sets as *uniformity surfaces.*[29]

4.2 Gradient energy

While the exchange energy establishes a preference for equilibrium states in which φ is homogeneously equal to either 0 or 1, it is constitutive dependence on $\boldsymbol{p}$ through the *gradient energy density* γ determined by

$$\gamma(\boldsymbol{F}, \varphi, \boldsymbol{p}) = \hat{W}(\boldsymbol{F}, \varphi, \boldsymbol{p}) - \hat{W}(\boldsymbol{F}, \varphi, \boldsymbol{0}) \tag{4.7}$$

that allows for these preferred order-parameter values to coexist and be connected by smooth layers. To account for orientation dependence in the response function $\hat{w}$ delivering the interfacial energy density w of the sharp-interface theory, we express dependence on $\boldsymbol{p} = |\boldsymbol{p}|\boldsymbol{n}$ in terms of separate dependencies on the variables $|\boldsymbol{p}|$ and $\boldsymbol{n}$, and, in particular, take the gradient energy to be quadratic in $|\boldsymbol{p}|$ but an arbitrary function of $\boldsymbol{n}$.[30] Letting

$$\boldsymbol{P} = \boldsymbol{1} - \boldsymbol{n} \otimes \boldsymbol{n} \tag{4.8}$$

denote the projector onto uniformity surfaces, we will incorporate deformational contributions to the interfacial energy density by allowing the gradient energy density to depend on the component

$$\boldsymbol{\Gamma} = \boldsymbol{F}\boldsymbol{P} \tag{4.9}$$

[29] Various facts concerning uniformity surfaces, that will be useful in the sequel, are collected in Appendix A.3.

[30] A basis for our assumption that γ be a quadratic function of $|\boldsymbol{p}|$ is discussed in Section 6.

of the deformation gradient tangential to uniformity surfaces, so that the gradient energy density accounts for deformation induced stretching of a uniformity surface in directions tangent to itself. Further, we require that the gradient energy density be independent of φ. Precisely, we assume that:

A2. the gradient energy density γ satisfies the functional equation

$$\gamma(\boldsymbol{F}_1, \varphi_1, \alpha \boldsymbol{p}) = \alpha^2 \gamma(\boldsymbol{F}_2, \varphi_2, \boldsymbol{p})$$

for all $\boldsymbol{F}_1$ and $\boldsymbol{F}_2$ such that $\boldsymbol{F}_1\boldsymbol{P} = \boldsymbol{F}_2\boldsymbol{P}$ (with $\boldsymbol{P} = \boldsymbol{1} - \boldsymbol{n}\otimes\boldsymbol{n}$ and $\boldsymbol{n} = \boldsymbol{p}/|\boldsymbol{p}|$), for all φ_1 and φ_2, for all $\boldsymbol{p}$, and for all α.

As a straightforward consequence of *A2*, we find that γ admits a representation of the form

$$\gamma(\boldsymbol{F}, \varphi, \boldsymbol{p}) = \tfrac{1}{2}|\boldsymbol{p}|^2 \lambda(\boldsymbol{\Gamma}, \boldsymbol{n}), \tag{4.10}$$

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

$$\lambda(\cdot, -\boldsymbol{n}) = \lambda(\cdot, \boldsymbol{n}) \tag{4.11}$$

for all unit vectors $\boldsymbol{n}$.

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 orientation and interfacial normal velocity dependence in the response function $\hat{b}$ delivering the kinetic coefficient b of the sharp-interface theory, $\hat{\beta}$ should depend on $(\boldsymbol{p}, \dot{\varphi}) = |\boldsymbol{p}|(\boldsymbol{n}, -V)$ through $(\boldsymbol{n}, -V)$; we do not, however, allow for a dependence of $\hat{\beta}$ on $|\boldsymbol{p}|$.[31] Further, we require that $\hat{\beta}$, like γ, depend on the deformation gradient $\boldsymbol{F}$ through at most $\boldsymbol{F}\boldsymbol{P} = \boldsymbol{\Gamma}$ and be independent of φ. Precisely, we assume that:

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

$$\hat{\beta}(\boldsymbol{F}_1, \varphi_1, \alpha \boldsymbol{p}, \alpha v) = \hat{\beta}(\boldsymbol{F}_1, \varphi_2, \boldsymbol{p}, v)$$

for all $\boldsymbol{F}_1$ and $\boldsymbol{F}_2$ such that $\boldsymbol{F}_1\boldsymbol{P} = \boldsymbol{F}_2\boldsymbol{P}$ (with $\boldsymbol{P} = \boldsymbol{1} - \boldsymbol{n}\otimes\boldsymbol{n}$ and $\boldsymbol{n} = \boldsymbol{p}/|\boldsymbol{p}|$), for all φ_1 and φ_2, for all $\boldsymbol{p}$, for all v, and for all α.

Employing *A3*, we find readily that $\hat{\beta}$ admits a representation in the form

$$\hat{\beta}(\boldsymbol{F}, \varphi, \boldsymbol{p}, \dot{\varphi}) = \tilde{\beta}(\boldsymbol{\Gamma}, \boldsymbol{n}, V). \tag{4.12}$$

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

4.4 Decomposition of fields into bulk and excess components

Since $\Psi(0) = \Psi(1) = 0$, the exchange energy density does not contribute sensibly to the energy of the bulk phases. It does, however, contribute to the energy of transition layers, wherein φ varies between $q_{\mathfrak{a}}$ and $q_{\mathfrak{b}}$. Thus, in light of the expressions (4.2) and (4.7) defining Ψ and γ, we are motivated to decompose the energy density as a sum

$$W = W^{\mathrm{bu}} + W^{\mathrm{xs}} \tag{4.13}$$

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

$$\begin{aligned} W^{\mathrm{bu}} &= \hat{W}^{\mathrm{bu}}(\boldsymbol{F}, \varphi) \\ &= \hat{W}(\boldsymbol{F}, \varphi, \boldsymbol{0}) - \hat{W}(\boldsymbol{U}_*, \varphi, \boldsymbol{0}) \\ &= \hat{W}(\boldsymbol{F}, \varphi, \boldsymbol{0}) - \Psi(\varphi) \end{aligned} \tag{4.14}$$

and

$$\begin{aligned} W^{\mathrm{xs}} &= \hat{W}^{\mathrm{xs}}(\boldsymbol{F}, \varphi, \boldsymbol{p}) \\ &= \hat{W}(\boldsymbol{F}, \varphi, \boldsymbol{p}) - \hat{W}^{\mathrm{bu}}(\boldsymbol{F}, \varphi) \\ &= \Psi(\varphi) + \tfrac{1}{2}|\boldsymbol{p}|^2 \lambda(\boldsymbol{\Gamma}, \boldsymbol{n}), \end{aligned} \tag{4.15}$$

respectively.

Together with the constitutive equations $(3.5)_2$ and $(3.5)_3$, the decomposition (4.13)–(4.15) of W leads immediately to natural decompositions of the deformational stress $\boldsymbol{S}$ and the microstress $\boldsymbol{\xi}$ into bulk and excess components. Specifically, we find that[32]

$$\boldsymbol{S} = \boldsymbol{S}^{\mathrm{bu}} + \boldsymbol{S}^{\mathrm{xs}} \qquad \text{and} \qquad \boldsymbol{\xi} = \boldsymbol{\xi}^{\mathrm{xs}}, \tag{4.16}$$

where, by virtue of the relations (A.30) and $(A.31)_2$ of Appendix A.3,

$$\left.\begin{aligned} \boldsymbol{S}^{\mathrm{bu}} = \frac{\partial}{\partial \boldsymbol{F}} \hat{W}^{\mathrm{bu}}(\boldsymbol{F}, \varphi), \qquad \boldsymbol{S}^{\mathrm{xs}} = \tfrac{1}{2}|\boldsymbol{p}|^2 \frac{\partial}{\partial \boldsymbol{\Gamma}} \lambda(\boldsymbol{\Gamma}, \boldsymbol{n}), \\ \boldsymbol{\xi}^{\mathrm{xs}} = |\boldsymbol{p}| \big(\lambda(\boldsymbol{\Gamma}, \boldsymbol{n}) \boldsymbol{n} - \tfrac{1}{2} \big(\frac{\partial}{\partial \boldsymbol{\Gamma}} \lambda(\boldsymbol{\Gamma}, \boldsymbol{n})\big)^{\mathrm{T}} \boldsymbol{F} \boldsymbol{n} + \tfrac{1}{2} \frac{D}{D\boldsymbol{n}} \lambda(\boldsymbol{\Gamma}, \boldsymbol{n})\big), \end{aligned}\right\} \tag{4.17}$$

Further, the decompositions (4.13), $(4.16)_1$, and $(4.16)_2$ of W, $\boldsymbol{S}$, and $\boldsymbol{\xi}$ yield, bearing in mind the definition $(3.8)_1$ of $\boldsymbol{C}$, a decomposition

$$\boldsymbol{C} = \boldsymbol{C}^{\mathrm{bu}} + \boldsymbol{C}^{\mathrm{xs}} \tag{4.18}$$

[32] 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.

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

$$\left.\begin{aligned} \boldsymbol{C}^{\rm bu} &= (W^{\rm bu} - \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2)\boldsymbol{1} - \boldsymbol{F}^T\boldsymbol{S}^{\rm bu}, \\ \boldsymbol{C}^{\rm xs} &= W^{\rm xs}\boldsymbol{1} - \boldsymbol{F}^T\boldsymbol{S}^{\rm xs} - \boldsymbol{p}\otimes\boldsymbol{\xi}^{\rm xs}. \end{aligned}\right\} \tag{4.19}$$

A useful alternative to the expression $(4.19)_2$ for the excess configurational stress $\boldsymbol{C}^{\rm xs}$ is

$$\boldsymbol{C}^{\rm xs} = W^{\rm xs}\boldsymbol{P} - \boldsymbol{\Gamma}^T\boldsymbol{S}^{\rm xs} + \boldsymbol{n}\otimes\boldsymbol{c}^{\rm xs} + \jmath^{\rm xs}\boldsymbol{n}\otimes\boldsymbol{n}, \tag{4.20}$$

with $\boldsymbol{c}^{\rm xs}$ and $\jmath^{\rm xs}$ defined by

$$\left.\begin{aligned} \boldsymbol{c}^{\rm xs} &= \boldsymbol{P}(\boldsymbol{C}^{\rm xs})^T\boldsymbol{n} = -\big((\boldsymbol{S}^{\rm xs})^T\boldsymbol{F}\boldsymbol{n} + |\boldsymbol{p}|\boldsymbol{P}\boldsymbol{\xi}^{\rm xs}\big), \\ \jmath^{\rm xs} &= \boldsymbol{n}\cdot(\boldsymbol{C}^{\rm xs}\boldsymbol{n}) = \Psi(\varphi) - \tfrac{1}{2}|\boldsymbol{p}|^2\lambda(\boldsymbol{\Gamma},\boldsymbol{n}). \end{aligned}\right\} \tag{4.21}$$

Further, using the expressions $(4.17)_2$ and $(4.17)_3$ for $\boldsymbol{S}^{\rm xs}$ and $\boldsymbol{\xi}^{\rm xs}$ in the first of (4.21), we determine a more convenient representation,

$$\boldsymbol{c}^{\rm xs} = -\tfrac{1}{2}|\boldsymbol{p}|^2\frac{D}{D\boldsymbol{n}}\lambda(\boldsymbol{\Gamma},\boldsymbol{n}), \tag{4.22}$$

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

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

$$\pi = \pi^{\rm bu} + \pi^{\rm xs}, \qquad \boldsymbol{f} = \boldsymbol{f}^{\rm xs}, \qquad \Delta = \Delta^{\rm xs}, \tag{4.23}$$

with

$$\left.\begin{aligned} \pi^{\rm bu} &= -\frac{\partial}{\partial\varphi}\hat{W}^{\rm bu}(\boldsymbol{F},\varphi), \qquad \pi^{\rm xs} = -\Psi'(\varphi) + |\boldsymbol{p}|\tilde{\beta}(\boldsymbol{\Gamma},\boldsymbol{n},V)V, \\ \boldsymbol{f}^{\rm xs} &= -|\boldsymbol{p}|^2\tilde{\beta}(\boldsymbol{\Gamma},\boldsymbol{n},V)V\boldsymbol{n}, \quad \Delta^{\rm xs} = |\boldsymbol{p}|^2\tilde{\beta}(\boldsymbol{\Gamma},\boldsymbol{n},V)V^2. \end{aligned}\right\} \tag{4.24}$$

Finally, using the expressions (4.15), $(4.17)_2$, $(4.21)_2$, (4.22), and $(4.24)_3$ for $W^{\rm xs}$, $\boldsymbol{S}^{\rm xs}$, $\jmath^{\rm xs}$, $\boldsymbol{c}^{\rm xs}$, and $\boldsymbol{f}^{\rm xs}$ in the relations $(4.17)_3$ and $(4.24)_2$ for the excess components of the microstress and internal microforce, we find that

$$\left.\begin{aligned} |\boldsymbol{p}|\boldsymbol{\xi}^{\rm xs} &= (W^{\rm xs} - \jmath^{\rm xs})\boldsymbol{n} - (\boldsymbol{S}^{\rm xs})^T\boldsymbol{F}\boldsymbol{n} - \boldsymbol{c}^{\rm xs}, \\ |\boldsymbol{p}|\pi^{\rm xs} &= -\tfrac{1}{2}\big(\nabla(W^{\rm xs} + \jmath^{\rm xs})\big)\cdot\boldsymbol{n} - \boldsymbol{f}^{\rm xs}\cdot\boldsymbol{n}. \end{aligned}\right\} \tag{4.25}$$

5 Scaling

In this section we scale the dependent and independent variables of the order-parameter based 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.

5.1 Preliminaries

We let μ and κ denote scale factors associated with the constitutive functions delivering the bulk and excess energy densities, respectively; for example,

$$\left.\begin{aligned} \mu &= \max_{\mathfrak{c}=\mathfrak{a},\mathfrak{b}} \{ \big| \frac{\partial^2}{\partial \boldsymbol{F}^2} \hat{W}^{\mathrm{bu}}(\boldsymbol{F}, \varphi_{\mathfrak{c}}(\boldsymbol{U}_*)) \big|_{\boldsymbol{F}=\boldsymbol{U}_{\mathfrak{c}}} \}, \\ \kappa &= \max_{\boldsymbol{n}\in\mathcal{K}} \{ \lambda(\mathbb{U}_{\mathfrak{S}}(\boldsymbol{n}), \boldsymbol{n}) \}, \end{aligned} \right\} \tag{5.1}$$

with $\boldsymbol{U}_{\mathfrak{c}}$ the natural stretch in phase $\mathfrak{c}$ and $\mathbb{U}_{\mathfrak{S}}(\boldsymbol{n})$ the natural interfacial stretch for $\boldsymbol{n} \in \mathcal{K}$.[33] Then, letting L denote a characteristic length and T a characteristic time, we assume that μ and κ yield a small dimensionless modulus

$$0 < \epsilon = \frac{\kappa}{\mu L^2} \ll 1, \tag{5.2}$$

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

$$\boldsymbol{x} = \frac{\boldsymbol{x}^*}{L}, \quad t = \frac{t^*}{T}, \quad \boldsymbol{y}(\boldsymbol{x}, t) = \frac{1}{L}\boldsymbol{y}^*(\boldsymbol{x}^*, t^*), \quad \varphi(\boldsymbol{x}, t) = \varphi^*(\boldsymbol{x}^*, t^*), \tag{5.3}$$

mass density

$$\varrho = \frac{L^2}{\mu T^2}\varrho^*, \tag{5.4}$$

and constitutive functions

$$\left.\begin{aligned} \hat{W}^{\mathrm{bu}}(\boldsymbol{F}, \varphi) &= \frac{1}{\mu}\hat{W}^{\mathrm{bu}*}(\boldsymbol{F}^*, \varphi^*), \\ \Psi(\varphi) &= \frac{\kappa}{\mu^2 L^2}\Psi^*(\varphi^*), \\ \lambda(\boldsymbol{\Gamma}, \boldsymbol{n}) &= \frac{1}{\kappa}\lambda^*(\boldsymbol{\Gamma}^*, \boldsymbol{n}^*), \\ \tilde{\beta}(\boldsymbol{\Gamma}, \boldsymbol{n}, V) &= \frac{L^2}{\kappa T}\tilde{\beta}^*(\boldsymbol{\Gamma}^*, \boldsymbol{n}^*, V^*), \end{aligned} \right\} \tag{5.5}$$

where the quantities without asterisks in (5.3), (5.4), and (5.5) are assumed to be of $O(1)$ in ϵ.

This scaling yields

$$\boldsymbol{W}^{\mathrm{bu}*} = \mu \boldsymbol{W}^{\mathrm{bu}}, \quad \boldsymbol{S}^{\mathrm{bu}*} = \mu \boldsymbol{S}^{\mathrm{bu}}, \quad \boldsymbol{C}^{\mathrm{bu}*} = \mu \boldsymbol{C}^{\mathrm{bu}}, \quad \pi^{\mathrm{bu}*} = \mu \pi^{\mathrm{bu}}, \tag{5.6}$$

[33] Cf. the discussion concluding Section 2.3.

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

$$\left.\begin{aligned} W^{\rm bu} &= \hat{W}^{\rm bu}(\boldsymbol{F},\varphi),\\ \boldsymbol{S}^{\rm bu} &= \frac{\partial}{\partial \boldsymbol{F}}\hat{W}^{\rm bu}(\boldsymbol{F},\varphi),\\ \boldsymbol{C}^{\rm bu} &= (W^{\rm bu} - \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2)\boldsymbol{1} - \boldsymbol{F}^T\boldsymbol{S}^{\rm bu},\\ \pi^{\rm bu} &= -\frac{\partial}{\partial\varphi}\hat{W}^{\rm bu}(\boldsymbol{F},\varphi), \end{aligned}\right\} \tag{5.7}$$

as well as

$$\left.\begin{aligned} W^{\rm xs*} = \epsilon\mu W^{\rm xs},\quad \boldsymbol{S}^{\rm xs*} = \epsilon\mu\boldsymbol{S}^{\rm xs},\quad \boldsymbol{C}^{\rm xs*} = \epsilon\mu\boldsymbol{C}^{\rm xs},\quad \boldsymbol{\xi}^{\rm xs*} = \epsilon\mu L\boldsymbol{\xi}^{\rm xs},\\ \pi^{\rm xs*} = \epsilon\mu\pi^{\rm xs},\quad \boldsymbol{f}^{\rm xs*} = \epsilon\frac{\mu}{L}\boldsymbol{f}^{\rm xs},\quad \Delta^{\rm xs*} = \epsilon\frac{\mu}{T}\Delta^{\rm xs}, \end{aligned}\right\} \tag{5.8}$$

with

$$\left.\begin{aligned} W^{\rm xs} &= |\boldsymbol{p}|^2\lambda(\boldsymbol{\Gamma},\boldsymbol{n}) + \jmath^{\rm xs},\\ \boldsymbol{S}^{\rm xs} &= \tfrac{1}{2}|\boldsymbol{p}|^2\frac{\partial}{\partial\boldsymbol{\Gamma}}\lambda(\boldsymbol{\Gamma},\boldsymbol{n}),\\ \boldsymbol{C}^{\rm xs} &= W^{\rm xs}\boldsymbol{P} - \boldsymbol{\Gamma}^T\boldsymbol{S}^{\rm xs} + \boldsymbol{n}\otimes\boldsymbol{c}^{\rm xs} + \jmath^{\rm xs}\boldsymbol{n}\otimes\boldsymbol{n},\\ \boldsymbol{\xi}^{\rm xs} &= |\boldsymbol{p}|^{-1}\big((W^{\rm xs} - \jmath^{\rm xs})\boldsymbol{n} - (\boldsymbol{S}^{\rm xs})^T\boldsymbol{F}\boldsymbol{n} - \boldsymbol{c}^{\rm xs}\big),\\ \pi^{\rm xs} &= -\epsilon^{-2}\Psi'(\varphi) + |\boldsymbol{p}|\tilde{\beta}(\boldsymbol{\Gamma},\boldsymbol{n},V)V,\\ \boldsymbol{f}^{\rm xs} &= -|\boldsymbol{p}|^2\tilde{\beta}(\boldsymbol{\Gamma},\boldsymbol{n},V)V\boldsymbol{n},\\ \Delta^{\rm xs} &= |\boldsymbol{p}|^2\tilde{\beta}(\boldsymbol{\Gamma},\boldsymbol{n},V)V^2, \end{aligned}\right\} \tag{5.9}$$

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

$$\boldsymbol{c}^{\rm xs} = -\tfrac{1}{2}|\boldsymbol{p}|^2\frac{D}{D\boldsymbol{n}}\lambda(\boldsymbol{\Gamma},\boldsymbol{n}) \quad\text{and}\quad \jmath^{\rm xs} = \epsilon^{-2}\Psi(\varphi) - \tfrac{1}{2}|\boldsymbol{p}|^2\lambda(\boldsymbol{\Gamma},\boldsymbol{n}) \tag{5.10}$$

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

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

$$dv = \frac{1}{L^3}dv^* \qquad\text{and}\qquad da = \frac{1}{L^2}da^* \tag{5.11}$$

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

5.2 Scaled integral laws expressing linear momentum balance, angular momentum balance, configurational momentum balance, and dissipation imbalance

The integral statements $(3.2)_1$, $(3.2)_2$, (3.12), and (3.3) expressing linear momentum balance, angular momentum balance, configurational momentum balance, and dissipation imbalance were written for the unscaled fields. Hence, we think of the terms appearing in these as carrying asterisks. If we use the scaling relations (5.3), (5.4), (5.6), (5.8), and (5.11) to convert these statements to nondimensional form, we find that they remain valid as is (i.e., without asterisks), but with the underlying fields given by (5.7), (5.9), and (5.10), so that the balances for linear, angular, and configurational momentum for $\mathcal{P}$ read

$$\left.\begin{aligned} \int_{\partial\mathcal{P}} (\boldsymbol{S}^{\mathrm{bu}} + \epsilon \boldsymbol{S}^{\mathrm{xs}})\boldsymbol{\nu}\, da &= \overline{\int_{\mathcal{P}} \varrho \dot{\boldsymbol{y}}\, dv}^{\cdot}, \\ \int_{\partial\mathcal{P}} \boldsymbol{y}\times(\boldsymbol{S}^{\mathrm{bu}} + \epsilon \boldsymbol{S}^{\mathrm{xs}})\boldsymbol{\nu}\, da &= \overline{\int_{\mathcal{P}} \boldsymbol{y}\times\varrho \dot{\boldsymbol{y}}\, dv}^{\cdot}, \\ \int_{\partial\mathcal{P}} (\boldsymbol{C}^{\mathrm{bu}} + \epsilon \boldsymbol{C}^{\mathrm{xs}})\boldsymbol{\nu}\, da + \int_{\mathcal{P}} \epsilon \boldsymbol{f}^{\mathrm{xs}}\, dv &= \overline{\int_{\mathcal{P}} \boldsymbol{q}\, dv}^{\cdot}, \end{aligned}\right\} \tag{5.12}$$

and the dissipation imbalance for $\mathcal{P}$ becomes

$$\int_{\partial\mathcal{P}} \left((\boldsymbol{S}^{\mathrm{bu}} + \epsilon \boldsymbol{S}^{\mathrm{xs}})\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}} + \epsilon \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\right) da \geq \overline{\int_{\mathcal{P}} (W^{\mathrm{bu}} + \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2 + \epsilon W^{\mathrm{xs}})\, dv}^{\cdot}. \tag{5.13}$$

5.3 Scaled local laws expressing linear momentum balance, angular momentum balance, configurational momentum balance, and dissipation balance

Proceeding as above, we may use the scaling relations (5.3), (5.4), (5.6), and (5.8) to obtain dimensionless versions,

$$\left.\begin{aligned} \operatorname{div}(\boldsymbol{S}^{\mathrm{bu}} + \epsilon \boldsymbol{S}^{\mathrm{xs}}) &= \varrho \ddot{\boldsymbol{y}}, \\ \boldsymbol{F}(\boldsymbol{S}^{\mathrm{bu}} + \epsilon \boldsymbol{S}^{\mathrm{xs}})^T &= (\boldsymbol{S}^{\mathrm{bu}} + \epsilon \boldsymbol{S}^{\mathrm{xs}})\boldsymbol{F}^T, \\ \operatorname{div}(\boldsymbol{C}^{\mathrm{bu}} + \epsilon \boldsymbol{C}^{\mathrm{xs}}) + \epsilon \boldsymbol{f}^{\mathrm{xs}} &= \dot{\boldsymbol{q}}, \end{aligned}\right\} \tag{5.14}$$

of the local balances $(3.4)_1$, $(3.4)_2$, and (3.10) for linear momentum, angular momentum, and configurational momentum as well as a dimensionless version

$$(\boldsymbol{S}^{\mathrm{bu}} + \epsilon \boldsymbol{S}^{\mathrm{xs}})\cdot\dot{\boldsymbol{F}} + \boldsymbol{\xi}^{\mathrm{xs}}\cdot\dot{\boldsymbol{p}} - (\pi^{\mathrm{bu}} + \epsilon\pi^{\mathrm{xs}})\dot{\varphi} - \dot{W}^{\mathrm{bu}} - \epsilon\dot{W}^{\mathrm{xs}} = \epsilon\Delta^{\mathrm{xs}} \tag{5.15}$$

of the local dissipation balance (3.6).

For later use, we observe that, in regions where $\boldsymbol{p}$ does not vanish the vectorial configurational momentum balance $(5.14)_3$ is, bearing in mind the expression $(5.9)_6$ for $\boldsymbol{f}^{\mathrm{xs}}$, equivalent to a scalar equation

$$(\operatorname{div}(\boldsymbol{C}^{\mathrm{bu}} + \epsilon \boldsymbol{C}^{\mathrm{xs}}) + \boldsymbol{f}^{\mathrm{xs}})\cdot\boldsymbol{n} = \dot{\boldsymbol{q}}\cdot\boldsymbol{n} \tag{5.16}$$

that enforces the balance of configurational momentum normal to uniformity surfaces.

Now, upon introducing the tensor field

$$\boldsymbol{L} = -(\nabla\boldsymbol{n})\boldsymbol{P}, \tag{5.17}$$

which determines the curvature of uniformity surfaces, and using once again $(5.7)_3$ and $(5.9)_3$, the normal configurational balance (5.16) can be written as

$$(\operatorname{div}\boldsymbol{C}^{\mathrm{bu}} - \dot{\boldsymbol{q}})\cdot\boldsymbol{n} + \epsilon\boldsymbol{C}^{\mathrm{xs}}\cdot\boldsymbol{L} + \epsilon\operatorname{div}\boldsymbol{c}^{\mathrm{xs}} + \epsilon\boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n} + \epsilon\operatorname{div}(\jmath^{\mathrm{xs}}\boldsymbol{n}) = 0. \tag{5.18}$$

Further, a direct but lengthy calculation using the expression $(5.9)_4$ for $\boldsymbol{\xi}^{\mathrm{xs}}$, the identities

$$\left.\begin{aligned} \boldsymbol{S}^{\mathrm{bu}}\cdot\dot{\boldsymbol{F}} + \big(\operatorname{div}(\boldsymbol{F}^T\boldsymbol{S}^{\mathrm{bu}})\big)\cdot(V\boldsymbol{n}) &= \boldsymbol{S}^{\mathrm{bu}}\cdot\mathring{\boldsymbol{F}} + (\operatorname{div}\boldsymbol{S}^{\mathrm{bu}})\cdot(V\boldsymbol{F}\boldsymbol{n}),\\ \boldsymbol{S}^{\mathrm{xs}}\cdot\big(\dot{\boldsymbol{F}} + \nabla(V\boldsymbol{F}\boldsymbol{n})\big) &= \boldsymbol{S}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{\Gamma}} - (\boldsymbol{\Gamma}^T\boldsymbol{S}^{\mathrm{xs}})\cdot(V\boldsymbol{L}),\\ \boldsymbol{C}^{\mathrm{xs}}\cdot\boldsymbol{L} &= W^{\mathrm{xs}}K - (\boldsymbol{\Gamma}^T\boldsymbol{S}^{\mathrm{xs}})\cdot\boldsymbol{L}, \end{aligned}\right\} \tag{5.19}$$

and the relation (A.28) determining ∇V shows that, wherever $\boldsymbol{p}$ does not vanish, the dimensionless local dissipation balance (5.15) can be written as[34]

$$\begin{aligned} &(\boldsymbol{S}^{\mathrm{bu}}\cdot\mathring{\boldsymbol{F}} - \mathring{W}^{\mathrm{bu}}) + \epsilon(\boldsymbol{S}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{\Gamma}} - \boldsymbol{c}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{n}} - (\boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n})V)\\ &\qquad - \epsilon\big(\mathring{W}^{\mathrm{xs}} - (W^{\mathrm{xs}} - \jmath^{\mathrm{xs}})\overline{\ln|\boldsymbol{p}|}^{\circ}\big) = \epsilon\Delta^{\mathrm{xs}}, \end{aligned} \tag{5.20}$$

where $\mathring{g}$ denotes the rate at which g changes following uniformity surfaces (cf. (A.27) of Appendix A.3).

5.4 Scaled local microforce balance

While we have omitted the microforce balance from the lists of scaled integral and local laws given, respectively, in Section 5.2 and Section 5.3, we do not intend to ignore that balance. Indeed, as we have noted in Section 3.4, granted linear momentum balance, configurational momentum balance and microforce

[34] Version (5.20) of the dimensionless dissipation balance is most easily obtained by appeal to the identity $\epsilon\operatorname{div}(\dot{\varphi}\boldsymbol{\xi}^{\mathrm{xs}}) = \epsilon\boldsymbol{\xi}^{\mathrm{xs}}\cdot\dot{\boldsymbol{p}} - (\pi^{\mathrm{bu}} + \epsilon\pi^{\mathrm{xs}})\dot{\varphi}$ (which follows on using the dimensionless local microforce balance (5.21) to simplify (5.15)).

balance are equivalent only in regions where $\boldsymbol{p}$ does not vanish. Thus, in regions, such as those far from any transition layers, where $\boldsymbol{p}$ might be expected to vanish, it is necessary to impose microforce balance in addition to configurational momentum balance.[35] For our purposes, it will be sufficient to impose microforce balance in the scaled local form

$$\epsilon(\operatorname{div}\boldsymbol{\xi}^{\mathrm{xs}}+\pi^{\mathrm{xs}})+\pi^{\mathrm{bu}}=0 \tag{5.21}$$

that results upon using (5.3), (5.6), and (5.8) to render $(3.4)_3$ dimensionless.

6 A constitutive connection

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

$$\left.\begin{aligned} \hat{W}^{\mathrm{a}}(\boldsymbol{F})&=\hat{W}^{\mathrm{bu}}(\boldsymbol{F},0), & \hat{W}^{\mathrm{b}}(\boldsymbol{F})&=\hat{W}^{\mathrm{bu}}(\boldsymbol{F},1),\\ \hat{\boldsymbol{S}}^{\mathrm{a}}(\boldsymbol{F})&=\frac{\partial}{\partial\boldsymbol{F}}\hat{W}^{\mathrm{bu}}(\boldsymbol{F},0), & \hat{\boldsymbol{S}}^{\mathrm{b}}(\boldsymbol{F})&=\frac{\partial}{\partial\boldsymbol{F}}\hat{W}^{\mathrm{bu}}(\boldsymbol{F},1), \end{aligned}\right\} \tag{6.1}$$

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

$$\left.\begin{aligned} \hat{w}(\mathbb{F},\mathbb{n})&=\sigma\sqrt{\lambda(\mathbb{F},\mathbb{n})}, & \hat{\mathbb{S}}(\mathbb{F},\mathbb{n})&=\sigma\frac{\partial}{\partial\mathbb{F}}\sqrt{\lambda(\mathbb{F},\mathbb{n})},\\ \hat{\mathbb{c}}(\mathbb{F},\mathbb{n})&=-\sigma\frac{D}{D\mathbb{n}}\sqrt{\lambda(\mathbb{F},\mathbb{n})}, & \hat{b}(\mathbb{F},\mathbb{n},V_{\mathbb{e}})&=\frac{\sigma\tilde{\beta}(\mathbb{F},\mathbb{n},V_{\mathbb{e}})}{\sqrt{\lambda(\mathbb{F},\mathbb{n})}}, \end{aligned}\right\} \tag{6.2}$$

with the *conversion modulus*[36] σ a constant determined by

$$\sigma=\int_0^1\sqrt{2\Psi(\varphi)}\,d\varphi. \tag{6.3}$$

We emphasize that the connections (6.1) and (6.2) allow for the full level of constitutive generality encompassed by the sharp-interface theory. The bulk

[35] Strictly speaking, one may (as per discussion of Section 3.4) replace configurational momentum balance with microforce balance in regions where $\boldsymbol{p}$ vanishes. However, we will find that imposing both balances in such regions allows us to recover, without recourse to the linear momentum balance, the redundant bulk configurational momentum balance $(2.14)_3$ of the sharp-interface theory.

[36] We borrow the term *conversion modulus* from FRIED & GURTIN [16]—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 (6.3) would require a factor of $1/\sqrt{\lambda(\boldsymbol{F},\boldsymbol{n})}$ for σ to be completely analogous to the conversion modulus of FRIED & GURTIN [16].

relations (6.1) are motivated by our previous discussion and are consistent with the relation $(2.22)_2$ determining $\boldsymbol{S}$. While not at all obvious, the choices $(6.2)_{1,4}$ of interfacial free-energy $\hat{w}$ and kinetic coefficient $\hat{b}$ will be justified from the ensuing asymptotic analysis; given $\hat{w}$, the choices $(6.2)_{2,3}$ are predicated upon the relations $(2.23)_{2,3}$ determining $\mathbb{S}$ and $\mathbb{c}$.

Examining the first of (6.2) and suppressing dependence of $\hat{w}$ on $\mathbb{F}$, we arrive at support for that part of assumption *A2* which requires that the gradient energy density γ be homogeneous of degree two in its dependence on $\boldsymbol{p}$. Indeed, in considering the dependence on orientation of the response function delivering the surface-energy density of a crystalline solid, it is standard to require that the extension of that function to all nonzero vectors be homogeneous of degree one.[37] Appealing to the representation (4.10) for γ through λ and the relation $(6.2)_1$ between $\hat{w}$ and λ, we see that postulating that γ be homogeneous of degree two in its dependence on $\boldsymbol{p}$ ensures that the extension of $\hat{w}$ to all nonvanishing vectors possesses appropriate homogeneity. Similarly, the assumption that γ depend on $\boldsymbol{F}$ through only $\boldsymbol{\Gamma}$ is consistent with the requirement that $\hat{w}$ depend on $\boldsymbol{F}$ through only the $\mathbb{F}$. Analogous remarks commending those aspects of assumption *A3* which require $\tilde{\beta}$ to be homogeneous of degree zero in $\boldsymbol{p}$ and to depend on $\boldsymbol{F}$ through only $\boldsymbol{\Gamma}$ follow from the last of (6.2).

7 Decomposition of the reference region. Expansions

Hereafter, we focus on a process 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 $\varphi(\boldsymbol{x},t,\epsilon) \approx 0$ and $\varphi(\boldsymbol{x},t,\epsilon) \approx 1$, respectively. We assume that the thickness $h(\epsilon)$ of $\mathcal{L}(\cdot,\epsilon)$ tends to zero with ϵ, but at slightly slower rate, viz.

$$\lim_{\epsilon\to 0+} h(\epsilon) = 0 \qquad \text{and} \qquad \lim_{\epsilon\to 0+} \epsilon^{-1} h(\epsilon) = +\infty, \tag{7.1}$$

and that the limit

$$\mathfrak{S} = \lim_{\epsilon\to 0+} \mathcal{L}(\cdot,\epsilon) \tag{7.2}$$

exists, with $\mathfrak{S}$ 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 (7.2) is that

$$\mathcal{B} = \mathcal{B}^{\mathfrak{a}}(t) \cup \mathfrak{S}(t) \cup \mathcal{B}^{\mathfrak{b}}(t), \tag{7.3}$$

[37] See, for example, the discussion of TAYLOR, CAHN & HANDWERKER [14].

where

$$\mathcal{B}^{\mathfrak{c}}(t) = \lim_{\epsilon \to 0+} \mathcal{R}^{\mathfrak{c}}(t, \epsilon) \tag{7.4}$$

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

Consistent with the foregoing, we insist that the motion $\boldsymbol{y}$ has a limit as $\epsilon \to 0+$, and that this limit coincides with a coherent motion $\boldsymbol{y}$ in which $\mathcal{B}$ is divided by a sharp phase interface $\mathfrak{S}$ into regions $\mathcal{B}^{\mathfrak{a}}$ and $\mathcal{B}^{\mathfrak{b}}$:

$$\lim_{\epsilon \to 0+} \boldsymbol{y}(\cdot, \cdot, \epsilon) = \boldsymbol{y}. \tag{7.5}$$

For each field g of interest, in particular for $g = \boldsymbol{y}$ and $g = \varphi$, we consider an *outer expansion*

$$g(\boldsymbol{x}, t, \epsilon) = g_0^{\text{out}}(\boldsymbol{x}, t) + \epsilon g_1^{\text{out}}(\boldsymbol{x}, t) + O(\epsilon^2), \tag{7.6}$$

assumed valid within $\mathcal{R}^{\mathfrak{c}}(t, \epsilon)$, $\mathfrak{c} = \mathfrak{a}, \mathfrak{b}$, and an *inner expansion*

$$g(\boldsymbol{x}, t, \epsilon) = g_0^{\text{in}}\big(r(\boldsymbol{x}, t), \not{z}(\boldsymbol{x}, t), t\big) + \epsilon g_1^{\text{in}}\big(r(\boldsymbol{x}, t), \not{z}(\boldsymbol{x}, t), t\big) + O(\epsilon^2), \tag{7.7}$$

assumed valid within $\mathcal{L}(t, \epsilon)$, with $(\ell, \not{z})$ a coordinate system corresponding to the surface $\mathfrak{S}$,[38] and

$$r(\boldsymbol{x}, t) = \epsilon^{-1} \ell(\boldsymbol{x}, t). \tag{7.8}$$

In letting the inner expansion depend on r rather than on ℓ, we, effectively, stretch the layer so that the coordinate normal to $\mathfrak{S}$ 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 phase interfaces are described—as layers of finite thickness—within the order-parameter based 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

$$\lim_{\ell(\boldsymbol{x}, t) \to 0\pm} g_0^{\text{out}}(\boldsymbol{x}, t) = \lim_{r \to \pm\infty} g_0^{\text{in}}(r, \not{z}, t) \tag{7.9}$$

relating the expansions within the overlap region.

8 Basic estimates

8.1 Estimates in bulk

Using the outer expansions of $\boldsymbol{y}$ and φ in the scaled local microforce balance (5.21) and neglecting terms of $O(1)$ and smaller in ϵ, we find that φ_0^{out} must

[38] We assume that, within the region $\mathcal{L}(\cdot, \epsilon)$, the mapping $\boldsymbol{x} \mapsto (\ell, \not{z})$ is one-to-one. Further details concerning the coordinate system $(\ell, \not{z})$ can be found in Appendix A.3.

satisfy

$$\Psi'(\varphi_0^{\text{out}}) = 0, \tag{8.1}$$

and hence, be constant in $\mathcal{R}^a$ and $\mathcal{R}^b$. By hypothesis, the constant values of φ_0^{out} on either side of $\mathcal{L}$ are required to lie outside of the spinodal. Drawing on the properties (4.4) of Ψ, we therefore conclude that

$$\varphi = \begin{cases} O(\epsilon) & \text{on} \quad \mathcal{R}^a, \\ 1 + O(\epsilon) & \text{on} \quad \mathcal{R}^b, \end{cases} \tag{8.2}$$

that

$$\Psi'(\varphi) = o(1) \quad \text{on} \quad \mathcal{R}^a \cup \mathcal{R}^b, \tag{8.3}$$

that

$$\Psi(\varphi) = o(\epsilon) \quad \text{on} \quad \mathcal{R}^a \cup \mathcal{R}^b, \tag{8.4}$$

and, further, that

$$\dot{\varphi}, \boldsymbol{p}, \dot{\boldsymbol{p}} = O(\epsilon) \quad \text{on} \quad \mathcal{R}^a \cup \mathcal{R}^b. \tag{8.5}$$

Next, the limit (7.5) relating the motions $\boldsymbol{y}$ and $\boldsymbol{y}$ implies that $\boldsymbol{y}_0^{\text{out}} = \boldsymbol{y}$. We therefore have the estimate

$$\boldsymbol{y} = \boldsymbol{y} + O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^a \cup \mathcal{R}^b, \tag{8.6}$$

from which we obtain

$$\left.\begin{aligned} \dot{\boldsymbol{y}} &= \dot{\boldsymbol{y}} + O(\epsilon) \quad \text{on} \quad \mathcal{R}^a \cup \mathcal{R}^b, & \boldsymbol{F} &= \boldsymbol{F} + O(\epsilon) \quad \text{on} \quad \mathcal{R}^a \cup \mathcal{R}^b, \\ \ddot{\boldsymbol{y}} &= \ddot{\boldsymbol{y}} + O(\epsilon) \quad \text{on} \quad \mathcal{R}^a \cup \mathcal{R}^b, & \dot{\boldsymbol{F}} &= \dot{\boldsymbol{F}} + O(\epsilon) \quad \text{on} \quad \mathcal{R}^a \cup \mathcal{R}^b. \end{aligned}\right\} \tag{8.7}$$

Together with the relations (6.1) connecting $\hat{W}^c$ and $\hat{\boldsymbol{S}}^c$ to $\hat{W}^{bu}$ and $\hat{\boldsymbol{S}}^{bu}$ and the expressions $(5.7)_1$, $(5.7)_2$, and $(5.7)_3$ for W^{bu}, $\boldsymbol{S}^{bu}$, and $\boldsymbol{C}^{bu}$, the bulk estimates (8.2) and $(8.7)_2$ for φ and $\boldsymbol{F}$ yield

$$\left.\begin{aligned} W^{bu} &= W + O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^a \cup \mathcal{R}^b, \\ \boldsymbol{S}^{bu} &= \boldsymbol{S} + O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^a \cup \mathcal{R}^b, \\ \boldsymbol{C}^{bu} &= \boldsymbol{C} + O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^a \cup \mathcal{R}^b. \end{aligned}\right\} \tag{8.8}$$

Similarly, the expression $(5.7)_4$ for π^{bu}, (8.2) and $(8.7)_2$ imply that

$$\pi^{bu} = O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^a \cup \mathcal{R}^b. \tag{8.9}$$

Further, on recalling the definition $(3.8)_2$ for the dimensional configurational momentum density $\boldsymbol{q}$, the scaling (5.3) for the dependent and independent variables, and the expression (5.4) for the scaled mass density ϱ, the bulk estimates $(8.7)_{1,2}$ imply that

$$\boldsymbol{q} = \boldsymbol{q} + O(\epsilon) \qquad \text{on} \qquad \mathcal{R}^{\mathrm{a}} \cup \mathcal{R}^{\mathrm{b}}. \tag{8.10}$$

Finally, drawing on the estimates (8.3), (8.4), $(8.5)_2$, and (8.7) and the expressions (5.9) and (5.10) for the excess fields, we conclude that

$$W^{\mathrm{xs}}, \boldsymbol{S}^{\mathrm{xs}}, \boldsymbol{C}^{\mathrm{xs}}, \boldsymbol{\xi}^{\mathrm{xs}}, \pi^{\mathrm{xs}}, \boldsymbol{f}^{\mathrm{xs}}, \Delta^{\mathrm{xs}}, \boldsymbol{c}^{\mathrm{xs}}, \jmath^{\mathrm{xs}} = o(1) \quad \text{on} \quad \mathcal{R}^{\mathrm{a}} \cup \mathcal{R}^{\mathrm{b}}, \tag{8.11}$$

whereby each of those fields is negligible in bulk.

8.2 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 $\mathfrak{S}$ and the coordinate $\mathscr{z}$ on $\mathfrak{S}$. Specifically, given a scalar field g, the identity (A.22) and the relation (7.8) between ℓ and r imply that

$$\nabla g = \epsilon^{-1} \acute{g} \mathscr{n} + \nabla_{\mathfrak{S}} g, \tag{8.12}$$

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

$$\acute{g}(r, \mathscr{z}, t) = \frac{\partial}{\partial r} g(r, \mathscr{z}, t). \tag{8.13}$$

8.2.1 Preliminary results

Bearing in mind the bulk estimate (8.6) for $\boldsymbol{y}$, the requirement that $\boldsymbol{y}$ obey the matching condition implies that $\boldsymbol{y}_0^{\mathrm{in}} = \mathscr{y}$, and we, therefore, obtain

$$\boldsymbol{y} = \mathscr{y} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{8.14}$$

Hence, applying the expression (8.12) for the gradient of a vector field within the layer to the inner expansion of $\boldsymbol{y}$, we find that $\boldsymbol{F}$ admits the estimate

$$\boldsymbol{F} = \mathbb{F} + \acute{\boldsymbol{y}}_1^{\mathrm{in}} \otimes \mathscr{n} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}, \tag{8.15}$$

so that, from the expressions for $(5.7)_1$, $(5.7)_2$, $(5.7)_3$, and $(5.7)_4$ for W^{bu}, $\boldsymbol{S}^{\mathrm{bu}}$, $\boldsymbol{C}^{\mathrm{bu}}$, and π^{bu},

$$W^{\mathrm{bu}}, \boldsymbol{S}^{\mathrm{bu}}, \boldsymbol{C}^{\mathrm{bu}}, \pi^{\mathrm{bu}} = O(1) \qquad \text{on} \qquad \mathcal{L}, \tag{8.16}$$

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

Further, the gradient decomposition (8.12), the definition (A.1) of the normal time-rate following $\mathfrak{S}$, and the identity $\dot{r} = -\epsilon^{-1}V_{\mathfrak{S}}$, which follows from the expression $(A.25)_2$ for $\dot{\ell}$ and the relation (7.8) between ℓ and r, imply the estimate

$$\dot{\boldsymbol{y}} = \mathring{\dot{y}} - V_{\mathfrak{S}}\boldsymbol{y}_1^{\prime\,\mathrm{in}} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{8.17}$$

Next, applying (8.12) to the inner expansion of φ, we obtain

$$\boldsymbol{p} = \epsilon^{-1}\varphi_0^{\prime\,\mathrm{in}}\boldsymbol{n} + \nabla_{\mathfrak{S}}\varphi_0^{\mathrm{in}} + \varphi_1^{\prime\,\mathrm{in}}\boldsymbol{n} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}, \tag{8.18}$$

whereby

$$|\boldsymbol{p}|^2 = \epsilon^{-2}|\varphi_0^{\prime\,\mathrm{in}}|^2 + 2\epsilon^{-1}\varphi_0^{\prime\,\mathrm{in}}\varphi_1^{\prime\,\mathrm{in}} + O(1) \qquad \text{on} \qquad \mathcal{L} \tag{8.19}$$

and

$$|\boldsymbol{p}| = \epsilon^{-1}|\varphi_0^{\prime\,\mathrm{in}}| + \big(\mathrm{sgn}(\varphi_0^{\prime\,\mathrm{in}})\big)\varphi_1^{\prime\,\mathrm{in}} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{8.20}$$

Together, (8.18) and (8.20) yield

$$\boldsymbol{n} = \frac{\boldsymbol{p}}{|\boldsymbol{p}|} = \big(\mathrm{sgn}(\varphi_0^{\prime\,\mathrm{in}})\big)\boldsymbol{n} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}, \tag{8.21}$$

so that

$$\boldsymbol{P} = \boldsymbol{1} - \boldsymbol{n}\otimes\boldsymbol{n} = \mathbb{P} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}, \tag{8.22}$$

and, bearing in mind (8.15),

$$\boldsymbol{\Gamma} = \boldsymbol{F}\boldsymbol{P} = \mathbb{F} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{8.23}$$

Further, from (8.18) and (A.26), we deduce that

$$\begin{aligned}\nabla\nabla\varphi = \epsilon^{-2}\varphi_0^{\prime\prime\,\mathrm{in}}\boldsymbol{n}\otimes\boldsymbol{n} + \epsilon^{-1}\big((\nabla_{\mathfrak{S}}\varphi_0^{\prime\,\mathrm{in}})\otimes\boldsymbol{n} + \boldsymbol{n}\otimes(\nabla_{\mathfrak{S}}\varphi_0^{\prime\,\mathrm{in}})\big)\\ - \epsilon^{-1}\varphi_0^{\prime\,\mathrm{in}}\mathbb{L} + \epsilon^{-1}\varphi_1^{\prime\prime\,\mathrm{in}}\boldsymbol{n}\otimes\boldsymbol{n} + O(1) \quad \text{on} \quad \mathcal{L},\end{aligned} \tag{8.24}$$

which, granted the identity $\nabla\boldsymbol{n} = |\boldsymbol{p}|^{-1}\boldsymbol{P}(\nabla\boldsymbol{p})$ and (8.22), implies that

$$\boldsymbol{L} = -(\nabla\boldsymbol{n})\boldsymbol{P} = \big(\mathrm{sgn}(\varphi_0^{\prime\,\mathrm{in}})\big)\mathbb{L} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{8.25}$$

Finally, appealing once again to the identity $\dot{r} = -\epsilon^{-1}V_{\mathfrak{S}}$, we also find that

$$\dot{\varphi} = -\epsilon^{-1}V_{\mathfrak{S}}\varphi_0^{\prime\,\mathrm{in}} + O(1) \qquad \text{on} \qquad \mathcal{L}, \tag{8.26}$$

which, in combination with (8.18), leads to

$$V = -\frac{\dot{\varphi}}{|\boldsymbol{p}|} = \big(\mathrm{sgn}(\varphi_0^{\prime\,\mathrm{in}})\big)V_{\mathfrak{S}} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L}. \tag{8.27}$$

8.2.2 Partition of energy

Using the estimates (8.15), (8.17), (8.18), (8.21), (8.24), and (8.26) in the scaled local microforce balance (5.21) and imposing (4.11), which requires that λ be an even function of $\boldsymbol{n}$, we find, on neglecting terms of $O(\epsilon^{-1})$ and smaller, that φ_0^{in} must satisfy the differential equation

$$\overline{\Psi(\varphi_0^{\text{in}}) - \tfrac{1}{2}\lambda(\mathbb{F},\mathbb{n})|\acute{\varphi}_0^{\text{in}}|^2} = 0 \tag{8.28}$$

on $\mathbb{R}$; moreover, the result (8.2) concerning the outer expansion of φ and the matching condition (7.9) imply that φ_0^{in} must also obey the boundary conditions

$$\lim_{r\to-\infty} \varphi_0^{\text{in}}(r,\cdot,\cdot) = 0 \qquad \text{and} \qquad \lim_{r\to+\infty} \varphi_0^{\text{in}}(r,\cdot,\cdot) = 1. \tag{8.29}$$

Since Ψ is a double-well potential with equal minima at $\varphi = 0$ and $\varphi = 1$, the boundary-value problem comprised by (8.28) and (8.29) has a unique solution. Further, that solution satisfies the *energy-partition relation*

$$\Psi(\varphi_0^{\text{in}}) = \tfrac{1}{2}\lambda(\mathbb{F},\mathbb{n})|\acute{\varphi}_0^{\text{in}}|^2 \tag{8.30}$$

and is therefore of the form

$$\varphi_0^{\text{in}}(r,\mathbb{z},t) = \phi\big(\eta(r,\mathbb{z},t)\big), \tag{8.31}$$

with

$$\eta(r,\mathbb{z},t) = \frac{r}{\sqrt{\lambda\big(\mathbb{F}(\mathbb{z},t),\mathbb{n}(\mathbb{z},t)\big)}} \tag{8.32}$$

and ϕ the solution of the boundary value problem

$$\left.\begin{aligned} &\frac{d}{d\eta}\phi(\eta) = \sqrt{2\Psi\big(\phi(\eta)\big)} \qquad \forall \eta \in \mathbb{R}, \\ &\lim_{\eta\to-\infty}\phi(\eta) = 0, \qquad \lim_{\eta\to+\infty}\phi(\eta) = 1. \end{aligned}\right\} \tag{8.33}$$

An important consequence of (8.31)–(8.33) is that

$$\acute{\varphi}_0^{\text{in}} > 0 \tag{8.34}$$

on $\mathbb{R}$, whereby the estimates (4.6), (4.5), and (5.17) for $\boldsymbol{n}$, V, and $\boldsymbol{L}$ simplify to

$$\left.\begin{aligned} \boldsymbol{n} &= \mathbb{n} + O(\epsilon) \quad \text{on} \quad \mathcal{L}, \\ V &= V_{\mathfrak{E}} + O(\epsilon) \quad \text{on} \quad \mathcal{L}, \\ \boldsymbol{L} &= \mathbb{L} + O(\epsilon) \quad \text{on} \quad \mathcal{L}, \end{aligned}\right\} \tag{8.35}$$

and our assumption that $|\boldsymbol{p}|$ does not vanish within the layer is justified—to most significant order in ϵ.

Next, (8.31), (8.33), and fact that both Ψ and its derivative vanish at $\varphi = 0$ and $\varphi = 1$ imply that there is a constant $\alpha > 0$ such that

$$\varphi_0^{\mathrm{in}}(r,\cdot,\cdot) = O(e^{-\alpha|r|}) \qquad \text{as} \quad |r| \to \infty; \tag{8.36}$$

φ_0^{in} is therefore, as a function of r, square integrable on $\mathbb{R}$; in fact, using (8.31) and (8.33), we find that

$$\int_{-\infty}^{+\infty} \sqrt{\lambda(\mathbb{F},\mathbb{n})}\,|\varphi_0^{\mathrm{in}}|^2\,dr = \int_0^1 \sqrt{2\Psi(\varphi)}\,d\varphi. \tag{8.37}$$

8.2.3 Interfacial thickness

Drawing on (8.34) to solve the energy-partition relation (8.30) for φ_0^{in}, separating variables, integrating over r from $-\epsilon^{-1}h(\epsilon)$ to $\epsilon^{-1}h(\epsilon)$, and appealing to the connection (6.2) between λ and $\hat{w}$, we obtain an estimate

$$h(\epsilon) = \tfrac{1}{2}\epsilon\hat{w}(\mathbb{F},\mathbb{n})\Big(\int_0^1 \sqrt{2\Psi(\varphi)}\,d\varphi\Big)^{-1}\Big(\int_\epsilon^{1-\epsilon} \frac{d\varphi}{\sqrt{2\Psi(\varphi)}}\Big) + o(h(\epsilon)), \tag{8.38}$$

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

8.2.4 Further results

Bearing in mind $(8.35)_{1,2}$ and using the definition (A.27) of the time derivative following uniformity surfaces, we deduce an estimate

$$\mathring{\boldsymbol{n}} = \dot{\boldsymbol{n}} + (\nabla\boldsymbol{n})(V\boldsymbol{n}) = \mathring{\mathbb{n}} + O(\epsilon) \qquad \text{on} \qquad \mathcal{L} \tag{8.39}$$

that relates the rate at which $\boldsymbol{n}$ changes following uniformity surfaces to the normal time derivative $\mathring{\mathbb{n}}$ of the orientation $\mathbb{n}$ of $\mathfrak{S}$. Similarly, employing the estimates (8.17) and (8.23) for $\dot{\boldsymbol{y}}$ and $\boldsymbol{\Gamma}$, $(8.35)_{1,2}$, and (A.5), we find that

$$\left.\begin{aligned} \mathring{\boldsymbol{y}} &= \dot{\boldsymbol{y}} + \boldsymbol{F}(V\boldsymbol{n}) = \mathring{\mathbb{y}} + O(\epsilon) && \text{on} \quad \mathcal{L}, \\ \mathring{\boldsymbol{\Gamma}} &= \dot{\boldsymbol{\Gamma}} + (\nabla\boldsymbol{\Gamma})(V\boldsymbol{n}) = \mathring{\mathbb{F}} + O(\epsilon) && \text{on} \quad \mathcal{L}, \end{aligned}\right\} \tag{8.40}$$

while, by the estimates (8.15) and (8.19) for $\boldsymbol{F}$ and $|\boldsymbol{p}|^2$,

$$\mathring{\boldsymbol{F}}, \overline{\ln|\boldsymbol{p}|} = O(1) \qquad \text{on} \qquad \mathcal{L}. \tag{8.41}$$

Next, recalling the expression $(5.10)_2$ for $\jmath^{\mathrm{xs}}$, the energy-partition relation (8.30) implies, together with the estimates (8.19), (8.23), and $(8.35)_1$, for $|\boldsymbol{p}|^2$, $\boldsymbol{\Gamma}$, and $\boldsymbol{n}$ that[39]

$$\epsilon \jmath^{\mathrm{xs}} = \epsilon^{-1}\Psi(\varphi) - \tfrac{1}{2}\epsilon|\boldsymbol{p}|^2\lambda(\boldsymbol{\Gamma},\boldsymbol{n}) = O(1) \qquad \text{on} \qquad \mathcal{L}, \tag{8.42}$$

so that, by appealing to (8.23), (8.19), $(8.35)_1$, and the expression $(5.9)_1$ for W^{xs}, we obtain

$$\epsilon W^{\mathrm{xs}} = \epsilon^{-1}\big(\sqrt{\lambda(\mathbb{F},\mathbb{n})}|\varphi_0^{\mathrm{in}}|^2\big)\sqrt{\lambda(\mathbb{F},\mathbb{n})} + O(1) \quad \text{on} \quad \mathcal{L}. \tag{8.43}$$

Thus, the connection $(6.2)_1$ between $\hat{w}$ and λ allows the estimate

$$\epsilon W^{\mathrm{xs}} = \epsilon^{-1}\chi w + O(1) \qquad \text{on} \qquad \mathcal{L}, \tag{8.44}$$

with χ defined by

$$\chi = \sigma^{-1}\sqrt{\lambda(\mathbb{F},\mathbb{n})}|\varphi_0^{\mathrm{in}}|^2. \tag{8.45}$$

Similarly, drawing on the expressions $(5.9)_2$, $(5.9)_3$, $(5.10)_1$, $(5.9)_6$, and $(5.9)_7$ for $\boldsymbol{S}^{\mathrm{xs}}$, $\boldsymbol{C}^{\mathrm{xs}}$, $\boldsymbol{c}^{\mathrm{xs}}$, $\boldsymbol{f}^{\mathrm{xs}}$, and Δ^{xs}, the relations (6.2) connecting $\hat{w}$, $\hat{\mathbb{S}}$, $\hat{\mathbb{c}}$, and $\hat{b}$ with λ and $\tilde{\beta}$, and the equations (2.30) and (2.25) determining $\mathbb{f}$ and δ, we extract the estimates

$$\left.\begin{aligned}
\epsilon\boldsymbol{S}^{\mathrm{xs}} &= \epsilon^{-1}\chi\mathbb{S} + O(1) \qquad \text{on} \qquad \mathcal{L},\\
\epsilon\boldsymbol{C}^{\mathrm{xs}} &= \epsilon^{-1}\chi\mathbb{C} + O(1) \qquad \text{on} \qquad \mathcal{L},\\
\epsilon\boldsymbol{c}^{\mathrm{xs}} &= \epsilon^{-1}\chi\mathbb{c} + O(1) \qquad \text{on} \qquad \mathcal{L},\\
\epsilon\boldsymbol{f}^{\mathrm{xs}} &= \epsilon^{-1}\chi\mathbb{f} + O(1) \qquad \text{on} \qquad \mathcal{L},\\
\epsilon\Delta^{\mathrm{xs}} &= \epsilon^{-1}\chi\delta + O(1) \qquad \text{on} \qquad \mathcal{L}.
\end{aligned}\right\} \tag{8.46}$$

Finally, for later reference, we note that χ as defined in (8.45) obeys the relation

$$\epsilon^{-1}\int_{-h(\epsilon)}^{h(\epsilon)} \chi\, d(\epsilon r) = 1 + o(1), \tag{8.47}$$

which follows from the definition (6.3) of σ, the limit $(7.1)_2$ whereby the interfacial thickness h approaches zero more slowly than ϵ, the far-field estimate (8.36) for φ_0^{in}, and the integral relation (8.37).

[39] Multiplying appropriately by ϵ in (8.42), we obtain the estimate (1.7) provided in the Introduction.

9 Asymptotic limit of the fundamental integral laws of the order-parameter based theory

Our purpose here is to demonstrate the consonance of the integral laws of the order-parameter based and sharp-interface theories. 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 $\mathcal{R}^a(t,\epsilon)$ and $\mathcal{R}^b(t,\epsilon)$ 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.

In particular, granted that the constitutive equations of the sharp-interface theory are given by (6.1) and (6.2), we find that

i. the terms comprising the scaled linear momentum balance $(5.12)_1$ of the order-parameter based theory admit the estimates

$$\left.\begin{aligned} \int_{\partial\mathcal{P}} \boldsymbol{S}^{\mathrm{bu}}\boldsymbol{\nu}\, da &= \int_{\partial\mathcal{P}} \boldsymbol{S}\boldsymbol{\nu}\, da + o(1), \\ \epsilon\int_{\partial\mathcal{P}} \boldsymbol{S}^{\mathrm{xs}}\boldsymbol{\nu}\, da &= \int_{\partial\mathfrak{Q}} \mathbb{S}\boldsymbol{m}\, dl + o(1), \\ \int_{\mathcal{P}} \varrho\dot{\boldsymbol{y}}\, dv &= \int_{\mathcal{P}} \varrho\dot{\boldsymbol{y}}\, dv + o(1), \end{aligned}\right\} \tag{9.1}$$

and hence, as the thickness of the layer vanishes, that balance corresponds to the linear momentum balance $(2.12)_1$ of the sharp-interface theory;

ii. the terms comprising the scaled angular momentum balance $(5.12)_2$ of the order-parameter based theory admit the estimates

$$\left.\begin{aligned} \int_{\partial\mathcal{P}} \boldsymbol{y}\times\boldsymbol{S}^{\mathrm{bu}}\boldsymbol{\nu}\, da &= \int_{\partial\mathcal{P}} \boldsymbol{y}\times\boldsymbol{S}\boldsymbol{\nu}\, da + o(1) \\ \epsilon\int_{\partial\mathcal{P}} \boldsymbol{y}\times\boldsymbol{S}^{\mathrm{xs}}\boldsymbol{\nu}\, da &= \int_{\partial\mathfrak{Q}} \boldsymbol{y}\times\mathbb{S}\boldsymbol{m}\, dl + o(1), \\ \int_{\mathcal{P}} \boldsymbol{y}\times\varrho\dot{\boldsymbol{y}}\, dv &= \int_{\mathcal{P}} \boldsymbol{y}\times\varrho\dot{\boldsymbol{y}}\, dv + o(1), \end{aligned}\right\} \tag{9.2}$$

and hence, as the thickness of the layer vanishes, that balance corresponds to the angular momentum balance $(2.12)_2$ of the sharp-interface theory;

iii. the terms comprising the scaled configurational momentum balance $(5.12)_3$ of the order-parameter based theory admit the estimates

$$\left.\begin{aligned}
&\int_{\partial\mathcal{P}} \boldsymbol{C}^{\mathrm{bu}}\boldsymbol{\nu}\,da = \int_{\partial\mathcal{P}} \boldsymbol{C}\boldsymbol{\nu}\,da + o(1),\\
&\epsilon\int_{\partial\mathcal{P}} \boldsymbol{C}^{\mathrm{xs}}\boldsymbol{\nu}\,da = \int_{\partial\Omega} \mathbb{C}\mathfrak{m}\,dl + o(1),\\
&\epsilon\int_{\mathcal{P}} \boldsymbol{f}^{\mathrm{xs}}\,dv = \int_{\Omega} \mathfrak{f}\,da + o(1),\\
&\int_{\mathcal{P}} \boldsymbol{q}\,dv = \int_{\mathcal{P}} \boldsymbol{q}\,dv + o(1),
\end{aligned}\right\} \tag{9.3}$$

and hence, as the thickness of the layer vanishes, that balance corresponds to the configurational momentum balance $(2.12)_3$ of the sharp-interface theory;[40]

iv. the terms comprising the scaled dissipation imbalance (5.13) of the order-parameter based theory admit the estimates

$$\left.\begin{aligned}
&\int_{\partial\mathcal{P}} \boldsymbol{S}^{\mathrm{bu}}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}\,da = \int_{\partial\mathcal{P}} \boldsymbol{S}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}\,da + o(1),\\
&\epsilon\int_{\partial\mathcal{P}} \left(\boldsymbol{S}^{\mathrm{xs}}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}} + \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\right) da\\
&\qquad\qquad = \int_{\partial\Omega} \left(\mathbb{S}\mathfrak{m}\cdot\mathring{\dot{y}} + \mathbb{C}\mathfrak{m}\cdot(V_{\mathfrak{S}}\mathfrak{n}) + wU_{\partial\Omega}\right) dl + o(1),\\
&\int_{\mathcal{P}} W^{\mathrm{bu}}\,dv = \int_{\mathcal{P}} W\,dv + o(1),\\
&\int_{\mathcal{P}} \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2\,dv = \int_{\mathcal{P}} \tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2\,dv + o(1),\\
&\epsilon\int_{\mathcal{P}} W^{\mathrm{xs}}\,dv = \int_{\Omega} w\,da + o(1),
\end{aligned}\right\} \tag{9.4}$$

and hence, as the thickness of the layer vanishes, that imbalance corresponds to the dissipation imbalance (2.13) of the sharp-interface theory.

[40] We recall that the bulk configurational force $\boldsymbol{f}$ of the sharp-interface theory vanishes (cf. (2.27)).

We consider only the estimates (9.4) associated with the dissipation imbalance (5.13), since to establish these we will call upon all ingredients necessary to verify (9.1)–(9.3). 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

$$\int_{\partial\mathcal{P}} g\, da = \int_{\partial\mathcal{P}\setminus\mathcal{L}} g\, da + o(1) \qquad \text{and} \qquad \int_{\mathcal{P}} g\, dv = \int_{\mathcal{P}\setminus\mathcal{L}} g\, dv + o(1) \tag{9.5}$$

for any field g that is of $O(1)$ in ϵ on $\mathcal{P}$. Hence, $(9.4)_1$, $(9.4)_3$, and $(9.4)_4$ follow directly from the results $(8.16)_2$, (8.17), and $(8.16)_1$ showing that $\boldsymbol{S}^{\mathrm{bu}}$, $\dot{\boldsymbol{y}}$, and $\boldsymbol{W}^{\mathrm{bu}}$ are of $O(1)$ on $\mathcal{L}$ and those, $(8.7)_1$, $(8.8)_1$, and $(8.8)_2$ determining the specific forms for the expansions of $\dot{\boldsymbol{y}}$, $\boldsymbol{W}^{\mathrm{bu}}$, and $\boldsymbol{S}^{\mathrm{bu}}$, on $\mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}$.

Next, we attend to $(9.4)_2$. Since each uniformity surface crosses $\partial\mathcal{P}$ transversely, $\boldsymbol{n}$ and $\boldsymbol{\nu}$ satisfy $0 \leq |\boldsymbol{n}\cdot\boldsymbol{\nu}| < 1$ 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

$$\boldsymbol{\nu} = (\boldsymbol{n}\cdot\boldsymbol{\nu})\boldsymbol{n} + (\boldsymbol{m}\cdot\boldsymbol{\nu})\boldsymbol{m}, \tag{9.6}$$

where

$$\boldsymbol{m} = \frac{\boldsymbol{P}\boldsymbol{\nu}}{\sqrt{1 - |\boldsymbol{n}\cdot\boldsymbol{\nu}|^2}} \tag{9.7}$$

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

$$\int_{\partial\mathcal{P}} \boldsymbol{g}\cdot\boldsymbol{\nu}\, da = \int_{\partial\mathcal{P}\setminus(\partial\mathcal{P}\cap\mathcal{L})} \boldsymbol{g}\cdot\boldsymbol{\nu}\, da + \int_{\partial\mathcal{P}\cap\mathcal{L}} \big((\boldsymbol{n}\otimes\boldsymbol{n})\boldsymbol{g}\big)\cdot\boldsymbol{\nu}\, da + \int_{\partial\mathcal{P}\cap\mathcal{L}} \boldsymbol{g}\cdot\boldsymbol{m}\, dA, \tag{9.8}$$

where the measure

$$dA = \boldsymbol{m}\cdot\boldsymbol{\nu}\, da \tag{9.9}$$

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

$$\left.\begin{aligned} \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{n}) &= -(W^{\mathrm{xs}} - \jmath^{\mathrm{xs}})V, \\ \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{m}) &= \boldsymbol{S}^{\mathrm{xs}}\boldsymbol{m}\cdot\big(\boldsymbol{F}(V\boldsymbol{n})\big) + \boldsymbol{C}^{\mathrm{xs}}\boldsymbol{m}\cdot(V\boldsymbol{n}), \end{aligned}\right\} \tag{9.10}$$

the first of which follows from the expression $(5.9)_4$ for $\boldsymbol{\xi}^{\mathrm{xs}}$ and the second of which issues from the definition (9.7) of $\boldsymbol{m}$, $(5.9)_4$, and the expression $(5.9)_3$ for

$\boldsymbol{C}^{\mathrm{xs}}$, the identity (9.8) allows us to express the left-hand-side of $(9.4)_2$ in the form

$$\int_{\partial\mathcal{P}} \left(\boldsymbol{S}^{\mathrm{xs}}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}} + \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\right) da = \int_{\partial\mathcal{P}\setminus(\mathcal{P}\cap\mathcal{L})} \left(\boldsymbol{S}^{\mathrm{xs}}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}} + \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\right) da$$
$$+ \int_{\partial\mathcal{P}\cap\mathcal{L}} \left(\boldsymbol{S}^{\mathrm{xs}}\boldsymbol{m}\cdot\hat{\dot{\boldsymbol{y}}} + \boldsymbol{C}^{\mathrm{xs}}\boldsymbol{m}\cdot(V\boldsymbol{n}) + (W^{\mathrm{xs}} - \jmath^{\mathrm{xs}})U\right) dA, \tag{9.11}$$

where

$$U = -\frac{(\boldsymbol{n}\cdot\boldsymbol{\nu})V}{\sqrt{1-|\boldsymbol{n}\cdot\boldsymbol{\nu}|^2}} \tag{9.12}$$

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

Immediate consequences of the results $(8.5)_1$, $(8.11)_2$, and $(8.11)_4$ concerning the orders of $\dot{\varphi}$, $\boldsymbol{S}^{\mathrm{xs}}$, and $\boldsymbol{\xi}^{\mathrm{xs}}$ are the estimates

$$\int_{\partial\mathcal{P}\setminus(\mathcal{P}\cap\mathcal{L})} \boldsymbol{S}^{\mathrm{xs}}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}\, da = o(1) \qquad \text{and} \qquad \int_{\partial\mathcal{P}\setminus(\mathcal{P}\cap\mathcal{L})} \boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\, da = o(1), \tag{9.13}$$

which imply that the first term on the right-hand-side of (9.11) is negligible.

It remains to show that the second term on the right-hand-side of (9.11) actually yields the right-hand-side of $(9.4)_2$. Toward this, we first record the estimates

$$\boldsymbol{m} = \mathfrak{m} + O(\epsilon) \qquad \text{and} \qquad U = U_{\partial\Omega} + O(\epsilon), \tag{9.14}$$

that follow from the definitions (9.7), and (9.12) of $\boldsymbol{m}$, and U, the estimates $(8.35)_1$, $(8.35)_2$, and (8.22) for $\boldsymbol{n}$, V, and $\boldsymbol{P}$, and the definitions (2.10), and (2.11) for $\boldsymbol{m}$ and $U_{\partial\Omega}$. Proceeding, we observe that, given a field $\boldsymbol{g}$ that satisfies

$$\boldsymbol{g} = \epsilon^{-1}\chi g + O(1) \quad \text{on} \quad \mathcal{L}, \tag{9.15}$$

with g independent of the coordinate r normal to $\mathfrak{S}$, the identity (8.47) for χ implies that

$$\epsilon \int_{\partial\mathcal{P}\cap\mathcal{L}} \boldsymbol{g}\, dA = \int_{\partial\Omega} \Big(\int_{-h(\epsilon)}^{h(\epsilon)} g\, d(\epsilon r) \Big)\, dl = \int_{\partial\Omega} g\, dl + o(1). \tag{9.16}$$

Thus, along with $(8.35)_1$, $(8.35)_2$, and (9.14), the estimates $(8.40)_1$, $(8.46)_1$,

$(8.46)_2$, (8.44), and (8.42) for $\mathring{\boldsymbol{y}}$, $\boldsymbol{S}^{\mathrm{xs}}$, $\boldsymbol{C}^{\mathrm{xs}}$, W^{xs}, and $\jmath^{\mathrm{xs}}$ yield

$$\left.\begin{aligned}
&\epsilon \int_{\partial\mathcal{P}\cap\mathcal{L}} \boldsymbol{S}^{\mathrm{xs}}\boldsymbol{m}\cdot\mathring{\boldsymbol{y}}\, dA = \int_{\partial\Omega} \mathbb{S}\boldsymbol{m}\cdot\mathring{\boldsymbol{y}}\, dl + o(1),\\
&\epsilon \int_{\partial\mathcal{P}\cap\mathcal{L}} \boldsymbol{C}^{\mathrm{xs}}\boldsymbol{m}\cdot(V\boldsymbol{n})\, dA = \int_{\partial\Omega} \mathbb{C}\boldsymbol{m}\cdot(V_{\mathfrak{S}}\mathfrak{n})\, dl + o(1),\\
&\epsilon \int_{\partial\mathcal{P}\cap\mathcal{L}} W^{\mathrm{xs}}U\, dA = \int_{\partial\Omega} wU_{\partial\Omega}\, dl + o(1),\\
&\epsilon \int_{\partial\mathcal{P}\cap\mathcal{L}} \jmath^{\mathrm{xs}}U\, dA = o(1),
\end{aligned}\right\} \tag{9.17}$$

whereby $(9.4)_2$ holds.

Finally, bearing in mind the estimates $(8.11)_1$ and (8.44) for W^{xs}, the identity

$$\int_{\mathcal{P}} g\, dv = \int_{\Omega} \Big(\int_{-h(\epsilon)}^{h(\epsilon)} g\, d(\epsilon r)\Big)\, da + o(1) = \int_{\Omega} g\, da + o(1), \tag{9.18}$$

which follows from (8.47) for any field g that is of $o(1)$ on $\mathcal{R}^{\mathfrak{a}}\cap\mathcal{R}^{\mathfrak{b}}$ and satisfies (9.15) with g independent of the coordinate r normal to $\mathfrak{S}$, implies $(9.4)_5$.

10 Asymptotic limit of the local balance laws of the order-parameter based theory

Here, we aim to demonstrate the consonance of the local balance laws of the order-parameter based and sharp-interface theories. Specifically, granted that the constitutive equations of the sharp-interface theory are given by (6.1) and (6.2), we find that

i. on $\mathcal{R}^{\mathfrak{a}}\cup\mathcal{R}^{\mathfrak{b}}$ the terms comprising scaled field equation $(5.14)_1$ imposing linear momentum balance for the order-parameter based theory admit the estimates

$$\left.\begin{aligned}
\operatorname{div}\boldsymbol{S}^{\mathrm{bu}} = \operatorname{div}\boldsymbol{S} + o(1), \qquad \varrho\ddot{\boldsymbol{y}} = \varrho\ddot{\boldsymbol{y}} + o(1),\\
\epsilon\operatorname{div}\boldsymbol{S}^{\mathrm{xs}} = o(1),
\end{aligned}\right\} \tag{10.1}$$

so that, as the thickness of the layer vanishes, that balance yields the bulk linear momentum balance $(2.14)_1$ of the sharp-interface theory; further,

the terms of $(5.14)_1$ obey the relations

$$\left.\begin{aligned} \int_{-h(\epsilon)}^{h(\epsilon)} \operatorname{div} \boldsymbol{S}^{\mathrm{bu}}\, d(\epsilon r) &= [\![\boldsymbol{S}\boldsymbol{n}]\!] + o(1), \\ \epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \operatorname{div} \boldsymbol{S}^{\mathrm{xs}}\, d(\epsilon r) &= \operatorname{div}_{\mathfrak{S}} \mathbb{S} + o(1), \\ \int_{-h(\epsilon)}^{h(\epsilon)} \varrho \ddot{\boldsymbol{y}}\, d(\epsilon r) &= -\varrho V_{\mathfrak{S}} [\![\dot{\boldsymbol{y}}]\!] + o(1), \end{aligned}\right\} \tag{10.2}$$

and the integral across the layer of the scaled field equation imposing linear momentum balance for the order-parameter based theory equation yields, as the thickness of that layer vanishes, the interfacial linear momentum balance $(2.15)_1$ of the sharp-interface theory;

ii. on $\mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}$ the terms comprising scaled field equation $(5.14)_2$ imposing angular momentum balance for the order-parameter based theory admit the estimates

$$\boldsymbol{F}(\boldsymbol{S}^{\mathrm{bu}})^T = \boldsymbol{F}\boldsymbol{S}^T + o(1), \qquad \epsilon \boldsymbol{F}(\boldsymbol{S}^{\mathrm{xs}})^T = o(1), \tag{10.3}$$

so that, as the thickness of the layer vanishes, that balance yields the bulk angular momentum balance $(2.14)_2$ of the sharp-interface theory; further, the terms of $(5.14)_2$ obey the relations

$$\left.\begin{aligned} \epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{F}(\boldsymbol{S}^{\mathrm{xs}})^T\, d(\epsilon r) &= \mathbb{F}\mathbb{S}^T + o(1), \\ \int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{F}(\boldsymbol{S}^{\mathrm{bu}})^T\, d(\epsilon r) &= o(1), \end{aligned}\right\} \tag{10.4}$$

and the integral across the layer of the scaled field equation imposing angular momentum balance for the order-parameter based theory equation yields, as the thickness of that layer vanishes, the interfacial angular momentum balance $(2.15)_2$ of the sharp-interface theory;

iii. on $\mathcal{R}^{\mathfrak{a}} \cup \mathcal{R}^{\mathfrak{b}}$ the terms comprising scaled field equation $(5.14)_3$ imposing configurational momentum balance for the order-parameter based theory admit the estimates

$$\left.\begin{aligned} \operatorname{div} \boldsymbol{C}^{\mathrm{bu}} &= \operatorname{div} \boldsymbol{C} + o(1), & \dot{\boldsymbol{q}} &= \dot{\boldsymbol{q}} + o(1), \\ \epsilon \operatorname{div} \boldsymbol{C}^{\mathrm{xs}} &= o(1), & \epsilon \boldsymbol{f}^{\mathrm{xs}} &= o(1), \end{aligned}\right\} \tag{10.5}$$

so that, as the thickness of the layer vanishes, that balance yields the bulk configurational momentum balance $(2.14)_3$ of the sharp-interface theory; further, the terms of the tangential component of $(5.14)_3$ obey the relations

$$\left.\begin{aligned}
&\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{P}\,\mathrm{div}\,\boldsymbol{C}^{\mathrm{bu}}\,d(\epsilon r) = \mathbb{P}[\![\boldsymbol{C}\mathfrak{n}]\!] + o(1),\\
&\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{P}\,\mathrm{div}\,\boldsymbol{C}^{\mathrm{xs}}\,d(\epsilon r) = \mathbb{P}\,\mathrm{div}_{\mathfrak{S}}\,\mathbb{C} + o(1),\\
&\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{P}\dot{\boldsymbol{q}}\,d(\epsilon r) = -V_{\mathfrak{S}}\mathbb{P}[\![\boldsymbol{q}]\!] + o(1),
\end{aligned}\right\} \tag{10.6}$$

while the terms of normal component (5.18) of $(5.14)_3$ obey the relations

$$\left.\begin{aligned}
&\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{n}\cdot\mathrm{div}\,\boldsymbol{C}^{\mathrm{bu}}\,d(\epsilon r) = \mathfrak{n}\cdot[\![\boldsymbol{C}\mathfrak{n}]\!] + o(1),\\
&\int_{-h(\epsilon)}^{h(\epsilon)} \dot{\boldsymbol{q}}\cdot\boldsymbol{n}\,d(\epsilon r) = -V_{\mathfrak{S}}[\![\boldsymbol{q}\cdot\mathfrak{n}]\!] + o(1),\\
&\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{C}^{\mathrm{xs}}\cdot\boldsymbol{L}\,d(\epsilon r) = \mathbb{C}\cdot\mathbb{L} + o(1),\\
&\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} \mathrm{div}\,\boldsymbol{c}^{\mathrm{xs}}\,d(\epsilon r) = \mathrm{div}_{\mathfrak{S}}\,\mathbb{c} + o(1),\\
&\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n}\,d(\epsilon r) = \mathfrak{f}\cdot\mathfrak{n} + o(1),\\
&\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} \mathrm{div}(\jmath^{\mathrm{xs}}\boldsymbol{n})\,d(\epsilon r) = o(1),
\end{aligned}\right\} \tag{10.7}$$

and the integral across the layer of the scaled field equation imposing configurational momentum balance for the order-parameter based theory equation yields, as the thickness of that layer vanishes, the interfacial configurational momentum balance $(2.15)_3$ of the sharp-interface theory;

iv. on $\mathcal{R}^a \cup \mathcal{R}^b$ the terms comprising the scaled dissipation balance (5.15) of the order-parameter based theory admit the estimates

$$\left.\begin{aligned} \boldsymbol{S}^{\mathrm{bu}}\cdot\boldsymbol{F} = \boldsymbol{S}\cdot\dot{\boldsymbol{F}} + o(1), \qquad \dot{W}^{\mathrm{bu}} = \dot{W} + o(1), \\ \epsilon\boldsymbol{S}^{\mathrm{xs}}\cdot\boldsymbol{F}, \epsilon\boldsymbol{\xi}^{\mathrm{xs}}\cdot\dot{\boldsymbol{p}}, \pi^{\mathrm{bu}}\dot{\varphi}, \epsilon\pi^{\mathrm{xs}}\dot{\varphi}, \epsilon\dot{W}^{\mathrm{xs}}, \epsilon\Delta^{\mathrm{xs}} = o(1), \end{aligned}\right\} \tag{10.8}$$

so that, as the thickness of the layer vanishes, that balance yields the bulk dissipation balance (cf. (2.16) and the remark following the bulk constitutive equations (2.22) of the sharp-interface theory) of the sharp-interface theory; further, the terms comprising the alternate form (5.20) of the scaled dissipation balance obey the relations

$$\left.\begin{aligned} &\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{S}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{I}}\, d(\epsilon r) = \mathbb{S}\cdot\mathring{\mathbb{F}} + o(1), \\ &\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{c}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{n}}\, d(\epsilon r) = \mathbb{c}\cdot\mathring{\mathbb{n}} + o(1), \\ &\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} (\boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n})V\, d(\epsilon r) = (\mathbb{f}\cdot\mathbb{n})V_{\mathbb{e}} + o(1), \\ &\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} (\mathring{W}^{\mathrm{xs}} - (W^{\mathrm{xs}} - \jmath^{\mathrm{xs}})\overset{\circ}{\overline{\ln|\boldsymbol{p}|}})\, d(\epsilon r) = \mathring{w} + o(1), \\ &\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} \Delta^{\mathrm{xs}}\, d(\epsilon r) = \delta + o(1), \\ &\epsilon\int_{-h(\epsilon)}^{h(\epsilon)} \boldsymbol{S}^{\mathrm{bu}}\cdot\mathring{\boldsymbol{F}}\, d(\epsilon r) = o(1), \quad \epsilon\int_{-h(\epsilon)}^{h(\epsilon)} \mathring{W}^{\mathrm{bu}}\, d(\epsilon r) = o(1), \end{aligned}\right\} \tag{10.9}$$

and the integral across the layer of that balance yields, as the thickness of that layer vanishes, the interfacial dissipation balance (2.24) of the sharp-interface theory.

We establish only the estimates (10.5)–(10.7) associated with the configurational momentum balance $(5.14)_3$. The remaining estimates (10.1), (10.2), (10.3), (10.4), (10.8), and (10.9) follow similarly.

To begin, we observe that the bulk results (10.5) are direct consequences of the estimates $(8.8)_3$, $(8.11)_3$, $(8.11)_6$, and (8.10) for $\boldsymbol{C}^{\mathrm{bu}}$, $\boldsymbol{C}^{\mathrm{xs}}$, $\boldsymbol{f}^{\mathrm{xs}}$, and $\boldsymbol{q}$ on $\mathcal{R}^a \cup \mathcal{R}^b$.

Next, we consider the results (10.6) involving the terms appearing in the tangential component of the configurational momentum balance $(5.14)_3$. First, bearing in mind $(8.16)_3$, whereby $\boldsymbol{C}^{\mathrm{bu}}$ is of $O(1)$ on $\mathcal{L}$, we obtain

$$\operatorname{div} \boldsymbol{C}^{\mathrm{bu}} = \epsilon^{-1} \dot{\boldsymbol{C}}^{\mathrm{bu}} \boldsymbol{n} + O(1) \tag{10.10}$$

on $\mathcal{L}$. Thus, $(10.6)_1$ follows from the estimate (8.22) for $\boldsymbol{P}$ on $\mathcal{L}$, the estimate $(8.8)_3$ for $\boldsymbol{C}^{\mathrm{bu}}$ on $\mathcal{R}^{\mathrm{a}} \cup \mathcal{R}^{\mathrm{b}}$, and the matching condition (7.9).

Proceeding, the estimate $(8.46)_2$ for $\boldsymbol{C}^{\mathrm{xs}}$ on $\mathcal{L}$ implies that

$$\epsilon \operatorname{div} \boldsymbol{C}^{\mathrm{xs}} = \epsilon^{-1} \operatorname{div}_{\mathcal{S}} (\chi \mathbb{C}) + O(1) \tag{10.11}$$

on $\mathcal{L}$, which, in conjunction with the integral identity (8.47) involving χ and the estimate (8.22) for $\boldsymbol{P}$ on $\mathcal{L}$, yields $(10.6)_2$.

Further, the estimates (8.14) and (8.15) for $\dot{\boldsymbol{y}}$ and $\boldsymbol{F}$ on $\mathcal{L}$ give

$$\dot{\boldsymbol{q}} = -\varrho \boldsymbol{F}^T \dot{\boldsymbol{y}} = -\epsilon^{-1} V_{\mathcal{S}} \dot{\boldsymbol{q}} + O(1) \tag{10.12}$$

on $\mathcal{L}$, whereby $(10.6)_3$ follows from the estimate (8.22) for $\boldsymbol{P}$ on $\mathcal{L}$, the estimate (8.10) for $\boldsymbol{q}$ on $\mathcal{R}^{\mathrm{a}} \cup \mathcal{R}^{\mathrm{b}}$, and the matching condition (7.9).

Next, we consider the results (10.7) involving the terms appearing in the normal component (5.16) of the configurational momentum balance $(5.14)_3$. First, we note that $(10.7)_1$ and $(10.7)_2$ follow from (10.10), (10.12), the estimate $(8.35)_1$ for $\boldsymbol{n}$ on $\mathcal{L}$, the estimates $(8.8)_3$ and (8.10) for $\boldsymbol{C}^{\mathrm{bu}}$ and $\boldsymbol{q}$ on $\mathcal{R}^{\mathrm{a}} \cup \mathcal{R}^{\mathrm{b}}$, and the matching condition (7.9).

Continuing, the estimates $(8.46)_2$, $(8.46)_3$, $(8.46)_4$, $(8.35)_1$, and $(8.35)_3$ for $\boldsymbol{C}^{\mathrm{xs}}$, $\boldsymbol{c}^{\mathrm{xs}}$, $\boldsymbol{f}^{\mathrm{xs}}$, $\boldsymbol{n}$, and $\boldsymbol{L}$ on $\mathcal{L}$ imply that, on $\mathcal{L}$,

$$\left.\begin{aligned} \epsilon \boldsymbol{C}^{\mathrm{xs}} \cdot \boldsymbol{L} &= \epsilon^{-1} \chi \mathbb{C} \cdot \mathbb{L} + O(1), \\ \epsilon \operatorname{div} \boldsymbol{c}^{\mathrm{xs}} &= \epsilon^{-1} \operatorname{div}_{\mathcal{S}} (\chi \mathbb{c}) + O(1), \\ \epsilon \boldsymbol{f}^{\mathrm{xs}} \cdot \boldsymbol{n} &= \epsilon^{-1} \chi \mathbb{f} \cdot \mathbb{n} + O(1), \end{aligned}\right\} \tag{10.13}$$

so that, by appeal to the integral identity (8.47) involving χ, $(10.7)_3$, $(10.7)_4$, and $(10.7)_5$ follow.

It remains to verify $(10.7)_6$, which we do following an argument due to FRIED & GURTIN [16]. Specifically, we observe that

$$\epsilon \operatorname{div}(j^{\mathrm{xs}} \boldsymbol{n}) = (\jmath^{\mathrm{xs}}) \mathbb{n} \cdot \boldsymbol{n} + \epsilon (\nabla_{\mathcal{S}} j^{\mathrm{xs}}) \cdot \boldsymbol{n} - \epsilon j^{\mathrm{xs}} K = \jmath^{\mathrm{xs}} + O(1) \tag{10.14}$$

on $\mathcal{L}$, and

$$\epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \operatorname{div}(j^{\mathrm{xs}} \boldsymbol{n}) \, d(\epsilon r) = \epsilon \int_{-h(\epsilon)}^{h(\epsilon)} \jmath^{\mathrm{xs}} \, dr + o(1). \tag{10.15}$$

Thus, to establish $(10.7)_6$ it is sufficient to demonstrate that, as $\epsilon \to 0$,

$$\epsilon \jmath^{\mathrm{xs}}(\pm\epsilon^{-1}h(\epsilon),\cdot,\cdot) = o(1). \tag{10.16}$$

To establish (10.16), we expand $\jmath^{\mathrm{xs}}$ to deduce that

$$\begin{aligned}\epsilon^2\jmath^{\mathrm{xs}} = \Psi(\varphi_0^{\mathrm{in}}) + \epsilon\Psi'(\varphi_0^{\mathrm{in}})\varphi_1^{\mathrm{in}} \\ - \acute{\varphi}_0^{\mathrm{in}}(\acute{\varphi}_0^{\mathrm{in}} + 2\epsilon\acute{\varphi}_1^{\mathrm{in}})\big(\tfrac{1}{2}\lambda(\mathbb{F},\mathfrak{n}) + O(\epsilon)\big) + O(\epsilon^2)\end{aligned} \tag{10.17}$$

on $\mathcal{L}$. Thus, on recalling the assumption $(7.1)_2$, whereby $\epsilon^{-1}h(\epsilon) \to \infty$ as $\epsilon \to 0$, the requirements $\Psi'(0) = 0$ and $\Psi'(1) = 0$, the energy partition relation (8.30), and the far-field bound (8.36) on $\acute{\varphi}_0^{\mathrm{in}}$, (10.15) follows.

11 Asymptotic limit of a power identity for the order-parameter based theory

Here, we derive a power identity relevant to the order-parameter based theory and then show that this identity is consonant with the power identity (2.21) of the sharp-interface theory.

A simple consequence of the results $(9.4)_1$, $(9.4)_2$, and $(9.17)_3$ established in determining the asymptotic limit of the scaled dissipation imbalance (5.13) of the order-parameter based theory is that, as $\epsilon \to 0$,

$$\begin{aligned}\int_{\partial\mathcal{P}} \big((\boldsymbol{S}^{\mathrm{bu}} + \epsilon\boldsymbol{S}^{\mathrm{xs}})\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}} + \epsilon\boldsymbol{\xi}^{\mathrm{xs}}\cdot(\dot{\varphi}\boldsymbol{\nu})\big)\,da - \epsilon\int_{\partial\mathcal{P}\cap\mathcal{L}} W^{\mathrm{xs}}U\,dA \\ = \int_{\partial\mathcal{P}} \boldsymbol{S}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}\,da + \int_{\partial\mathfrak{Q}} \big(\mathbb{S}\mathfrak{m}\cdot\mathring{\mathfrak{y}} + \mathbb{C}\mathfrak{m}\cdot(V_{\mathfrak{S}}\mathfrak{n})\big)\,dl + o(1),\end{aligned} \tag{11.1}$$

whereby the surfeit of the total power expended on $\partial\mathcal{P}$ by the tractions associated with the bulk and excess deformational stresses $\boldsymbol{S}^{\mathrm{bu}}$ and $\boldsymbol{S}^{\mathrm{xs}}$ and 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 $\partial\mathcal{P}$ and $\partial\mathfrak{Q}$ by the tractions associated with the bulk and interfacial deformational stresses $\boldsymbol{S}$ and $\mathbb{S}$ and the configurational stress $\mathbb{C}$. Thus, bearing in mind the form of the power identity (2.21) for the sharp-interface theory, we develop a power identity for the left-hand-side of (11.1).

Toward this identity, we first apply the divergence theorem to the first term on the left-hand-side of (11.1) and use the scaled local linear momentum balance

$(5.14)_1$ to yield

$$\int_{\partial\mathcal{P}} \big((\boldsymbol{S}^{\rm bu}+\epsilon\boldsymbol{S}^{\rm xs})\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}+\epsilon\boldsymbol{\xi}^{\rm xs}\cdot(\dot{\varphi}\boldsymbol{\nu})\big)\,da-\overline{\int_{\mathcal{P}}\tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2\,dv}$$
$$=\int_{\mathcal{P}}\big((\boldsymbol{S}^{\rm bu}+\epsilon\boldsymbol{S}^{\rm xs})\cdot\dot{\boldsymbol{F}}+\epsilon\,{\rm div}(\dot{\varphi}\boldsymbol{\xi}^{\rm xs})\big)\,dv. \quad (11.2)$$

Next, we decompose the integral on the right-hand-side of (11.2) into integrals over $\mathcal{P}\setminus\mathcal{L}$ and $\mathcal{P}\cap\mathcal{L}$. In the integral over $\mathcal{P}\setminus\mathcal{L}$ we expand the term $\epsilon\,{\rm div}(\dot{\varphi}\boldsymbol{\xi}^{\rm xs})$ and use the scaled local microforce balance (5.21) to give

$$\int_{\mathcal{P}\setminus\mathcal{L}}\big((\boldsymbol{S}^{\rm bu}+\epsilon\boldsymbol{S}^{\rm xs})\cdot\dot{\boldsymbol{F}}+\epsilon\,{\rm div}(\dot{\varphi}\boldsymbol{\xi}^{\rm xs})\big)\,dv$$
$$=\int_{\mathcal{P}\setminus\mathcal{L}}\big((\boldsymbol{S}^{\rm bu}+\epsilon\boldsymbol{S}^{\rm xs})\cdot\dot{\boldsymbol{F}}+\epsilon\boldsymbol{\xi}^{\rm xs}\cdot\dot{\boldsymbol{p}}-(\pi^{\rm bu}+\epsilon\pi^{\rm xs})\dot{\varphi}\big)\,dv. \quad (11.3)$$

In the integral over $\mathcal{P}\cap\mathcal{L}$, we use the expression $(5.9)_4$ for $\boldsymbol{\xi}^{\rm xs}$, the identities (5.19) and the relation (A.28) to obtain

$$\int_{\mathcal{P}\cap\mathcal{L}}\big((\boldsymbol{S}^{\rm bu}+\epsilon\boldsymbol{S}^{\rm xs})\cdot\dot{\boldsymbol{F}}+\epsilon\,{\rm div}(\dot{\varphi}\boldsymbol{\xi}^{\rm xs})\big)\,dv=-\epsilon\int_{\mathcal{P}\cap\mathcal{L}}\big(\varpi+{\rm div}(W^{\rm xs}V\boldsymbol{n})\big)\,dv, \quad (11.4)$$

with ϖ given by

$$\varpi=(\epsilon^{-1}\nabla W^{\rm bu}+\boldsymbol{f}^{\rm xs})\cdot(V\boldsymbol{n})+W^{\rm xs}KV$$
$$-\epsilon^{-1}\boldsymbol{S}^{\rm bu}\cdot\hat{\boldsymbol{F}}-\boldsymbol{S}^{\rm xs}\cdot\hat{\boldsymbol{\Gamma}}+\boldsymbol{c}^{\rm xs}\cdot\hat{\boldsymbol{n}}+\jmath^{\rm xs}\overset{\diamond}{\overline{\ln|\boldsymbol{p}|}}. \quad (11.5)$$

Thus, consolidating (11.2), (11.3), and (11.4), and using the result

$$\int_{\mathcal{P}\cap\mathcal{L}}{\rm div}(W^{\rm xs}V\boldsymbol{n})\,dv=-\int_{\partial\mathcal{P}\cap\mathcal{L}}W^{\rm xs}U\,dA+\int_{\mathcal{P}\cap\partial\mathcal{L}}W^{\rm xs}V\boldsymbol{n}\cdot\boldsymbol{\nu}\,da, \quad (11.6)$$

which follows from the divergence theorem, the representation (9.6) for $\boldsymbol{\nu}$, and the definitions (9.9) and (9.12) of dA and U, we arrive at a power identity,

$$\int_{\partial\mathcal{P}}\big((\boldsymbol{S}^{\rm bu}+\epsilon\boldsymbol{S}^{\rm xs})\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}+\epsilon\boldsymbol{\xi}^{\rm xs}\cdot(\dot{\varphi}\boldsymbol{\nu})\big)\,da-\epsilon\int_{\partial\mathcal{P}\cap\mathcal{L}}W^{\rm xs}U\,dA$$
$$-\overline{\int_{\mathcal{P}}\tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2\,dv}=\int_{\mathcal{P}\setminus\mathcal{L}}\big((\boldsymbol{S}^{\rm bu}+\epsilon\boldsymbol{S}^{\rm xs})\cdot\dot{\boldsymbol{F}}+\epsilon\boldsymbol{\xi}^{\rm xs}\cdot\dot{\boldsymbol{p}}-(\pi^{\rm bu}+\epsilon\pi^{\rm xs})\dot{\varphi}\big)\,dv$$
$$-\epsilon\int_{\mathcal{P}\cap\mathcal{L}}\varpi\,dv-\epsilon\int_{\mathcal{P}\cap\partial\mathcal{L}}W^{\rm xs}(V\boldsymbol{n})\cdot\boldsymbol{\nu}\,da, \quad (11.7)$$

for the order-parameter based theory.

Now, from $(9.4)_4$ and (11.1), the left-hand-side of the power identity (11.7) differs, in the limit of decreasing transition layer thickness, from the left-hand-side of the power identity (2.21) 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 (6.1) and (6.2), we find that

i. the term of (11.7) involving integration over $\mathcal{P} \setminus \mathcal{L}$ obeys

$$\int_{\mathcal{P}\setminus\mathcal{L}} ((\boldsymbol{S}^{\text{bu}} + \epsilon \boldsymbol{S}^{\text{xs}})\cdot\dot{\boldsymbol{F}} + \epsilon\boldsymbol{\xi}^{\text{xs}}\cdot\dot{\boldsymbol{p}} - (\pi^{\text{bu}} + \epsilon\pi^{\text{xs}})\dot{\varphi})\, dv = \int_{\mathcal{P}\setminus\mathfrak{Q}} \boldsymbol{S}\cdot\dot{\boldsymbol{F}}\, dv + o(1), \tag{11.8}$$

and, hence, as the thickness of the layer vanishes, that term reckons the conventional stress power expended on $\mathcal{P} \setminus \mathfrak{Q}$ by the action of the bulk deformational stress $\boldsymbol{S}$ over $\dot{\boldsymbol{F}}$;

ii. the term of (11.7) involving integration over $\mathcal{P} \cap \mathcal{L}$ obeys

$$\epsilon \int_{\mathcal{P}\cap\mathcal{L}} \varpi\, dv = \int_{\mathfrak{Q}} ((\llbracket W \rrbracket + \mathfrak{f}\cdot\mathfrak{n})V_{\mathfrak{S}} + wK_{\mathfrak{S}}V_{\mathfrak{S}} - \mathbb{S}\cdot\mathring{\mathbb{F}} + \mathfrak{c}\cdot\mathring{\mathfrak{n}})\, da + o(1) \tag{11.9}$$

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 $\llbracket W \rrbracket + \mathfrak{f}\cdot\mathfrak{n}$ over $V_{\mathfrak{S}}$, altering the interfacial area through the action of $wK_{\mathfrak{S}}$ over $V_{\mathfrak{S}}$, deformation of the interface within its tangent plane via the action of the interfacial deformational stress $\mathbb{S}$ over $\mathring{\mathbb{F}}$, and altering the orientation of the interface resulting from the action of the configurational shear $\mathfrak{c}$ over $\mathring{\mathfrak{n}}$;[41]

iii. the term of (11.7) involving integration over $\mathcal{P} \cap \partial\mathcal{L}$ obeys

$$\epsilon \int_{\mathcal{P}\cap\partial\mathcal{L}} W^{\text{xs}}(V\boldsymbol{n})\cdot\boldsymbol{\nu}\, da = o(1) \tag{11.10}$$

and, hence, as the thickness of the layer vanishes, that term contributes nothing to the power.

To verify (11.8), we merely employ the estimates $(8.8)_2$, $(8.11)_2$, $(8.11)_4$, (8.9), $(8.11)_5$, $(8.7)_4$, $(8.5)_3$, and $(8.5)_1$ for $\boldsymbol{S}^{\text{bu}}$, $\boldsymbol{S}^{\text{xs}}$, $\boldsymbol{\xi}^{\text{xs}}$, π^{bu}, π^{xs}, $\dot{\boldsymbol{F}}$, $\dot{\boldsymbol{p}}$, and $\dot{\varphi}$ on $\mathcal{R}^a \cup \mathcal{R}^b$, whereby

$$\int_{\mathcal{P}\setminus\mathcal{L}} \boldsymbol{S}^{\text{bu}}\cdot\dot{\boldsymbol{F}}\, dv = \int_{\mathcal{P}\setminus\mathfrak{Q}} \boldsymbol{S}\cdot\dot{\boldsymbol{F}}\, dv + o(1) \tag{11.11}$$

[41] This delineation of the manner in which power is expended by the evolution of $\mathfrak{Q}$ through $\mathcal{P}$ is due to GURTIN [20, 22].

and

$$\left.\begin{aligned} &\epsilon\int_{\mathcal{P}\setminus\mathcal{L}} \boldsymbol{S}^{\mathrm{xs}}\cdot\dot{\boldsymbol{F}}\,dv = o(1), && \int_{\mathcal{P}\setminus\mathcal{L}} \pi^{\mathrm{bu}}\dot{\varphi}\,dv = o(1),\\ &\epsilon\int_{\mathcal{P}\setminus\mathcal{L}} \boldsymbol{\xi}^{\mathrm{xs}}\cdot\dot{\boldsymbol{p}}\,dv = o(1), && \epsilon\int_{\mathcal{P}\setminus\mathcal{L}} \pi^{\mathrm{xs}}\dot{\varphi}\,dv = o(1), \end{aligned}\right\} \tag{11.12}$$

as $\epsilon \to 0$.

Next, to establish (11.9), we actually show that

$$\left.\begin{aligned} &\int_{\mathcal{P}\cap\mathcal{L}} (\nabla W^{\mathrm{bu}})\cdot\boldsymbol{n}\,dv = \int_{\mathfrak{Q}} [\![W]\!] V_{\mathfrak{S}}\,da + o(1),\\ &\epsilon\int_{\mathcal{P}\cap\mathcal{L}} (\boldsymbol{f}^{\mathrm{xs}}\cdot\boldsymbol{n})V\,dv = \int_{\mathfrak{Q}} (\mathbb{f}\cdot\mathbb{n})V_{\mathfrak{S}}\,da + o(1),\\ &\epsilon\int_{\mathcal{P}\cap\mathcal{L}} W^{\mathrm{xs}}KV\,dA = \int_{\mathfrak{Q}} wK_{\mathfrak{S}}V_{\mathfrak{S}}\,da + o(1),\\ &\epsilon\int_{\mathcal{P}\cap\mathcal{L}} \boldsymbol{S}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{\Gamma}}\,dv = \int_{\mathfrak{Q}} \mathbb{S}\cdot\mathring{\mathbb{F}}\,da + o(1),\\ &\epsilon\int_{\mathcal{P}\cap\mathcal{L}} \boldsymbol{c}^{\mathrm{xs}}\cdot\mathring{\boldsymbol{n}}\,dv = \int_{\mathfrak{Q}} \mathbb{c}\cdot\mathring{\mathbb{n}}\,da + o(1), \end{aligned}\right\} \tag{11.13}$$

and that

$$\int_{\mathcal{P}\cap\mathcal{L}} \boldsymbol{S}^{\mathrm{bu}}\cdot\mathring{\boldsymbol{F}}\,dv = o(1), \qquad \epsilon\int_{\mathcal{P}\cap\mathcal{L}} \jmath^{\mathrm{xs}}\overset{\circ}{\overline{\ln|\boldsymbol{p}|}}\,dv = o(1). \tag{11.14}$$

Toward (11.13), we first record the identity

$$\int_{\mathcal{P}\cap\mathcal{L}} g\,dv = \int_{\mathfrak{Q}} \Big(\int_{-h(\epsilon)}^{h(\epsilon)} g\,d(\epsilon r)\Big)\,da, \tag{11.15}$$

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 (11.15),

$$(\nabla W^{\mathrm{bu}})\cdot\boldsymbol{n} = \epsilon^{-1}\acute{W}^{\mathrm{bu}} + O(1), \tag{11.16}$$

the matching condition (7.9), and the estimate $(8.8)_1$ for W^{bu} on $\mathcal{R}^{\mathfrak{a}}\cup\mathcal{R}^{\mathfrak{b}}$, we obtain $(11.13)_1$. Similarly, $(11.13)_{2\text{–}5}$ follow from (11.15), the estimates $(8.35)_1$,

$(8.35)_2$, $(8.35)_3$, (8.39), $(8.40)_2$, (8.44), $(8.46)_1$, $(8.46)_3$, and $(8.46)_4$ for $\boldsymbol{n}$, V, $\boldsymbol{L}$, $\mathring{\boldsymbol{n}}$, $\mathring{\boldsymbol{\Gamma}}$, W^{xs}, $\boldsymbol{S}^{\mathrm{xs}}$, $\boldsymbol{c}^{\mathrm{xs}}$, and $\boldsymbol{f}^{\mathrm{xs}}$, and the integral identity (8.47) involving χ. Next, on recalling that the volume of $\mathcal{P}\cap\mathcal{L}$ is bounded by $h(\epsilon)$ (cf. the argument used to justify (9.5)), the results (11.14) follow from the estimates $(8.16)_2$ and (8.42) for $\boldsymbol{S}^{\mathrm{bu}}$ and $\jmath^{\mathrm{xs}}$ in tandem with the results $(8.41)_1$ and $(8.41)_2$, whereby the time rates, following uniformity surfaces, of $\boldsymbol{F}$ and $\ln|\boldsymbol{p}|$ are of $O(1)$ on $\mathcal{L}$.

Finally, concerning (11.10), we observe first that $\mathcal{P}\cap\partial\mathcal{L}$ belongs to the overlap region $\mathcal{L}\cap(\mathcal{R}^{\mathrm{a}}\cup\mathcal{R}^{\mathrm{b}})$ where the outer and inner expansions agree. Thus, the bulk estimate $(8.11)_1$ for W^{xs} and the estimates $(8.35)_1$ and $(8.35)_2$ for $\boldsymbol{n}$ and V on $\mathcal{L}$ imply that $W^{\mathrm{xs}}(V\boldsymbol{n})\cdot\boldsymbol{\nu} = o(1)$ on $\mathcal{P}\cap\partial\mathcal{L}$, and (11.10) follows immediately.

12 Discussion

Our asymptotic analysis shows that an order-parameter based regularization of the sharp-interface theory determined by the constitutive response functions $\hat{W}^{\mathrm{a}}$, $\hat{W}^{\mathrm{b}}$, $\hat{w}$, and $\hat{b}$, is obtained by selecting $\hat{W}^{\mathrm{bu}}$, $\hat{W}^{\mathrm{xs}}$, and $\hat{\beta}$ to be of the form

$$\left.\begin{aligned}\hat{W}^{\mathrm{bu}}(\boldsymbol{F},\varphi) &= (1-z(\varphi))\hat{W}^{\mathrm{a}}(\boldsymbol{F}) + z(\varphi)\hat{W}^{\mathrm{b}}(\boldsymbol{F}),\\ \hat{W}^{\mathrm{xs}}(\boldsymbol{F},\varphi,\boldsymbol{p}) &= \epsilon^{-1}\Psi(\varphi) + \frac{\epsilon}{2\sigma^2}|\boldsymbol{p}|^2\hat{w}^2(\boldsymbol{\Gamma},\boldsymbol{n}),\\ \hat{\beta}(\boldsymbol{F},\varphi,\boldsymbol{p},\dot{\varphi}) &= \frac{\epsilon}{\sigma^2}\hat{b}(\boldsymbol{\Gamma},\boldsymbol{n},V)\hat{w}(\boldsymbol{\Gamma},\boldsymbol{n}),\end{aligned}\right\} \tag{12.1}$$

where V, $\boldsymbol{n}$, $\boldsymbol{P}$, and $\boldsymbol{\Gamma}$ are given by (4.5), (4.6), (4.8), and (4.9), and with Ψ any double-well potential satisfying (4.4), and z a monotonic function taking $\mathbb{R}$ into the interval $[0,1]$ and consistent with $z(0)=0$ and $z(1)=1$ (cf. Fig. 3).

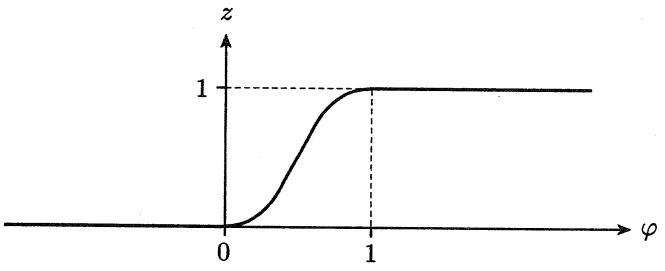

Figure 3. Graph depicting the qualitative properties of z.

So long as Ψ and z possess the qualitative properties described above, the asymptotic correspondence established here does not depend on the particular features of these functions. Because this allows for choices of Ψ and z that

facilitate analysis and/or computation, this freedom should be viewed not as a defect, but, rather, as a strength of the order-parameter based regularization.

In closing, we observe that our results may also be viewed as an independent derivation of the theory of GURTIN & STRUTHERS. Specifically, granted constitutive equations consistent with (1.1)–(1.3) and an appropriate scaling, the order-parameter based theory yields, as an asymptotic limit, a sharp-interface theory coincident with that proposed by GURTIN & STRUTHERS. This suggests that, with different constitutive assumptions and/or scalings, the order-parameter based theory might provide a framework for deriving sharp-interface theories that, unlike the theory of GURTIN & STRUTHERS, remain unestablished. In particular, we have in mind theories in which the interfacial structure incorporates effects, such as those associated with curvature and orientation-rate, that are ignored in the sharp-interface theory considered here.

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A Appendices

A.1 Differentiation on moving surfaces

Since the interface $\mathcal{S}$ evolves with time, time-rates of fields intrinsic to $\mathcal{S}$ must be calculated with care. For this reason, GURTIN & STRUTHERS [2] have introduced the *time derivative of any interfacial field g following the normal trajectories of $\mathcal{S}$*:

$$\mathring{g}(\boldsymbol{x},t) = \frac{d}{d\tau} g(\boldsymbol{z}(\boldsymbol{x},\tau),\tau)\Big|_{\tau=t}, \tag{A.1}$$

where $\boldsymbol{z}$ satisfies the differential equation

$$\dot{\boldsymbol{z}} = V_{\mathcal{S}}(\boldsymbol{z},\cdot)\boldsymbol{m}(\boldsymbol{z},\cdot), \tag{A.2}$$

subject to the condition

$$\boldsymbol{z}(t) = \boldsymbol{z} \tag{A.3}$$

requiring that the trajectory passes through $\boldsymbol{z} \in \mathcal{S}(t)$ at time t. For brevity, we refer to $\mathring{g}$ as *the normal time-rate of g*.

Associated with each continuous bulk field $\boldsymbol{g}$, whose gradient and rate may suffer finite jumps across $\mathcal{S}$, we may introduce an interfacial vector-field $\mathbb{g}$ defined through

$$\mathbb{g} = \boldsymbol{g}|_{\mathcal{S}}. \tag{A.4}$$

Straightforward calculations then show that the surface gradient $\nabla_{\mathcal{S}}\mathbb{g}$ and normal time-rate $\mathring{\mathbb{g}}$ of such a field $\mathbb{g}$ are given by

$$\nabla_{\mathcal{S}}\mathbb{g} = \langle\!\langle \nabla \boldsymbol{g} \rangle\!\rangle \mathbb{P} \qquad \text{and} \qquad \mathring{\mathbb{g}} = \langle\!\langle \dot{\boldsymbol{g}} \rangle\!\rangle + V_{\mathcal{S}} \langle\!\langle (\nabla \boldsymbol{g}) \mathbb{n} \rangle\!\rangle, \tag{A.5}$$

where $\mathbb{P} = \boldsymbol{1} - \mathbb{n}\otimes\mathbb{n}$ is the projector onto $\mathcal{S}$.

Next, suppose that a scalar-valued interfacial field g is given as a function $\hat{g}$ depending on $\mathbb{F}$ and $\mathbb{n}$. Then, letting $\mathbb{E} = \langle\!\langle \boldsymbol{F} \rangle\!\rangle$, the unique decomposition

$$\mathbb{E} = \mathbb{F} + \mathbb{E}\mathbb{n}\otimes\mathbb{n} \tag{A.6}$$

allows us to write

$$\check{g}(\mathbb{E}, \mathbb{n}) = \hat{g}(\mathbb{F}, \mathbb{n}). \tag{A.7}$$

whereby a straightforward calculation furnishes the result

$$\big(\frac{\partial}{\partial \mathbb{E}} \check{g}(\mathbb{E}, \mathbb{n})\big)\mathbb{n} = \boldsymbol{0}, \tag{A.8}$$

which, in turn, implies the identities

$$\frac{\partial}{\partial \mathbb{E}} \check{g}(\mathbb{E}, \mathbb{n}) = \big(\frac{\partial}{\partial \mathbb{E}} \check{g}(\mathbb{E}, \mathbb{n})\big)\mathbb{P} = \frac{\partial}{\partial \mathbb{F}} \hat{g}(\mathbb{F}, \mathbb{n}). \tag{A.9}$$

Given a unit vector $\boldsymbol{k} \neq \mathbb{n}$, let $\boldsymbol{Q}(\boldsymbol{k}, \mathbb{n})$ denote the rotation of $\boldsymbol{k}$ into $\mathbb{n}$ about the axis orthogonal to both $\boldsymbol{k}$ and $\mathbb{n}$, with $\boldsymbol{Q}(\mathbb{n}, \mathbb{n}) = \boldsymbol{1}$. Then, the *derivative of $\hat{g}$ with respect to $\mathbb{n}$ following the surface* $\mathcal{S}$, as introduced by GURTIN & STRUTHERS [2], is defined by (cf. [2])

$$\big(\frac{D}{D\mathbb{n}} \hat{g}(\mathbb{F}, \mathbb{n})\big)\cdot\boldsymbol{\kappa} = \big(\frac{D}{D\mathbb{n}} \check{g}(\mathbb{E}, \mathbb{n})\big)\cdot\boldsymbol{\kappa} = \frac{\partial}{\partial \alpha} \check{g}\big(\mathbb{E}\boldsymbol{Q}(\boldsymbol{k}(\alpha), \mathbb{n}), \boldsymbol{k}(\alpha)\big)\big|_{\alpha=0}, \tag{A.10}$$

with $\boldsymbol{k}(0) = \mathbb{n}$ and $\boldsymbol{k}'(0) = \boldsymbol{\kappa}$.

This derivative allows us to calculate the surface gradient and the normal time-rate of g in terms of $\hat{g}(\mathbb{F}, \mathbb{n})$. To do so, we begin by noting the identity

$$\frac{D}{D\mathbb{n}} \check{g}(\mathbb{E}, \mathbb{n}) = \frac{\partial}{\partial \mathbb{n}} \check{g}(\mathbb{E}, \mathbb{n}) + \big(\frac{\partial}{\partial \mathbb{E}} \check{g}(\mathbb{E}, \mathbb{n})\big)^{T} \mathbb{E}\mathbb{n}, \tag{A.11}$$

which follows directly from (A.7)–(A.10). Then, working with $\check{g}$, we have

$$\mathring{g} = \big(\frac{\partial}{\partial \mathbb{E}} \check{g}(\mathbb{E}, \mathbb{n})\big)\cdot\mathring{\mathbb{E}} + \big(\frac{\partial}{\partial \mathbb{n}} \check{g}(\mathbb{E}, \mathbb{n})\big)\cdot\mathring{\mathbb{n}}, \tag{A.12}$$

so that, bearing in mind the identity

$$\mathring{\mathbb{E}}\mathbb{P} = \mathring{\mathbb{F}} + \mathbb{E}n\otimes\mathring{n} + \mathbb{E}\mathring{n}\otimes n, \tag{A.13}$$

we obtain

$$\mathring{g} = \big(\frac{\partial}{\partial\mathbb{E}}\check{g}(\mathbb{E},n)\big)\cdot\mathring{\mathbb{F}} + \big(\frac{\partial}{\partial n}\check{g}(\mathbb{E},n) + \big(\frac{\partial}{\partial\mathbb{E}}\check{g}(\mathbb{E},n)\big)^T\mathbb{E}n\big)\cdot\mathring{n}, \tag{A.14}$$

which, by virtue of (A.9)–(A.11), yields

$$\mathring{g} = \big(\frac{D}{Dn}\hat{g}(\mathbb{F},n)\big)\cdot\mathring{n} + \big(\frac{\partial}{\partial\mathbb{F}}\hat{g}(\mathbb{F},n)\big)\cdot\mathring{\mathbb{F}}. \tag{A.15}$$

Similarly, we find that

$$\nabla_{\mathfrak{S}}g = -\mathbb{L}^T\big(\frac{D}{Dn}\hat{g}(\mathbb{F},n)\big) + \big(\nabla_{\mathfrak{S}}(\mathbb{F}^T)\big)\big(\frac{\partial}{\partial\mathbb{F}}\hat{g}(\mathbb{F},n)\big). \tag{A.16}$$

A.2 A power identity for the sharp-interface theory

Here we verify the power identity (2.21) of the sharp-interface theory.

Toward this, we first note that, by virtue of the local bulk and interfacial statements $(2.14)_1$ and $(2.15)_1$ of linear momentum balance

$$\int_{\partial\mathcal{P}}\boldsymbol{S}\boldsymbol{\nu}\cdot\dot{\boldsymbol{y}}\,da = \overbrace{\int_{\mathcal{P}}\tfrac{1}{2}\varrho|\dot{\boldsymbol{y}}|^2\,dv}^{\cdot} + \int_{\mathcal{P}\setminus\Omega}\boldsymbol{S}\cdot\dot{\boldsymbol{F}}\,dv + \int_{\Omega}\big([\![\boldsymbol{S}n\cdot\dot{\boldsymbol{y}}]\!] + \tfrac{1}{2}\varrho[\![|\dot{\boldsymbol{y}}|^2]\!]V_{\mathfrak{S}}\big)\,da. \tag{A.17}$$

Further, the interfacial linear momentum balance $(2.15)_1$ yields

$$\int_{\partial\Omega}\mathbb{S}n\cdot\mathring{\mathbb{y}}\,dl = -\int_{\Omega}\big(\mathring{\mathbb{y}}\cdot(\varrho[\![\dot{\boldsymbol{y}}]\!]V_{\mathfrak{S}} - [\![\boldsymbol{S}n]\!]) - \mathbb{S}\cdot(\nabla_{\mathfrak{S}}(\mathring{\mathbb{y}}))\big)\,da, \tag{A.18}$$

while the normal configurational balance (2.31) implies

$$\int_{\partial\Omega}\mathbb{c}\cdot(V_{\mathfrak{S}}\mathbb{m})\,dl = -\int_{\Omega}\big((n\cdot[\![\boldsymbol{C}n]\!] + [\![\boldsymbol{q}\cdot n]\!] + \mathbb{C}\cdot\mathbb{L} + \mathbb{f}\cdot n)V_{\mathfrak{S}} + \mathbb{c}\cdot\mathring{n}\big)\,da. \tag{A.19}$$

Finally, on combining (A.17), (A.18), and (A.19) and employing the relations

$$\left.\begin{aligned}
\tfrac{1}{2}\varrho[\![|\dot{\boldsymbol{y}}|^2]\!] &= \tfrac{1}{2}\varrho[\![|\boldsymbol{F}n|^2]\!]V_{\mathfrak{S}}^2 + \varrho[\![\dot{\boldsymbol{y}}]\!]\cdot\mathring{\mathbb{y}},\\
\mathring{\mathbb{y}}\cdot[\![\boldsymbol{S}n]\!] &= [\![\boldsymbol{S}n\cdot\dot{\boldsymbol{y}}]\!] + n\cdot[\![\boldsymbol{F}^T\boldsymbol{S}n]\!]V_{\mathfrak{S}},\\
n\cdot[\![\boldsymbol{C}n]\!] + [\![\boldsymbol{q}\cdot n]\!] &= [\![W]\!] - n\cdot[\![\boldsymbol{F}^T\boldsymbol{S}n]\!] + \tfrac{1}{2}\varrho[\![|\boldsymbol{F}n|^2]\!]V_{\mathfrak{S}}^2,\\
\mathbb{S}\cdot\big(\nabla_{\mathfrak{S}}(\mathring{\mathbb{y}})\big) &= \mathbb{S}\cdot\mathring{\mathbb{F}} - (\mathbb{F}^T\mathbb{S})\cdot(V_{\mathfrak{S}}\mathbb{L}),\\
\mathbb{C}\cdot\mathbb{L} &= wK_{\mathfrak{S}} - (\mathbb{F}^T\mathbb{S})\cdot\mathbb{L},
\end{aligned}\right\} \tag{A.20}$$

we arrive at the power identity (2.21).

A.3 Facts concerning uniformity surfaces

Assume that the layer $\mathcal{L}$ of the order-parameter based theory contains the interface $\mathcal{S}$ 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 $\mathcal{S}(t)$, 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

$$\nabla\mathbb{z}=\mathbb{P}, \tag{A.21}$$

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

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

$$\nabla g=\big((\nabla g)\cdot\mathbb{n}\big)\mathbb{n}+\nabla_{\mathcal{S}}g, \tag{A.22}$$

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

$$\big(\nabla g(\ell,\mathbb{z},t)\big)\cdot\mathbb{n}(\mathbb{z},t)=\frac{\partial}{\partial\ell}g(\ell,\mathbb{z},t), \tag{A.23}$$

and

$$\nabla_{\mathcal{S}}g(\ell,\mathbb{z},t)=\frac{\partial}{\partial\mathbb{z}}g(\ell,\mathbb{z},t), \tag{A.24}$$

respectively.

In terms of the surface-related coordinate system $(\ell,\mathbb{z})$, 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

$$\nabla\ell=\mathbb{n}\qquad\text{and}\qquad\dot{\ell}=-V_{\mathcal{S}}. \tag{A.25}$$

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

$$\mathbb{L}=-\nabla\mathbb{n}. \tag{A.26}$$

Next, given a scalar-valued field g,

$$\mathring{g}=\dot{g}+(\nabla g)\cdot(V\boldsymbol{n}), \tag{A.27}$$

represents its time derivative following the normal trajectories of uniformity surfaces.[42] By appealing to this definition, we find, in particular, that

$$\mathring{\boldsymbol{n}}+(\overline{\ln|\boldsymbol{p}|})\boldsymbol{n}=-\nabla V. \tag{A.28}$$

[42] Here, V and $\boldsymbol{n}$ are as introduced in (4.5) and (4.6).

Finally, suppose that

$$g = \check{g}(\boldsymbol{F}, \boldsymbol{p}) = \hat{g}(\boldsymbol{\Gamma}, \boldsymbol{n}). \tag{A.29}$$

Then, using the definition (A.11), with m replaced by $\boldsymbol{n}$, we find that

$$|\boldsymbol{p}| \frac{\partial}{\partial \boldsymbol{p}} \check{g}(\boldsymbol{F}, \boldsymbol{p}) = \frac{D}{D\boldsymbol{n}} \hat{g}(\boldsymbol{\Gamma}, \boldsymbol{n}) - \big(\frac{\partial}{\partial \boldsymbol{\Gamma}} \hat{g}(\boldsymbol{\Gamma}, \boldsymbol{n})\big)^T \boldsymbol{F}\boldsymbol{n}, \tag{A.30}$$

with

$$\big(\frac{D}{D\boldsymbol{n}} \hat{g}(\boldsymbol{\Gamma}, \boldsymbol{n})\big) \cdot \boldsymbol{n} = 0, \qquad \big(\frac{\partial}{\partial \boldsymbol{\Gamma}} \hat{g}(\boldsymbol{\Gamma}, \boldsymbol{n})\big)\boldsymbol{n} = \boldsymbol{0}, \tag{A.31}$$

and

$$\frac{\partial}{\partial \boldsymbol{F}} \check{g}(\boldsymbol{F}, \boldsymbol{p}) = \frac{\partial}{\partial \boldsymbol{\Gamma}} \hat{g}(\boldsymbol{\Gamma}, \boldsymbol{n}). \tag{A.32}$$

Further, an argument similar to that resulting in (A.16) yields

$$\nabla g = -\boldsymbol{L}^T \big(\frac{D}{D\boldsymbol{n}} \hat{g}(\boldsymbol{\Gamma}, \boldsymbol{n})\big) + \big(\nabla(\boldsymbol{\Gamma}^T)\big)\big(\frac{\partial}{\partial \boldsymbol{\Gamma}} \hat{g}(\boldsymbol{\Gamma}, \boldsymbol{n})\big), \tag{A.33}$$

with $\boldsymbol{L}$ as defined in (5.17).

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