NONLOCAL MODELS OF PHASE TRANSITIONS IN SOLIDS

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Abstract

A framework is presented for constructing phase field models of multiphase thermoelastic solids. The theory allows for nonlocal interactions. Our development uses concepts analogous to those of classical thermodynamics, and is thus an extension of classical irreversible thermodynamics. Particular models within this framework are examined, by formal asymptotic layer analyses, from the point of view of determining the dynamics and other properties of their phase interfaces. In particular, relations of Gibbs-Thomson type are derived.

1 Introduction

The basic physics of complicated materials is still only partially known. This is especially true of dynamical nonequilibrium phenomena. In an effort at least to gain a conceptual basis for the better understanding of these nonequilibrium processes, a number of phase-field models using thermodynamic concepts have been constructed in recent years (Penrose-Fife [12], Alt-Pawlow [2], Wang-Sekerka et al [18], Ahmad-Wheeler et al [1], Bates-Fife et al [4], Charach-Fife [7]), and in some cases applied to specific nonequilibrium settings such as hypercooled solidification and the rapid solidification of alloys. These concepts are analogous to those in simpler equilibrium situations, where they are more rigorously applicable.

In phase-field theories, a continuous, possibly multicomponent, conserved or nonconserved field function (referred to as order parameter or phase field parameter) is used to characterize the phase of a material. The state of the material is described by the temperature, order parameter and maybe some other state variables. One then proceeds on the basis of some irreversible thermodynamic theory to derive evolution equations for the state.

In this paper, we follow this procedure for materials which can exist in different phases, incorporating (possibly short-range) nonlocal and thermoelastic effects. The framework which we design is general, anticipating later applications to specific scenarios.

However, we do examine two special cases in greater detail. One of them is when the interactions are local, but involve elastic energies, which are most often neglected in phase field theories. The other case is for materials with nonlocal interactions expressed by integrals and influence functions. Recognizing that the most important issues relating to the dynamics of multiphase materials lie in the properties of interfaces between phases, we ask what the theory in those two cases predicts about interfaces.

According to the theory given in [16] and [17], the local Helmholtz free energy density of a material may be influenced by the global concentration and temperature distributions in quasi-static binary alloys and elastic solids. Our concern with the possible existence of nonlocal (long-range) effects even outside of quasi-static conditions is the motivation for our construction of a general theory in which such effects are allowed.

In our treatment, the multiphase elastic solid experiences small deformations during changes of state. The Cauchy strain tensor field ϵ_{ij}, the temperature field T and a phase field parameter ϕ, where ϕ in general has many components, are chosen as independent state variables that completely characterize the physical state of the solid.

The nonlocal features are embodied in the solid's Helmholtz free energy density function, which takes the form:

$$f(\mathbf{x}) = \tilde{f}(\epsilon_{ij}, [T], [\phi])(\mathbf{x}). \qquad \boxed{\text{HF1}} \tag{1}$$

The brackets appearing here in the arguments of the constitutive function $\tilde{f}$ indicate the global functional dependences of $\tilde{f}$ on T and ϕ. This postulated free energy density is used as the basis for the construction of equations governing the evolution of the state of the system. Some previous analysis of models with functional dependence on order parameter can be found in [5] and [13].

More conventional and more familiar local Helmholtz free density functions $f = \tilde{f}(\epsilon_{ij}, T, \phi)$ constitute a special case of (1), obtained by employing the evaluational functional $\delta_{\mathbf{x}}$; namely,

$$\tilde{f}(\epsilon_{ij}, T, \phi) = \tilde{f}(\epsilon_{ij}, \delta_{\mathbf{x}}[T], \delta_{\mathbf{x}}[\phi]), \qquad \boxed{\text{LHF}} \tag{2}$$

where the action of $\delta_{\mathbf{x}}$ on a continuous function ψ is given by $\delta_{\mathbf{x}}[\psi] = \psi(\mathbf{x})$.

The paper is organized as follows. In Section 2, we introduce a general framework using concepts from equilibrium thermodynamics that accommodates the postulated nonlocal effects of temperature and phase parameter. The concept of entropy density, as it appears in classical irreversible thermodynamics, is extended by the introduction of the notion of pseudo-entropy density. A generalized entropy principle is then proposed and a generalized Gibbs relation formulated. Classical irreversible thermodynamics is verified to be a particular case of our general theory.

In Section 3, using the framework developed in Section 2, we derive basic equations governing the evolution of the state variables under the assumption that rates of change of phase decay rapidly as one approaches the equilibrium far field. We also exhibit special cases of the general formulation when the Helmholtz free energy density assumes specific forms. Its dependence on the order parameter field includes specific nonlocal dependence on possibly higher derivatives of that field.

In Section 4, we study phase interface dynamics in a two-phase quasi-static solid when only local effects are present, but the Helmholtz free energy depends on derivatives of the order parameter. The dimensionless basic equations obtained in this case are subjected to an asymptotic layer analysis, and a generalized Gibbs-Thomson type relation is thereby derived. In Section 5, a nonlocal analogue of the foregoing dimensionless Helmholtz free energy density is postulated. A Gibbs-Thomson type relation analogous to the one in Section 4 is obtained. The paper ends with an overview and discussion of various issues in Section 6.

2 The general theory

Our object is to derive general equations governing the time evolution of the state of the material. In order to do this, we utilize several other fields in addition to those mentioned before. They can be connected with the primary fields in various ways. Except for ρ, the following densities are per unit mass. The additional quantities are mass density ϱ, internal energy density e, velocity $\mathbf{v} = (v_1, v_2, v_3)$, heat density q, the energy density p induced by phase transformations, a body force $\mathbf{F} = (F_1, F_2, F_3)$, and a contact force represented by $\sigma_{ji}n_j$ [1], where σ_{ij} is the stress tensor and $\mathbf{n} = (n_1, n_2, n_3)$ is the outward unit normal vector on the bounding surface Σ of V. Later we introduce a pseudo-entropy density s as well.

2.1 Balance laws

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We begin the general theory with the derivation of basic balance equations, starting with that of the total energy density.

Let $V(t)$ be a portion of the solid which changes in accordance with the deformation of the material it encloses. The total energy of that portion of the solid is defined to be the sum of its internal energy $\mathcal{E}$ and kinetic energy $\mathcal{K}$. The total energy density balance equation is taken to be

$$\frac{d}{dt}(\mathcal{E} + \mathcal{K}) = \frac{d}{dt}\mathcal{Q} - \frac{d}{dt}\mathcal{W} + \frac{d}{dt}\mathcal{P}, \tag{3}$$

where $\mathcal{Q}$ is the heat content, $\mathcal{W}$ is the work done by the solid, and $\mathcal{P}$ is the energy of phase. Thus

$$\mathcal{E} = \int_{V(t)} \varrho e \; dV, \quad \mathcal{Q} = \int_{V(t)} \varrho q \; dV, \quad \mathcal{P} = \int_{V(t)} \varrho p \; dV. \tag{4}$$

The kinetic energy is given by

$$\mathcal{K} = \frac{1}{2}\int_{V(t)} \varrho v_i v_i \, dV$$

and the time rate of change of the work done by the body force and contact force is given by

$$-\frac{d}{dt}\mathcal{W} = \int_{\Sigma(t)} (\sigma_{ji}n_j)v_i \; d\Sigma + \int_{V(t)} \varrho F_i v_i \; dV, \tag{5}$$

where $\Sigma(t)$ is the bounding surface of $V(t)$.

Since the elementary volumes change their size and shape in time when deformation is underway, for an arbitary quantity b, we have

$$\frac{d}{dt}\int_{V(t)} b \; dV = \int_{V(t)} (\frac{d}{dt}b) \; dV + \int_{V(t)} b \; \frac{d}{dt}(dV), \tag{6}$$

where $\frac{d}{dt}(dV) = v_{i,i} \; dV$ (cf. e.g., [3]). Therefore the total energy balance equation can be written in local dynamic form:

$$\begin{aligned} &\dot{\varrho}e + \varrho(\dot{e} + ev_{i,i}) + \varrho v_i \dot{v}_i + \frac{1}{2}v_i v_i(\dot{\varrho} + \varrho v_{i,i}) \\ &= \dot{\varrho}q + \varrho(\dot{q} + qv_{i,i}) + \sigma_{ji,j}v_i + \sigma_{ji}v_{i,j} + \varrho F_i v_i + \dot{\varrho}p + \varrho(\dot{p} + pv_{i,i}), \qquad \boxed{\text{1stl3}} \end{aligned} \tag{7}$$

[1] Einstein's convention for summation of repeated indices is used in this paper.

where the upper dot stands for the material (Lagrangian) time derivative [2].

Requiring that (7) remain invariant under rigid motion of the solid, we obtain, in the usual way, the

Balance equation of mass, equation of motion, and symmetry of the stress tensor:

$$\dot{\varrho} = -\varrho v_{i,i}, \quad \sigma_{ji,j} + \varrho F_i - \varrho \dot{v}_i = 0, \quad \sigma_{ij} = \sigma_{ji}. \qquad \boxed{\text{rtinv}} \tag{8}$$

By (8) and $\sigma_{ij} v_{i,j} = \sigma_{ij}(\dot{\epsilon}_{ij} + \dot{\omega}_{ij}) = \sigma_{ij}\dot{\epsilon}_{ij}$, where $\dot{\epsilon}_{ij}$ is the symmetric part and $\dot{\omega}_{ij}$ is the anti-symmetric part of $v_{i,j}$, equation (7) is reduced to the

First internal energy balance equation:

$$\varrho \dot{e} = \varrho \dot{q} + \sigma_{ij}\dot{\epsilon}_{ij} + \varrho \dot{p}. \qquad \boxed{\text{ebe}} \tag{9}$$

By definition, $\dot{\epsilon}_{ij}$ is the Cauchy strain tensor rate. Moreover the left side of (7), which represents the rate of change of the total energy density, is reduced to $\varrho \dot{e} + \varrho v_i \dot{v}_i$.

We require that energy be conserved in the sense that the total energy content within an arbitrary volume in the solid can only change if energy flows into (or out of) the volume through its boundary, i.e.,

$$\frac{d}{dt}(\mathcal{E} + \mathcal{K}) = -\int_{\Sigma} \mathbf{J}_{tot}\ \mathbf{n}\ d\Sigma, \tag{10}$$

where $\mathbf{J}_{tot}$ is the total energy density flux. Thus by (8) and Gauss' theorem, we have the conservation of total energy in local dynamic form:

$$\varrho \dot{e} + \varrho v_i \dot{v}_i = -\nabla \cdot \mathbf{J}_{tot}, \qquad \boxed{\text{cte}} \tag{11}$$

where $\mathbf{J}_{tot}$ is the total energy density flux.

Multiplying equation $(8)_2$ by v_i and using the identity $(\sigma_{ij} v_i)_{,j} = \sigma_{ij,j} v_i + \sigma_{ij} v_{i,j}$, we obtain $\varrho v_i \dot{v}_i = (\sigma_{ij} v_i)_{,j} - \sigma_{ij} v_{i,j} + \varrho F_i v_i$. Introducing this relation into (11), we arrive at the

Second internal energy balance equation:

$$\varrho \dot{e} = -\nabla \cdot \mathbf{J}_e + \sigma_{ij}\dot{\epsilon}_{ij} - \varrho F_i v_i, \qquad \boxed{\text{ebe2}} \tag{12}$$

where $\mathbf{J}_e = \mathbf{J}_{tot} + \sigma_{i.} v_i$. Here $\mathbf{J}_e$ is considered to be the internal energy density flux, while $\sigma_{ij}\dot{\epsilon}_{ij} - \varrho F_i v_i$ is the internal power supply density induced by deformation and body force.

2.2 Entropy and Helmholtz free energy

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At this point we develop the concept of pseudo-entropy density and some associated nonlocal thermodynamical principles, in order to accommodate the nonlocal action embodied in equation (1). We first review the entropy concept in classical irreversible thermodynamics, in which nonlocal effects are not considered.

In classical irreversible thermodynamics, a physical system in a nonequilibrium state is conceived as being divided into a series of little cells which are approximately in instantaneous

[2] An index after comma denotes partial derivative.

equilibrium. This assumption is called the hypothesis of local equilibrium. Entropy S can therefore be defined locally as in equilibrium thermodynamics, and is thus a local state function. As a result, the time rate of change of the entropy density is given by the ratio of the rate of change of heat density to the temperature, i.e.,

$$\dot{S} = \dot{q}/T. \qquad \boxed{\text{Sdot}} \tag{13}$$

To incorporate the possible nonlocal effects of temperature into the theory, we introduce a generalized entropy density. For a fixed global physical state, we assume that there is associated a field function s that maps V to a set of functionals acting on temperature field functions. In place of (13), we assume that during changes of state, the rates of change $\dot{s}$ and $\dot{q}$ at $\mathbf{x}$ are given by

$$\dot{q}(\mathbf{x}) = \langle \dot{s}(\mathbf{x}), T \rangle. \qquad \boxed{\text{dqdst}} \tag{14}$$

The angular bracket pair will always denote the action of functionals on field functions. This function s is called the **pseudo-entropy density**.

As a further analogue of classical thermodynamics, in which the Helmholtz free energy f is related to e, S, and T by $f = e - ST$, we now define

$$f(\mathbf{x}) = e(\mathbf{x}) - \langle s(\mathbf{x}), T \rangle. \qquad \boxed{\text{fest}} \tag{15}$$

From (9) and (15), we obtain

$$\varrho \dot{e} = \varrho \langle \dot{s}, T \rangle + \sigma_{ij} \dot{\epsilon}_{ij} + \varrho \dot{p} \qquad \boxed{\text{gibbs}} \tag{16}$$

and

$$\dot{f} = \langle -s, \dot{T} \rangle + \frac{1}{\varrho} \sigma_{ij} \dot{\epsilon}_{ij} + \dot{p}. \qquad \boxed{\text{df}} \tag{17}$$

2.3 Constitutive relations

As mentioned before, we follow other phase field theories in taking the phase of the material to be described by a continuous order parameter ϕ.

Equation (17) suggests that the Helmholtz free energy density be given by a constitutive function $\tilde{f}$ taking the form of equation (1) when nonlocal effects of the phase are also allowed. We so assume. We now restate the equation (1) using a more mathematically precise terminology.

Let $V \subset R^3$ be the space occupied by the elastic solid. Let Ω_T be a Banach space of scalar field functions on V, and Ω_ϕ be a Banach space of k-component field functions on V. The state of the solid is described by (ϵ_{ij}, T, ϕ), where ϵ_{ij} is the (local) Cauchy strain tensor, $T \in \Omega_T$ is the temperature, and $\phi \in \Omega_\phi$ is a k-component conserved/nonconserved order parameter that we also call a phase function.

For each $\mathbf{x}$, let

$$\tilde{f}(\epsilon_{ij}, [T], [\phi])(\mathbf{x}) : R^{3\times 3} \times \Omega_T \times \Omega_\phi \to R \tag{18}$$

be F-differentiable on its domain. We identify this function with $f(\mathbf{x})$. Dependence of our various functions on time will not be noted explicitly, although time derivatives continue to be symbolized by dots. The variation of f with t comes about through the t-variation of ϵ, T, and ϕ. Thus

$$\dot{f} = \langle f_T, \dot{T} \rangle + f_{\epsilon_{ij}} \dot{\epsilon}_{ij} + \langle f_\phi, \dot{\phi} \rangle. \qquad \boxed{\text{df2}} \tag{19}$$

As a result, by comparing (17) and (19), we obtain the further constitutive relations:

$$-f_T = s, \quad \varrho f_{\epsilon_{ij}} = \sigma_{ij}, \quad \dot{p} = \langle f_\phi, \dot{\phi} \rangle. \qquad \boxed{\text{cr}} \tag{20}$$

Note that f_T and f_ϕ are the partial F-derivatives of f with respect to T and ϕ, and $f_{\epsilon_{ij}}$ is the usual function derivative of f with respect to ϵ_{ij}. At each $\mathbf{x} \in V$, $f_T(\mathbf{x}) \in \Omega_T^*$ and $f_\phi(\mathbf{x}) \in \Omega_\phi^*$, where Ω_T^* and Ω_ϕ^* are continuous dual spaces of Ω_T and Ω_ϕ.

Let $\theta = \frac{1}{T}$, T being the temperature on the Kelvin scale, positive and bounded away from zero. Inspired by (13) and (14), we now choose the function

$$\theta \langle \dot{s}, T \rangle = \dot{q}/T, \tag{21}$$

in the nonlocal theory, as our analogue of the quantity $\dot{S}$ in classical irreversible thermodynamics. This appears to be the most natural choice. Multiplying (12) and (16) by θ and combining the resulting equations, we obtain, within our theory, the expression:

$$\varrho \theta \langle \dot{s}, T \rangle = -\theta \nabla \cdot \mathbf{J}_e - \varrho \theta \langle f_\phi, \dot{\phi} \rangle - \varrho \theta F_i v_i. \qquad \boxed{\text{tsdt}} \tag{22}$$

2.4 Analogue of second law

$\boxed{\text{2ndlaw}}$ We now set $F_i = 0$ and formulate an analogue of the entropy principle in classical irreversible thermodynamics. First, we recall the procedure.

Let $\dot{S}$ be the time rate of change of entropy density. The quantity $\varrho \dot{S}$ is decomposed in such a way that $\varrho \dot{S} = -\nabla \cdot \mathbf{J}_S + \sigma$, where $\mathbf{J}_S$ is the entropy flux and σ represents the time rate of local entropy production per unit volume. As an analogue of the second law in equilibrium thermodynamics, an entropy principle which requires that σ be nonnegative during changes of state is postulated. On the other hand, the entropy flux represents the entropy transport in the system and its surroundings. The integral $-\int_\Sigma \mathbf{J}_S \cdot \mathbf{n}\, d\Sigma$, where Σ is the bounding surface of V and $\mathbf{n}$ is the outward unit normal vector on Σ, represents the time rate of the entropy obtained by transport from the surroundings of V.

As stated, the analogue of $\dot{S}$ is now $\theta \langle \dot{s}, T \rangle$. We will need to envisage the quantity $\varrho \theta \langle \dot{s}, T \rangle$ as the sum of a transport term (analogous to $\nabla \cdot J_S$) and a production term (analogous to σ). According to (22), at a fixed material point $\mathbf{x}$ this quantity depends on the global rate of phase change, i.e. on $[\dot{\phi}]$. We may speak of this dependence as giving rise to a phase-change-induced transport and a phase-change-induced production.

Postulate:

This nonlocal dependence of $\varrho \theta \langle \dot{s}, T \rangle$ on ϕ gives rise to a transport of the quantity $\varrho \theta \langle \dot{s}, T \rangle$, and on the other hand, the local production of $\varrho \theta \langle \dot{s}, T \rangle$ due to phase changes depends only on the *local* rate of phase change $\dot{\phi}(\mathbf{x})$.

Let h be the transport of the quantity $\varrho \theta \langle \dot{s}, T \rangle$ due to the nonlocal effect of $\dot{\phi}$ on $\varrho \theta \langle \dot{s}, T \rangle$. Since this transport is restricted to the solid, it follows by a global conservation law that $\int_V h = 0$.

In our applications, we generally assume a restriction on f, which will in each case be shown to be natural. The assumption is that the functional pairing expressed by the second term on the right of (22) be realized by integration with an ordinary function. More specifically, there exists a multicomponent function ζ on V such that

$$\int_V \varrho(\mathbf{x})\theta(\mathbf{x})\langle f_\phi(\mathbf{x}), \psi\rangle d\mathbf{x} = \int_V \zeta(\mathbf{x})\psi(\mathbf{x})d\mathbf{x}, \ \forall \ \psi \in \mathcal{D}, \qquad \boxed{\text{rep}} \tag{23}$$

where $\zeta(\mathbf{x})\psi(\mathbf{x})$ is the Euclidean inner product and the $\mathcal{D} \subset \Omega_\phi$ will be specified according to applications.

Let

$$h = \varrho\theta\langle f_\phi, \dot{\phi}\rangle - \zeta\dot{\phi} \qquad \boxed{\text{444}}. \tag{24}$$

Clearly, $\int_V h = 0$ if $\dot{\phi} \in \mathcal{D}$. According to our stated postulate regarding the transport and production of the quantity $\varrho\theta\langle \dot{s}, T\rangle$ due to phase changes, while h is regarded as the transport of $\varrho\theta\langle \dot{s}, T\rangle$, the quantity $\zeta\dot{\phi}$ is regarded as the production of $\varrho\theta\langle \dot{s}, T\rangle$ due to phase changes.

To complete the formulation of our analogue of the second law, we observe that

$$-\theta\nabla \cdot \mathbf{J}_e = -\nabla \cdot (\theta\mathbf{J}_e) + \nabla\theta \cdot \mathbf{J}_e.$$

Putting this and (24) into (22), we may identify $-\nabla \cdot (\theta\mathbf{J}_e)$ as the transport of $\varrho\theta\langle \dot{s}, T\rangle$ due to the flux $\theta\mathbf{J}_e$, and moreover take $\nabla\theta \cdot \mathbf{J}_e - \zeta\dot{\phi}$ to be our analogue of local entropy production when $F = 0$. We therefore postulate:

Generalized Entropy Principle. The quantity

$$\sigma = \nabla\theta \cdot \mathbf{J}_e - \zeta\dot{\phi}, \qquad \boxed{\text{ep}} \tag{25}$$

where ζ is defined in (23), is required to be nonnegative. $\boxed{\text{gep}}$

2.5 The role of classical theory

$\boxed{\text{class}}$ It will be shown below that phenomenological relations between fluxes and thermodynamic forces can be chosen in such a way as to keep σ nonnegative. The basic equations are then constructed by using the balance equations of mass $(8)_1$, momentum $(8)_2$, and internal energy (12), and the phenomenological relations. We shall return to the construction of basic equations in the next section. Meanwhile, we conclude this section by fitting classical irreversible thermodynamics into the nonlocal theory.

According to the hypothesis of local equilibrium, the entropy density in the classical case is a well defined state variable and the internal energy density is a function of the entropy density and other state variables such as the strain tensor and the order parameter. The Helmholtz free energy density defined by $f = e - ST$ is given by a constitutive function $\tilde{f}$ of the temperature T and the other suppressed state variables such that $f = \tilde{f}(T)$.

To fit this case into the scheme of our nonlocal theory, we let $\Omega_T = C_b(V)$, the Banach space of all bounded continuous scalar functions on V with the sup-norm. At each $\mathbf{x} \in V$, the pseudo-entropy density s defined in terms of S by

$$s(\mathbf{x}) = S(\mathbf{x})\delta_{\mathbf{x}} \in \Omega_T^*, \quad \forall \ \mathbf{x} \in V, \qquad \boxed{\text{ssd}} \tag{26}$$

where $\langle \delta_{\mathbf{x}}, T \rangle = T(\mathbf{x})$, for all $T \in \Omega_T = C_b(V)$. With this pseudo-entropy density, the Helmholtz free energy density defined according to (15), $f(\mathbf{x}) = e(\mathbf{x}) - \langle S(\mathbf{x})\delta_{\mathbf{x}}, T \rangle$, is the same as it is in classical irreversible thermodynamics, and $\tilde{f}([T])(\mathbf{x}) = \tilde{f}(\delta_{\mathbf{x}}[T])$. Reviving the suppressed state variables of the Helmholtz free energy density, we have equation (2).

In this particular case, ζ in (25) is given by $\varrho\theta\tilde{f}_\phi$, where $\tilde{f}_\phi$ is the usual function partial derivative of $\tilde{f}$ with respect to ϕ. This is the same as the entropy production obtained in classical irreversible thermodynamics. Therefore the nonlocal theory, including our generalized entropy principle, is an adequate extension of classical irreversible thermodynamics.

3 Basic equations of evolution

In this section we consider an isotropic solid occupying the whole space R^3 under the condition that the material remains in equilibrium in the far field. We assume that the phase is described by a scalar-valued nonconserved order parameter ϕ, which is a smooth bounded function of $(\mathbf{x}, t)$. The Helmholtz free energy density is assumed to be regular and its constitutive function takes a general form which allows for nonlocal dependence on the temperature and the order parameter. It will be useful to express this nonlocal dependence on ϕ as consisting of separate explicit nonlocal dependences on ϕ and its spatial derivatives up to some order. This involves no loss or gain of generality. Differential equations governing the change of state are then derived based on this free energy density under the assumption that the rate of phase change decays rapidly in some sense near the far field.

3.1 Helmholtz free energy densities

To put the above described scenario into our previous framework, let $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$, where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is the multi-index of the partial differential operator

$$D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \partial x_3^{\alpha_3}}.$$

Let n be a fixed positive integer and let

$$C_b^n(R^3) = \{\psi \in C_b(R^3) | D^\alpha \psi \in C_b(R^3), \ \forall \ |\alpha| \le n\},$$

where $C_b(R^3)$ is the set of bounded continuous functions on R^3. Then $C_b^n(R^3)$ is a Banach space with norm $\|\psi\| = \sum_{|\alpha| \le n} \|D^\alpha \psi\|_{sup}$. We take Ω_T to be $C_b(R^3)$ and Ω_ϕ to be $C_b^n(R^3)$.

Let $\mathcal{C}^0 \subset C(R^3)$ be some collection of continuous functions rapidly decaying at infinity. For example, $C_c(R^3)$, the set of continuous functions with compact support, is a possible choice for $\mathcal{C}^0$. Relative to $\mathcal{C}^0$, an n^{th} order continuously differentiable function ψ on R^3 is said to be rapidly decaying if $D^\alpha \psi \in \mathcal{C}^0$ for all $|\alpha| \le n$. The symbol $\mathcal{C}^n$ is used to denote the set of rapidly decaying n^{th} order continuously differentiable functions on R^3. We require the time rate of change of phase to decay rapidly in space in the sense that $\dot{\phi} \in \mathcal{C}^n$.

Let n^* be the total number of multiindices α such that $|\alpha| \le n$, and $\Phi = (\varphi_\alpha) \in (C_b(R^3))^{n^*}$ be an n^*-tuple of functions in $C_b(R^3)$. For each $\mathbf{x}$, let

$$\overline{f}(\epsilon_{ij}, [T], [\Phi])(\mathbf{x}) : R^{3\times 3} \times C_b^1(R^3) \times (C_b(R^3))^{n^*} \to R \qquad (27)$$

be F-differentiable. In line with (23), we make the following

Assumption on f:
For each fixed $\theta \in C_b(R^3)$ and α, there exists a (smooth enough) function $\zeta_\alpha \in C_b(R^3)$ such that

$$\int_{R^3} \zeta_\alpha(\mathbf{x})\psi(\mathbf{x})d\mathbf{x} = \int_{R^3} \varrho(\mathbf{x})\theta(\mathbf{x})\langle \overline{f}_{\varphi_\alpha}(\mathbf{x}), \psi\rangle d\mathbf{x}, \quad \forall\ \psi \in \mathcal{C}^n, \qquad \boxed{\text{flt}} \tag{28}$$

where $\overline{f}_{\varphi_\alpha}(\mathbf{x})$ is the F-derivative of $\overline{f}$ with respect to φ_α. In view of the rapidly decaying nature of $\psi \in \mathcal{C}^n$ we see by integration by parts that

$$\int_{R^3} \zeta_\alpha(\mathbf{x})D^\alpha\psi(\mathbf{x})\ d\mathbf{x} = \int_{R^3} (-1)^{|\alpha|}D^\alpha\zeta_\alpha(\mathbf{x})\psi(\mathbf{x})\ d\mathbf{x},\ \forall\ \psi\ \in \mathcal{C}^n. \qquad \boxed{\text{itje0}} \tag{29}$$

Our Helmholtz free energy density function is now assumed to take the form:

$$f(\mathbf{x}) = \tilde{f}(\epsilon_{ij}, [T], [\phi])(\mathbf{x}) = \overline{f}(\epsilon_{ij}, [T], [\mathbf{D}\phi])(\mathbf{x}), \qquad \boxed{\text{hfe1}} \tag{30}$$

where the symbol $\mathbf{D}\phi$ denotes the collection of all possible spatial partial derivatives of ϕ of order less than or equal to n. The free energy density in (30) is F-differentiable.

With this definition, the chain rule for F-derivative implies

$$\tilde{f}_\phi(\epsilon_{ij}, [T], [\phi])(\mathbf{x}) = \sum_{|\alpha|\le n} \overline{f}_{\varphi_\alpha}(\epsilon_{ij}, [T], [\mathbf{D}\phi])(\mathbf{x}) \circ D^\alpha. \qquad \boxed{\text{fsp}} \tag{31}$$

By (28), (29) and (31), we have

$$\int_{R^3} \varrho(\mathbf{x})\theta(\mathbf{x})\langle \tilde{f}_\phi(\mathbf{x}), \psi\rangle d\mathbf{x} = \sum_{|\alpha|\le n} \int_{R^3} (-1)^{|\alpha|}D^\alpha\zeta_\alpha(\mathbf{x})\psi(\mathbf{x})d\mathbf{x}, \qquad \boxed{\text{ifsp}} \tag{32}$$

for all $\psi \in \mathcal{C}^n$. Therefore the function ζ appearing in (23) and in the generalized entropy principle (25) takes the form

$$\zeta = \sum_{|\alpha|\le n} (-1)^{|\alpha|}D^\alpha\zeta_\alpha. \qquad \boxed{\text{zeta}} \tag{33}$$

3.2 Phenomenological relations

$\boxed{\text{phen}}$

In accordance with the expression (25) for σ given in the generalized entropy principle, (33), and the Curie principle in classical irreversible thermodynamics, we propose the following general choice of linear phenomenological relations between the fluxes and forces:

$$\mathbf{J}_e = L_1\nabla\theta, \quad \dot{\phi} = -c\ \zeta, \qquad \boxed{\text{pn1}} \tag{34}$$

where ζ is defined in (33), and L_1 and $c > 0$ are phenomenological coefficients (L_1 is a positive matrix). These coefficients may depend on state variables, and their positivity ensures that $\sigma \ge 0$. (cf. e.g., [9]).

3.3 The equations

Subtracting (12) from (16), we obtain the internal energy conduction equation in the following form:

$$\varrho\langle \dot{s}, T\rangle + \nabla \cdot \mathbf{J}_e = -\varrho\langle f_\phi, \dot{\phi}\rangle - \varrho\theta F_i v_i, \qquad \boxed{\text{inece}} \tag{35}$$

where f_ϕ is given by (31) and $\dot{s}$ can be obtained from $(20)_1$ with the given f.

In (34) we write $L_1 = T^2 A$, where A is a non-negative definite matrix and $c \geq 0$. As a result, the internal energy conduction equation becomes

$$\varrho\langle \dot{s}, T\rangle - \nabla \cdot (A\nabla T) = -\varrho\langle f_\phi, \dot{\phi}\rangle - \varrho\theta F_i v_i. \qquad \boxed{\text{inece1}} \tag{36}$$

In summary, for the Helmholtz free energy density in (30), the system of basic equations governing the evolution of state variables consists of (36), $(34)_2$, $(8)_1$, and $(8)_2$. This system is supplemented with the relation $(34)_1$, initial conditions and conditions in the far field. We shall consider the case that the body force is absent from now on for simplicity.

We now exhibit special cases, using specific postulated Helmholtz free energy densities. We first consider a local density of Ginzburg-Landau type, with added free energy induced by strain.

3.4 Example 1: A Ginzburg Landau model with strain energy

$\boxed{\text{ex1}}$

We begin with postulating the Helmholtz free energy density:

$$f = \tilde{f}(\epsilon_{ij}, T, \phi) = f'(\epsilon_{ij}, T, \phi) + \frac{1}{2}\upsilon|\nabla\phi|^2, \qquad \boxed{\text{efd}} \tag{37}$$

where υ is a nonnegative constant ([7]). The function f' is the bulk term, and the gradient term represents phase interface energy density (as in previous phase field theories).

Let T_o and ϕ_o be the uniform temperature and the order parameter of the solid in a stress free equilibrium state chosen as reference for defining strain. We assume the solid is homogeneous and isotropic. The expansion principle then says that when the solid is stress free and is allowed to expand freely due to uniform temperature change and phase change, the volume will change without creating stress. The bulk free energy density f' is thus further assumed to be of the form:

$$f'(\epsilon_{ij}, T, \phi) = f_0(T, \phi) + W, \qquad \boxed{\text{f0w}} \tag{38}$$

where

$$W = \frac{1}{2}\lambda\epsilon_{kk}^2 + G\epsilon_{ij}\epsilon_{ij} - b_1(T - T_o)\epsilon_{kk} - b_2(\phi - \phi_o)\epsilon_{kk}. \tag{39}$$

Here λ and G are Lame constants, and the b_1 and b_2 are nonnegative constants. The function f_0, which depends smoothly on T and ϕ, is the bulk free energy without deformation. Finally W represents the free energy induced by elastic effects in conformity with linear elasticity and the expansion principle.

Following a widely used convention of linear elasticity, the mass density of homogeneous materials is assumed in this example to be constant during the deformation. Without loss of generality, we assume $\varrho = 1$.

Let $\Omega_T = C_b(R^3)$ and $\Omega_\phi = C_b^1(R^3)$. As the case of classical irreversible thermodynamics, we regard the local free energy density in $(37)_2$ as a functional on $R^{3\times 3} \times C_b(R^3) \times C_b^1(R^3)$ by means of evaluational functionals. We know that this functional assumes the form of (30). By (20) and (28), we obtain respectively:

$$\begin{aligned} \sigma_{ij} &= \lambda\epsilon_{\alpha\alpha}\delta_{ij} + 2G\epsilon_{ij} - b_1(T - T_o)\delta_{ij} - b_2(\phi - \phi_o)\delta_{ij}, \\ \langle \dot{s}, T\rangle &= c_v\dot{T} - f_{0_{T\phi}}\dot{\phi}T + b_1\dot{\epsilon}_{kk}T, \\ \zeta_\alpha = \theta f_{0_\phi} - b_2\theta\epsilon_{kk}, &\text{ if } |\alpha| = 0; \quad \zeta_\alpha = \upsilon\theta D^\alpha\phi, \text{ if } |\alpha| = 1, \end{aligned} \quad \boxed{\text{ssz}} \tag{40}$$

where $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$,

$$c_v = -f_{0_{TT}}T \quad \boxed{\text{spec-ht}} \tag{41}$$

is the specific heat per unit volume, and ζ_α is defined by (28). As a result, together with $(8)_2$, (35) and $(34)_2$, we arrive at the basic equations in this case:

$$\begin{aligned} \lambda\epsilon_{kk,i} + 2G\epsilon_{ik,k} - b_1T_{,i} - b_2(\phi - \phi_o)_{,i} - \dot{v}_i = 0, \\ c_v\dot{T} - \nabla\cdot(A\nabla T) = g, \\ \dot{\phi} = -c[\theta f_{0_\phi} - \upsilon\nabla\cdot(\theta\nabla\phi) - \theta b_2\epsilon_{kk}], \end{aligned} \quad \boxed{\text{bac2}} \tag{42}$$

where

$$g = f_{0_{T\phi}}\dot{\phi}T - b_1\dot{\epsilon}_{kk}T - f_{0_\phi}\dot{\phi} + b_2\epsilon_{kk}\dot{\phi} - \upsilon\nabla\phi\cdot\nabla\dot{\phi}. \tag{43}$$

3.5 Example 2: A nonlocal case.

$\boxed{\text{ex2}}$ In the second example, we let $\Omega_T = \Omega_\phi = C_b(R^3)$. A nonlocal Helmholtz free energy density taking the form

$$f'(\epsilon_{ij}, T, \phi) + \frac{1}{2}\int_{R^3} J(\mathbf{x}-\mathbf{y}, T(\mathbf{x}), T(\mathbf{y}))(\phi(\mathbf{y}) - \phi(\mathbf{x}))^2 d\mathbf{y} \quad \boxed{\text{nla}} \tag{44}$$

is used as the basis for constructing evolution equations. The second term in (44) is the free energy due to nonuniformities in ϕ, and is analogous to the second term in $(37)_2$.

We assume that the function f' here is the same as (38) in the first example. The weight function $J(\mathbf{x}, T_1, T_2)$ in (44) is a smooth function on $R^3 \times R \times R$ such that $J(\mathbf{x}, T_1, T_2) = J(-\mathbf{x}, T_1, T_2)$ and $J(\mathbf{x}, T_1, T_2) = J(\mathbf{x}, T_2, T_1)$. Hence the partial derivatives $J_{T_1} = J_{T_2}$ and $J_{T_1T_1} = J_{T_iT_j}$, for all $i, j = 1, 2$. Moreover, for each fixed $\mathbf{x} \in R^3$ and $T \in C_b(R^3)$, we assume that $J(\mathbf{x}-\mathbf{y}, T(\mathbf{x}), T(\mathbf{y}))$ as well as $J_{T_i}(\mathbf{x}-\mathbf{y}, T(\mathbf{x}), T(\mathbf{y}))$ and $J_{T_iT_j}(\mathbf{x}-\mathbf{y}, T(\mathbf{x}), T(\mathbf{y}))$, converge to 0 rapidly as $|\mathbf{y}| \to \infty$. Thus this nonlocal functional is F-differentiable on $R^3 \times R^{3\times 3} \times \Omega_T \times \Omega_\phi$. Unlike the gradient term in $(37)_2$, the nonlocal term defined in (44) depends on temperature. The mass density is still assumed to remain constant during deformation. Based on the mass conservation $(8)_1$, the elementary volume dV is independent of time.

As in the first example, we calculate σ_{ij}, $\dot{s}$ and f_ϕ based on this supposed nonlocal Helmholtz free energy density. While the stress tensor σ_{ij} is still given by $(40)_1$, we have

$$\langle \dot{s}, T\rangle = -f_{0_{TT}}T\dot{T} - f_{0_{T\phi}}\dot{\phi}T + b_1\dot{\epsilon}_{kk}T - \mathcal{M}_{11} - \mathcal{M}_{12}, \tag{45}$$

where

$$\mathcal{M}_{11}(\mathbf{x}) = \frac{1}{2}\int_{R^3} J_{T_1T_1}(\mathbf{x}-\mathbf{y},T(\mathbf{x}),T(\mathbf{y}))(\phi(\mathbf{y})-\phi(\mathbf{x}))^2(\dot{T}(\mathbf{x})+\dot{T}(\mathbf{y}))$$
$$(T(\mathbf{x})+T(\mathbf{y}))d\mathbf{y},$$

and

$$\mathcal{M}_{12}(\mathbf{x}) = \int_{R^3} J_{T_1}(\mathbf{x}-\mathbf{y},T(\mathbf{x}),T(\mathbf{y}))(\phi(\mathbf{y})-\phi(\mathbf{x}))(\dot{\phi}(\mathbf{y})-\dot{\phi}(\mathbf{x}))$$
$$(T(\mathbf{x})+T(\mathbf{y}))d\mathbf{y}.$$

Also we have

$$\langle f_\phi, \dot{\phi}\rangle = f_{0_\phi}\dot{\phi} - b_2\epsilon_{kk} + \mathcal{M}_2, \tag{46}$$

where

$$\mathcal{M}_2(\mathbf{x}) = \int_{R^3} J(\mathbf{x}-\mathbf{y},T(\mathbf{x}),T(\mathbf{y}))(\dot{\phi}(\mathbf{y})-\dot{\phi}(\mathbf{x}))(\phi(\mathbf{y})-\phi(\mathbf{x}))d\mathbf{y}.$$

Consequently, while the equation of motion in this case is the same as $(42)_1$, we have the internal energy conduction equation

$$-f_{0_{TT}}T\dot{T} - \mathcal{M}_{11} - \nabla\cdot(A\nabla T) = g, \qquad \boxed{\text{bac4}} \tag{47}$$

where

$$g = f_{0_{T\phi}}\dot{\phi} - b_1\dot{\epsilon}_{kk}T + \mathcal{M}_{12} - f_{0_\phi}\dot{\phi} + b_2\epsilon_{kk}\dot{\phi} - \mathcal{M}_2,$$

and the phase field equation

$$\dot{\phi} = -c[\theta f_{0_\phi} - \mathcal{M} - \theta b_2\epsilon_{kk}], \qquad \boxed{\text{bac5}} \tag{48}$$

where

$$\mathcal{M}(\mathbf{x}) = \int_{R^3} J(\mathbf{x}-\mathbf{y},T(\mathbf{x}),T(\mathbf{y}))(\theta(\mathbf{x})+\theta(\mathbf{y}))(\phi(\mathbf{y})-\phi(\mathbf{x}))d\mathbf{y}.$$

If the solid is quasi-static and there is a displacement potential, the balance equation of momentum $(42)_1$ becomes

$$\epsilon_{kk} = \frac{1}{\lambda+2G}[b_1(T-T_o)+b_2(\phi-\phi_o)]. \qquad \boxed{\text{ee}} \tag{49}$$

In other models, the internal energy conduction equation is often written as a linear equation, which amounts to the assumption that the dependence of the coefficients on T is negligble. This may be done in our model (47) as well.

4 Phase interface dynamics based on a local model

In this section, we study the phase interface dynamics of quasi-static two-phase solids whose free energy density is of the form $(37)_2$. The nonconserved scalar-valued order parameter ϕ takes values in the interval $[0,1]$.

Let $A = c_dI$, where c_d is the **internal energy conductivity** of the solid which is assumed to be constant and I is the identity matrix.

Following common practice, we take f_0 to be a double well function of ϕ. More specifically, we make the following

Assumptions on f_0:

(a) f_0 is a quadratic function of T when ϕ is fixed,

(b) for fixed T, it is a smooth double-well function of ϕ with two local minima at $\phi_\pm(T)$, where $\phi_-(T) < \phi_+(T)$, and one local maximum between $\phi_-(T)$ and $\phi_+(T)$,

(c) it is strictly convex on R except on a fixed interval $[q_0, q_1] \subset (0,1)$,

(d) $f_0(T, \phi_-(T)) = f_0(T, \phi_+(T))$ if and only if $T = \tau_c$,

(e) $f_0(\tau_c, \phi)$ is symmetric about $\frac{1}{2}(\phi_-(\tau_c) + \phi_+(\tau_c))$, and

(f) $f_{0_T}(\tau_c, \phi_+(\tau_c)) - f_{0_T}(\tau_c, \phi_-(\tau_c)) < 0$.

The two phases contained in the solid, phase zero and phase one, are identified with the intervals $\phi < q_0$ and $\phi > q_1$.

4.1 Dimensionless basic equations

We assume that the region occupied by phase zero is bounded during the time interval considered. Let l be a characteristic length of the phase zero region and ν be a characteristic value for the specific heat c_v. Then $\overline{\mathbf{x}} = \mathbf{x}/l$ and $\overline{t} = tc_d \,/\, l^2\nu$ are the dimensionless space and time variables. Moreover, $\overline{T}(\overline{\mathbf{x}}, \overline{t}) = T(\mathbf{x}, t)/T_o$, $\overline{\phi}(\overline{\mathbf{x}}, \overline{t}) = \phi(\mathbf{x}, t)$, and $\overline{\theta}(\overline{\mathbf{x}}, \overline{t}) = \theta(\mathbf{x}, t)/\theta_o$, where $\theta_o = 1/T_o$, are dimensionless state variables. We also define the dimensionless quantities: $\overline{\phi}_\pm(\overline{T}) = \phi_\pm(T)$, $\overline{c}_v(\overline{\phi}) = c_v(\phi)/\nu$ and $\overline{f}_0(\overline{T}, \overline{\phi}) = f_0(T, \phi)/\nu T_o$.

We define $\alpha = c_d \tau_c / c\,\nu$ and $\varepsilon^2 = \upsilon/\nu l^2 \tau_c$, where the constant c in α is from the equation $(42)_3$. Similar to the rescaling performed in [14], we rescale the thermoelastic parameters as follows: $\varepsilon\overline{\lambda} = \lambda/\nu\tau_c$, $\varepsilon\overline{G} = G/\nu\tau_c$, $\varepsilon\overline{b}_1 = b_1/\nu$ and $\varepsilon\overline{b}_2 = b_2/\nu\tau_c$. We suppress overbars on dimensionless variables and parameters. The nondimensionalized free energy density then reads:

$$\tilde{f}(\epsilon_{ij}, T, \phi) = f_0(T, \phi) + \frac{1}{2}\varepsilon^2 |\nabla\phi|^2 + \varepsilon W, \qquad \boxed{\text{dllhfe}} \tag{50}$$

where

$$W = \frac{1}{2}\lambda\epsilon_{kk}^2 + G\epsilon_{ij}\epsilon_{ij} - b_1(T-1)\epsilon_{kk} - b_2(\phi - \phi_o)\epsilon_{kk}.$$

We follow the widely used simplification in thermoelasticity that the internal energy conduction equation is linear in T; the rescaled dimensionless equations from (42) now read:

$$\begin{aligned} c_v(\phi)\dot{T} - \nabla^2 T &= -\iota_{0_\phi}\dot{\phi} - \varepsilon^2 \nabla\phi \cdot \nabla\dot{\phi} - \varepsilon b_1 \dot{\epsilon}_{kk} + \varepsilon b_2 \epsilon_{kk}\dot{\phi}, \\ \varepsilon^2 \alpha \dot{\phi} &= -\theta f_{0_\phi} + \varepsilon^2 \nabla \cdot (\theta \nabla\phi) - \varepsilon b_2 \theta \epsilon_{kk}, \qquad \boxed{\text{bac6}} \end{aligned} \tag{51}$$

where

$$\iota_0(\phi) = f_0(1, \phi) - f_{0_T}(1, \phi)$$

and the ϵ_{kk} are given by (49) with $T_o = 1$.

Thus ι_0 is the lowest order internal energy at $T = \tau_c$, as a function of ϕ.

4.2 Phase interface and asymptotic analysis

We now assume that $\epsilon \ll 1$ and that the width of the transition layer is $O(\varepsilon)$. This assumption will be consistent with our asymptotic analysis. Define the phase interface by the level surface $\Sigma(t;\varepsilon) = \{\mathbf{x} : \phi(\mathbf{x}, t, \varepsilon) = \hat{h}\}$, where $\hat{h} \in (q_0, q_1) \subset (0, 1)$.

4.2.1 Outer expansion

To pursue an asymptotic layer analysis, we assume that any state variable u can be expressed as

$$u = u(\mathbf{x}, t; \varepsilon) = u_0(\mathbf{x}, t) + \varepsilon u_1(\mathbf{x}, t) + O(\varepsilon^2), \qquad \boxed{\text{out}} \tag{52}$$

where $u_i \in O(1)$ for $i = 0, 1, 2$, when $\mathbf{x}$ is away from $\Sigma(t, \varepsilon)$. Equation (52) is called the outer expansion of u and u_i are called outer functions. Introducing the outer expansions of T, ϕ and θ into (51), then equating terms of the lowest individual ε powers, we obtain the $O(1)$ basic equations:

$$c_v(\phi_0)\dot{T}_0 - \nabla^2 T_0 = -\iota_{0_\phi}(\phi_0)\dot{\phi}_0, \quad -\theta_0 f_{0_\phi}(T_0, \phi_0) = 0. \qquad \boxed{\text{ord1}} \tag{53}$$

Knowing that, for each fixed T, $f_0(T, \phi)$ is a double-well function whose minima are at $\phi_\pm(T)$, we see that $(T_0, \phi_\pm(T_0))$ solves $(53)_2$. Therefore,

$$\phi_0(\mathbf{x}, t) = \phi_-(T_0(\mathbf{x}, t)), \text{ on } \mathbf{D}^0(t); \ \phi_0(\mathbf{x}, t) = \phi_+(T_0(\mathbf{x}, t)), \text{ on } \mathbf{D}^1(t), \qquad \boxed{\text{solphi0o}} \tag{54}$$

where $\mathbf{D}^0(t)$ is the region on the phase zero side of $\Sigma(t;\varepsilon)$, and $\mathbf{D}^1(t)$ is the region on the phase one side of $\Sigma(t;\varepsilon)$. With ϕ_0 given by (54), T_0 is determined by solving $(53)_1$ together with a given initial temperature field.

4.2.2 Inner expansion

Near $\Sigma(t;\varepsilon)$, we define the local coordinates (s_1, s_2, r) by

$$\mathbf{x} = \mathbf{x}(s_1, s_2, r) = \mathbf{p}(s_1, s_2) + r\mathbf{n}(s_1, s_2), \qquad \boxed{\text{lc}} \tag{55}$$

where $\mathbf{p}$ is a reparameterization of the phase interface surface and $\mathbf{n}$ is the unit normal vector toward the phase one region. Therefore we have

$$\nabla r = \mathbf{n}, \quad \nabla^2 r = \frac{-2H + 2rK}{1 - 2rH + r^2 K}, \qquad \boxed{\text{gt}} \tag{56}$$

where K is the Gaussian curvature and H is the mean curvature of $\Sigma(t;\varepsilon)$ (cf. [15]). The normal velocity v of the moving interface surface $\Sigma(t;\varepsilon)$ is thus given by $-r_t$, the negative of the partial time derivative of r.

The stretched local coordinates are defined by (s_1, s_2, ρ), where $\rho = \frac{r}{\varepsilon}$. In a close neighborhood of Σ, state variables u expressed in terms of the stretched local coordinates are assumed to be able to be expressed as

$$u = \tilde{u}(s_1, s_2, \rho; \varepsilon) = \tilde{u}_0(s_1, s_2, \rho) + \varepsilon \tilde{u}_1(s_1, s_2, \rho) + O(\varepsilon^2), \qquad \boxed{\text{inner}} \tag{57}$$

where $\tilde{u}_i \in O(1)$ for $i = 0, 1, 2$. The dependence on the time variable t is suppressed for simplicity here and afterwards. Equation (57) is called the inner expansion of u and $\tilde{u}_i$ are called inner functions.

The outer functions u_i in (52) and the inner functions $\tilde{u}_i$ in (57) should match in the overlapping region where both expansions are valid. The following standard matching conditions are derived from this requirement:

$$\tilde{u}_0(s_1, s_2, \pm\infty) = \hat{u}_0(s_1, s_2, 0\pm),$$

$$\tilde{u}_1(s_1, s_2, \pm\infty) = \hat{u}_1(s_1, s_2, 0\pm) + \rho \hat{u}_{0_r}(s_1, s_2, 0\pm) + O(1), \qquad \boxed{\text{match}} \tag{58}$$

as $\rho \to \pm\infty$, where $\hat{u}_i(s_1, s_2, 0\pm)$, $i = 0, 1$, are the limits of the $O(1)$ and $O(\varepsilon)$ outer functions as the interface surface is approached at (s_1, s_2) from both sides in the normal direction and $\hat{u}_{0_r}(s_1, s_2, 0\pm)$ are the corresponding limits of the normal derivatives (cf. [6]).

Assume that the Gaussian curvature K, the mean curvature H and the normal velocity v of $\Sigma(t;\varepsilon)$ may be expanded in powers of ε to second order. Namely $K = K(s_1, s_2; \varepsilon) = K_0(s_1, s_2) + \varepsilon K_1(s_1, s_2) + O(\varepsilon^2)$, $H = H(s_1, s_2; \varepsilon) = H_0(s_1, s_2) + \varepsilon H_1(s_1, s_2) + O(\varepsilon^2)$, and $v(s_1, s_2; \varepsilon) = v_0(s_1, s_2) + \varepsilon v_1(s_1, s_2) + O(\varepsilon^2)$ where K_i, H_i and v_i are of $O(1)$, for $i = 0, 1$. Using the chain rule for derivatives, (55) and (56), among other things, we transform (51) to equations with state variables in the stretched local coordinates. We introduce the inner expansions of T, ϕ and θ, as well as the ε expansions of H, K and v into these equations and expand the equations in powers of ε to second order. The $O(1)$ and $O(\varepsilon)$ inner basic equations are obtained by equating terms of the same orders in the expansions.

To lowest order, the $O(1)$ inner basic equations read:

$$\tilde{T}_{0_{\rho\rho}} = 0, \qquad -\frac{1}{\tilde{T}_0} f_{0_\phi}(\tilde{T}_0, \tilde{\phi}_0) - \frac{1}{\tilde{T}_0^2} \tilde{T}_{0_\rho} \tilde{\phi}_{0_\rho} + \frac{1}{\tilde{T}_0} \tilde{\phi}_{0_{\rho\rho}} = 0. \qquad \boxed{\text{ord1in}} \tag{59}$$

Since we seek a bounded solution for $\tilde{T}_0$, by $(59)_1$ we conclude that $\tilde{T}_0 = c$, a constant, for each fixed (s_1, s_2). Consequently $(59)_2$ is rewritten as

$$\tilde{\phi}_{0_{\rho\rho}} - f_{0_\phi}(c, \tilde{\phi}_0) = 0. \qquad \boxed{\text{phain1}} \tag{60}$$

Using (54) and $(58)_1$, we obtain that, for (s_1, s_2) fixed,

$$\tilde{\phi}_0(s_1, s_2, \rho) \to \phi_\pm(c), \quad \text{as} \quad \rho \to \pm\infty. \qquad \boxed{\text{bdypin1}} \tag{61}$$

Since $f_0(c, \cdot)$ has two equal local minima if and only if $c = \tau_c$, we have that $c = \tau_c$ if and only if there exists a unique solution of ψ of (60) such that (61) is verified and $\psi(0) = \hat{h}$ (cf. [11]). Thus

$$\tilde{T}_0(s_1, s_2, \rho) = \tau_c, \quad \tilde{\phi}_0(s_1, s_2, \rho) = \psi(\rho). \qquad \boxed{\text{o1is}} \tag{62}$$

By applying (58), we summarize: when the phase interface surface is approached from both sides, the $O(1)$ approximations of T and ϕ are

$$\hat{T}_0(s_1, s_2, 0\pm) = \tau_c, \qquad \hat{\phi}_0(s_1, s_2, 0\pm) = \phi_\pm(\tau_c). \qquad \boxed{\text{ipct0p0}} \tag{63}$$

We shall suppress the dependence on (s_1, s_2) for simplicity.

With the knowledge of (62), the $O(\varepsilon)$ inner basic equations read:

$$\tilde{T}_{1_{\rho\rho}} = -v_0[\iota_{0_\phi}(\psi)\psi_\rho + \psi_{\rho\rho}\psi_\rho], \qquad - f_{0_{\phi\phi}}(\tau_c, \psi)\tilde{\phi}_1 + \tilde{\phi}_{1_{\rho\rho}} = \omega, \qquad \boxed{\text{ordepin}} \tag{64}$$

where

$$\begin{aligned} \omega = & -\alpha\tau_c v_0 \psi_\rho + 2H_0\psi_\rho - \frac{1}{\tau_c} f_{0_\phi}(\tau_c, \psi)\tilde{T}_1 + f_{0_{\phi T}}(\tau_c, \psi)\tilde{T}_1 \\ & + \frac{1}{\tau_c}\tilde{T}_{1_\rho}\psi_\rho + \frac{1}{\tau_c}\tilde{T}_1\psi_{\rho\rho} + \frac{b_2}{\lambda + 2G}[b_1(\tau_c - 1) + b_2(\psi - \tilde{\phi}_o)]. \end{aligned} \tag{65}$$

4.2.3 Stefan condition

Integrating $(64)_1$, we obtain

$$\tilde{T}_{1_\rho} = -v_0[\iota_0(\psi) + \frac{1}{2}\psi_\rho^2] + c_1, \qquad \boxed{\text{tth1ro}} \tag{66}$$

where c_1 is an integration constant. Using $(58)_2$, we get

$$\hat{T}_{0_r}(0\pm) = -v_0 \ \iota_0(\phi_\pm(\tau_c)) + c_1. \qquad \boxed{\text{ict0r}} \tag{67}$$

Hence the jump condition of $\hat{T}_{0_r}$ across the phase interface is

$$[\hat{T}_{0_r}]_\Sigma = \hat{T}_r(0+) - \hat{T}_r(0-) = -v_0 \ \mathcal{L}_0, \qquad \boxed{\text{jumpt0r}} \tag{68}$$

where

$$\mathcal{L}_0 = \iota_0(\phi_+(\tau_c)) - \iota_0(\phi_-(\tau_c)) \qquad \boxed{\text{L0}} \tag{69}$$

is the $O(1)$ dimensionless latent heat density (the internal energy of the disordered minus the that of the ordered material) at $T = \tau_c$. We shall write $\iota_{0\pm}$ for $\iota_0(\phi_\pm(\tau_c))$.

A classical Stefan free boundary problem with variables T_0, ϕ_0 and v_0 is given by (53), (63) and (68). With initial and boundary conditions, this free boundary problem could be solved. Clearly, the c_1 in (67) (and also in (66)) is determined if T_0 and v_0 are known.

4.2.4 Gibbs-Thomson condition

Integrating (66), we obtain

$$\tilde{T}_1(\rho) = -v_0\gamma(\rho) + c_1\rho + c_2, \qquad \boxed{\text{tts1}} \tag{70}$$

where

$$\gamma(\rho) = \int_0^\rho \iota_0(\psi) + \frac{1}{2}\int_0^\rho \psi_\rho^2, \tag{71}$$

and c_1 and c_2 are constants. As $\rho \to \pm\infty$,

$$\int_0^\rho \iota_0(\psi) = \int_0^{\pm\infty} (\iota_0(\psi) - \iota_{0\pm}) + \rho\iota_{0\pm} + o(1). \qquad \boxed{\text{iq2}} \tag{72}$$

By (70), (72) and (58), we have

$$\hat{T}_1(0\pm) = -v_0 \left[\int_0^{\pm\infty} (\iota_0(\psi) - \iota_{0\pm}) + \frac{1}{2}\int_0^{\pm\infty} \psi_\rho^2\right] + c_2. \qquad \boxed{\text{icts1}} \tag{73}$$

Since ψ solves the equation (60), we have that ψ_ρ satisfies the homogeneous equation of $(64)_2$. Namely ψ_ρ is an eigenfunction with eigenvalue 0 of the operator defined by $\Lambda : \varphi \to \partial_{\rho\rho}\varphi - f_{0_{\phi\phi}}(\tau_c, \psi)\varphi$. By the solvability condition used in [6] and many other places, we know that $(64)_2$ has a solution if and only if

$$\int_R \omega\psi_\rho d\rho = 0 \qquad \boxed{\text{sc}} \tag{74}$$

(cf. [6]). Introducing (70) into (74), we obtain

$$c_2\ \hat{\mathcal{L}}_0 = -v_0(\alpha\tau_c\mathcal{A} + \Psi) + 2H_0\mathcal{A} + c_1\mathcal{B} + \mathcal{F}, \qquad \boxed{\text{c2}} \tag{75}$$

where

$$\begin{aligned}
\hat{\mathcal{L}}_0 &= f_{0_T}(\tau_c, \phi_-(\tau_c)) - f_{0_T}(\tau_c, \phi_+(\tau_c)) > 0,\\
\Psi &= \int_R \left[-\frac{1}{\tau_c} f_{0_\phi}(\tau_c, \psi) + f_{0_{\phi T}}(\tau_c, \psi) - \frac{1}{\tau_c}\psi_{\rho\rho}\right]\psi_\rho\gamma, \quad \mathcal{A} = \int_R \psi_\rho^2, \qquad \boxed{\text{calRel}}\\
\mathcal{B} &= \int_R \left[-\frac{1}{\tau_c} f_{0_\phi}(\tau_c, \psi) + f_{0_{\phi T}}(\tau_c, \psi) + \frac{1}{\tau_c}\psi_{\rho\rho}\right]\psi_\rho\rho + \frac{1}{\tau_c}\int_R \psi_\rho^2,\\
\mathcal{F} &= \frac{b_2}{\lambda + 2G}\left[b_1(\tau_c - 1)[\phi_0]_\Sigma + b_2\left(\frac{1}{2}[\phi_0^2]_\Sigma - \int_R \tilde{\phi}_o\psi_\rho\right)\right].
\end{aligned} \tag{76}$$

Here $\tilde{\phi}_o$ is the reference phase parameter in the stretched local coordinates near the phase interface and the symbol $[\phi_0]_\Sigma$ denotes $\phi_+(\tau_c) - \phi_-(\tau_c)$, and $[\phi_0^2]_\Sigma$ denotes $\phi_+^2(\tau_c) - \phi_-^2(\tau_c)$.

The constant c_2 in (70) is obtained from (75). The $\hat{\mathcal{L}}_0 > 0$ is the change of $O(1)$ internal energy density per unit mass at the critical temperature τ_c when the solid changes from phase zero to phase one.

In view of (76), Ψ is completely determined by ψ and τ_c. Since Ψ is also seen as a weighted average of γ, Ψ is related to the $O(\varepsilon)$ inner temperature.

Since $f_0(\tau_c, \cdot)$ is symmetric about a with $a = \frac{1}{2}(\phi_-(\tau_c) + \phi_+(\tau_c))$, $f_{0_\phi}(\tau_c, x + a)$ is an odd function of x. Since ψ solves (60), $\psi - a$ solves $\tilde{\phi}_{0_{\rho\rho}} - f_{0_\phi}(\tilde{\phi}_0 + a) = 0$. By the oddness of $-f_{0_\phi}(x + a)$, we have that $\psi - a$ is an odd function (cf. [6]). ψ_ρ is thus an even function. Therefore, $\int_0^\infty \psi_\rho^2 = \int_{-\infty}^0 \psi_\rho^2 = \frac{1}{2}\mathcal{A}$. Introducing (75) into (73), the interface condition of T_1 in (73) is determined. By (63), (73) and (75), the interface condition of T_1 is given by

$$\begin{aligned}
\hat{T}_1(0\pm) \;&=\; -v_0\Big[\int_0^{\pm\infty}(\iota_0(\psi) - \iota_{0_\pm})d\rho \pm \frac{1}{4}\mathcal{A} + \alpha\tau_c\mathcal{A}\hat{\mathcal{L}}_0^{-1} + \Psi\hat{\mathcal{L}}_0^{-1}\Big]\\
&\quad + 2H_0\mathcal{A}\mathcal{L}_0^{-1} + c_1\mathcal{B}\hat{\mathcal{L}}_0^{-1} + \mathcal{F}\hat{\mathcal{L}}_0^{-1}, \qquad \boxed{\text{tsspm}}
\end{aligned} \tag{77}$$

where $\hat{\mathcal{L}}_0^{-1}$ is the reciporocal of $\hat{\mathcal{L}}_0$. The temperature thus has an $O(\varepsilon)$ discontinuity across the phase interface. By (60), we have

$$\mathcal{A} = \int_R \psi_\rho^2 d\rho = \int_{\phi_-(\tau_c)}^{\phi_+(\tau_c)} \sqrt{2[f_0(\tau_c, \phi) - f_0(\tau_c, \phi_c)]}d\phi, \qquad \boxed{\text{A2}} \tag{78}$$

where $\phi_c = \phi_+(\tau_c)$ or $\phi_-(\tau_c)$. According to [11], the dimensionless surface tension is given by $\varepsilon\mathcal{A} + O(\varepsilon^2)$. This temperature discontinuity is caused in part by the change of internal energy density across the phase interface, and also surface tension effects expressed by $-\int_0^{\pm\infty}(\iota_0(\psi)-\iota_{0\pm})d\rho \mp \frac{1}{4}\mathcal{A}$.

Finally, we comment that since the free energy density function is defined up to a constant, we may choose it so that $\iota_{0_+} = \iota_0(\phi_+(\tau_c)) = \frac{1}{2}\mathcal{L}_0$. As a result, $\iota_{0_-} = \iota_0(\phi_-(\tau_c)) = -\frac{1}{2}\mathcal{L}_0$. By (67), we have

$$c_1 = \hat{T}_{0_r}(0\pm) \pm \frac{1}{2}\mathcal{L}_0 v_0. \qquad \boxed{\text{c12}} \tag{79}$$

By (79), equation (77) is therefore rewritten as

$$\hat{T}_1(0\pm) - \mathcal{B}\hat{T}_{0_r}(0\pm)\hat{\mathcal{L}}_0^{-1} - 2H_0\mathcal{A}\hat{\mathcal{L}}_0^{-1} - \mathcal{F}\hat{\mathcal{L}}_0^{-1}$$

$$= -v_0[\int_0^{\pm\infty}(\iota_0(\psi) \mp \frac{1}{2}\mathcal{L}_0)d\rho \pm \frac{1}{4}\mathcal{A} + \alpha\tau_c\mathcal{A}\hat{\mathcal{L}}_0^{-1} + \Psi\hat{\mathcal{L}}_0^{-1} \mp \frac{1}{2}\mathcal{B}\mathcal{L}_0\hat{\mathcal{L}}_0^{-1}]. \qquad \boxed{\text{gtr}} \tag{80}$$

Equation (80) is the Gibbs-Thomson relation for the phase interface. This relation connects the phase front normal velocity v_0 to the first order correction to the temperature on both sides of the phase interface, the mean curvature H_0 of the phase interface surface (third term on the left), the relaxation time α, the latent heat density $\mathcal{L}_0$ ($\hat{\mathcal{L}}_0$), the phase interface surface tension represented by $\mathcal{A}$ (78), and an elastic effect represented by $\mathcal{F}$ (76) (all, except for the temperature, to lowest order). Recall that the lowest order temperature is simply given by $(63)_1$. The more typical kinetic under-cooling (super-heating) condition is recovered when the temperature is constant in a neighborhood of a flat phase interface and the elastic effect is ignored.

5 Phase interface dynamics based on a nonlocal model

A dimensionless nonlocal free energy density is assumed with the gradient term in (50) replaced with its nonlocal analogue:

$$\frac{1}{2}\int_{R^3} J^\varepsilon(\mathbf{x}-\mathbf{y}, T(\mathbf{x}), T(\mathbf{y}))(\phi(\mathbf{y})-\phi(\mathbf{x}))^2 d\mathbf{y},$$

where $J^\varepsilon(\mathbf{x}, T_1, T_2) = \frac{1}{\varepsilon^3}J(\frac{\mathbf{x}}{\varepsilon}, T_1, T_2)$.

The characteristic range of this nonlocal influence function J^ε is $O(\epsilon)$, so that when ϵ is small (which we assume), the nonlocal effects die off rapidly with distance. We assume that J satisfies the smoothness, symmetry and decaying assumptions we made in the example in Section 3.5. Moreover, for any bounded set $\overline{V} \subset R^2$, there exists a $C > 0$ such that for all $(T_1, T_2) \in \overline{V}$,

$$J(\mathbf{x}, T_1, T_2) < C|\mathbf{x}|^{-5}, \quad J_{x_i}(\mathbf{x}, T_1, T_2) < C|\mathbf{x}|^{-6}. \qquad \boxed{\text{grate7}} \tag{81}$$

The basic equations derived from this free energy density take the form of (47) and (48) with J replaced with J^ε. The linearized internal energy conduction equation is obtained by replacing T by the dimensionless reference temperature 1 in (47).

5.1 Outer expansion

By performing an outer expansion on the equations, we obtain the same $O(1)$ outer basic equations as (53). Therefore the $O(1)$ outer approximation to the order parameter is given by (54).

5.2 Inner expansion; Stefan condition

For a point represented by (s_1, s_2) on the phase interface surface $\Sigma(t;\varepsilon)$, the vectors $(\mathbf{p}_{s_1}(s_1, s_2), \mathbf{p}_{s_2}(s_1, s_2), \mathbf{n}$ form a reference frame tied to the surface at (s_1, s_2) (cf. (55)). At fixed (s_1, s_2), define

$$\delta = |det(\mathbf{p}_{s_1}, \mathbf{p}_{s_2}, \mathbf{n})|,$$

$$k(\sigma_1, \sigma_2, \rho, T_1, T_2) = J(\mathbf{p}_{s_1}\sigma_1 + \mathbf{p}_{s_2}\sigma_2 + \mathbf{n}\rho, T_1, T_2). \qquad \boxed{\text{k}} \tag{82}$$

As in the case of the asymptotic layer analysis performed in Section 4, inner expansions of state variables are accomplished by expressing the state variables in terms of the stretched local coordinates. However, for reasons of simplicity we ignore the ε term and high order terms in the ε expansions of normal velocity v, mean curvature H and other geometric quantities of the phase interface surface. Expanding the inner equations in powers of ε to second order and equating terms of the same ε powers, we obtain the $O(1)$ and $O(\varepsilon)$ inner basic equations. The transformation and expansion of a typical term defined by an integral is shown in the appendix.

The $O(1)$ inner internal energy conduction equation is the same as the equation (59), therefore $\tilde{T}_0 = c$ for some constant c. With this condition, the $O(1)$ inner order parameter $\tilde{\phi}_0$ satisfies

$$-f_{0_\phi}(c, \tilde{\phi}_0) - 2\delta h * \tilde{\phi}_0 + 2\delta m\tilde{\phi}_0 = 0, \qquad \boxed{\text{nlo1p1}} \tag{83}$$

where

$$h(\rho) = \int_{R^2} k(\sigma_1, \sigma_2, \rho, c, c)\,d\sigma_1 d\sigma_2, \tag{84}$$

$$m = \int_R h(\rho)d\rho, \quad h * \tilde{\phi}_0(\rho) = \int_R h(\rho - \rho')\tilde{\phi}_0(\rho')d\rho'. \qquad \boxed{\text{mhp}} \tag{85}$$

Since J is an even function of $\mathbf{x}$, we have that h is even. By the evenness of h, Fubini's theorem and the Lebesgue dominated convergence theorem, we obtain $\int_R (h * \tilde{\phi}_0)\tilde{\phi}_{0_\rho} = \int_R (h * \tilde{\phi}_0)_\rho \tilde{\phi}_0$. Since the $O(1)$ outer approximation of the order parameter ϕ_0 is given by (54), we obtain by $(58)_1$ that $\tilde{\phi}_0(\pm\infty) = \phi_\pm(c)$. Integrating by parts and using the Lebesgue dominated convergence theorem, we obtain $\int_R (h * \tilde{\phi}_0)\tilde{\phi}_{0_\rho} = m[\phi_+^2(c) - \phi_-^2(c)] - \int_R (h * \tilde{\phi}_0)_\rho \tilde{\phi}_0$. Hence

$$\int_R (h * \tilde{\phi}_0)\tilde{\phi}_{0_\rho} = \frac{1}{2}m[\phi_+^2(c) - \phi_-^2(c)]. \qquad \boxed{\text{phispn}} \tag{86}$$

Multiplying (83) by $\tilde{\phi}_{0_\rho}$ and integrating it over R, we conclude by (86) that

$$f_0(c, \phi_+(c)) - f_0(c, \phi_-(c)) = 0. \qquad \boxed{\text{edmf0}} \tag{87}$$

The equation (87) implies that $\tilde{T}_0 = c = \tau_c$ when f_0 obeys the assumption that $f_0(T, \phi)$ has equal depth minimal at $\phi_\pm(T)$ if and only if $T = \tau_c$. For simplicity, we assume that $\phi_\pm(\tau_c) = 1, 0$ from now on.

Without loss of generality, we assume that the constant m defined in (85) is 1. Assume that h and $-f_{0_\phi}(\tau_c,\cdot)$ satisfy the hypotheses (H_1) through (H_3) in [5] and $-f_{0_{\phi\phi}}(\tau_c,\cdot) > -2\delta$ on R. Under this assumption, for each fixed s_1 and s_2, (83) together with $\tilde{\phi}_0(\pm\infty) = 1, 0$ and $\tilde{\phi}_0(0) = \hat{h}$, is uniquely solvable if and only if $\tilde{T}_0 = \tau_c$ (cf. [5]). We call the solution $\tilde{\phi}_0 = \psi^*$. We therefore have

$$\tilde{T}_0(s_1, s_2, \rho) = \tau_c, \quad \tilde{\phi}_0(s_1, s_2, \rho) = \psi^*(s_1, s_2, \rho). \qquad \boxed{\text{psitauc}} \tag{88}$$

According to $(58)_1$, we obtain the $O(1)$ approximations of T and ϕ as the phase interface surface is approached from the phase one side and phase zero side:

$$T_0(0\pm) = \tau_c, \quad \phi_0(0\pm) = 1, 0. \qquad \boxed{\text{tc10}} \tag{89}$$

For $i = 0, 1, 2$ let

$$\begin{aligned} \mathcal{H}_i(\rho) &= \int_{R^2} k_{T_i}(\sigma_1, \sigma_2, \rho, 1, 1) d\sigma_1 d\sigma_2, \\ h_i(\rho) &= \int_{R^2} k_{T_i}(\sigma_1, \sigma_2, \rho, \tau_c, \tau_c) d\sigma_1 d\sigma_2. \end{aligned} \tag{90}$$

When $i = 0$, this is taken to mean that there is no partial derivative of k involved. Since $J_{T_1} = J_{T_2}$, we have $\mathcal{H}_1 = \mathcal{H}_2$ and $h_1 = h_2$. We first define

$$\begin{aligned} g(\rho) &= \iota_{0_\phi}(\psi^*(\rho))\psi^*_\rho(\rho) \\ &+ \sum_{i=0}^{2}(-1)^r \delta \int_R \mathcal{H}_i(\rho')(\psi^*(\rho - \rho') - \psi^*(\rho))(\psi^*_\rho(\rho - \rho') - \psi^*_\rho(\rho))d\rho', \qquad \boxed{\text{zzg}} \end{aligned} \tag{91}$$

where $r = 0$ if $i = 0$, and $r = 1$ otherwise. Secondly,

$$\begin{aligned} w_1(\rho) &= 4H\delta \int_R h_0(\rho - \rho')(\psi^*(\rho') - \psi^*(\rho))\rho' d\rho' \\ &+ 2\sum_{l=1}^{3} \delta \int_{R^3} k_{\sigma_l}(\sigma_1', \sigma_2', \rho - \rho', \tau_c, \tau_c)\mathcal{Q}_l(\sigma_1', \sigma_2', \rho - \rho') \\ &(\psi^*(\rho') - \psi^*(\rho))d\sigma_1' d\sigma_2' d\rho', \qquad \boxed{\text{zzw}} \end{aligned} \tag{92}$$

(see appendix for $\mathcal{Q}_l$ cf. (109)). And thirdly,

$$w_2(\rho) = L(\tilde{T}_1)(\rho),$$

where the linear operator L is defined by

$$\begin{aligned} L(\varphi)(\rho) &= -\frac{1}{\tau_c} f_{0_\phi}(\tau_c, \psi^*)\varphi(\rho) + f_{0_{\phi T}}(\tau_c, \psi^*(\rho))\varphi(\rho) \\ &+ \sum_{i=0}^{2}(-\frac{1}{\tau_c})^r \delta \int_R h_i(\rho - \rho')(\psi^*(\rho') - \psi^*(\rho))(\varphi(\rho) + \varphi(\rho'))d\rho', \end{aligned} \tag{93}$$

where $r = 1$ if $i = 0$, and $r = 0$ otherwise.

With the knowledge of (88), the evenness of h_i and $\mathcal{Q}_l$, for $i = 0, 1, 2$ and $l = 1, 2, 3$, and also $\tilde{\theta}_1 = -\frac{1}{\tau_c^2}\tilde{T}_1$, the $O(\varepsilon)$ inner equations read:

$$\tilde{T}_{1_{\rho\rho}} = -vg, \quad - f_{0_{\phi\phi}}(\tau_c, \psi^*)\tilde{\phi}_1 - 2\delta h_0 * \tilde{\phi}_1 - 2\delta\tilde{\phi}_1 = \omega, \qquad \boxed{\text{ioepbt}} \tag{94}$$

where v is the $O(1)$ normal velocity of the phase interface and

$$\omega = -\alpha\tau_c v\psi_\rho^* + w_1 + w_2 + \frac{b_2}{\lambda + 2G}[b_1(\tau_c - 1) + b_2(\psi^* - \tilde{\phi}_o)]. \qquad \boxed{\text{ome}} \tag{95}$$

The quantity w_1 represents the part of ω which depends on the geometry of the phase interface represented by $\mathcal{Q}_l$ and H. The quantity w_2 represents the part of ω depending on $\tilde{T}_1$.

Let $e_1(\rho) = 1$ and $e_2(\rho) = \rho$. The functions e_1 and e_2 are fundamental solutions of the homogeneous differential equation $\tilde{T}_{1_{\rho\rho}} = 0$. The Wronskian $\mathcal{W}(e_1, e_2)$ of e_1 and e_2 is 1. By the method of variation of constants for a second order linear differential equation, the general solution of $(94)_1$ is given by

$$\tilde{T}_1(\rho) = -v\int_0^\rho (\rho - \xi)g(\xi)d\xi + c_1\rho + c_2. \qquad \boxed{\text{tts12}} \tag{96}$$

According to $(58)_2$, we obtain the following interface and jump conditions for $\hat{T}_{0_r}$ at the phase interface:

$$\hat{T}_{0_r}(0\pm) = -v(\int_0^{\pm\infty} g) + c_1, \quad [\hat{T}_{0_r}]_\Sigma = -v\int_R g. \qquad \boxed{\text{nljpt0r}} \tag{97}$$

It can be verified by Fubini's theorem that

$$\int_R g(\rho)d\rho = \iota_0(1) - \iota_0(0) = \mathcal{L}_0, \tag{98}$$

where $\mathcal{L}_0$ (69) is the $O(1)$ latent heat (cf. [8]). The jump condition given by $(97)_2$ may also be written as

$$[\hat{T}_{0_r}]_\Sigma = -v\mathcal{L}_0. \qquad \boxed{\text{nljpt0r2}} \tag{99}$$

A classical Stefan free boundary problem with variables T_0, ϕ_0 and v is formulated by (53), (89) and (99). This indicates that under the proposed nonlocal Helmholtz free energy density analogous to that given in (37), we have the same lowest order approximations of the temperature, order parameter and normal velocity of the phase interface surface as before in Section 4.

5.3 Generalized Gibbs-Thomson condition

We now derive a relation analogous to (80).

By (83) and $(94)_2$, we know that ψ_ρ^* satisfies the homogeneous equation of $(94)_2$. That is, ψ_ρ^* is an eigenfunction with eigenvalue 0 of the linear operator defined by $\Lambda : \varphi \to -f_{0_{\phi\phi}}(\tau_c, \psi^*)\varphi - 2\delta h_0 * \varphi - 2\delta\varphi$. According to the solvability condition in [5], (94) has a solution only if

$$\int_R \omega\psi_\rho^* = 0. \qquad \boxed{\text{wp7}} \tag{100}$$

Let

$$\gamma^*(\rho) = \int_0^\rho (\rho - \xi) g(\xi) d\xi, \quad I(\rho) = \rho.$$

Introducing (95) and (96) into (100), we obtain

$$c_2 \hat{\mathcal{L}}_0^* = -v(\alpha\tau_c \mathcal{A}^* + \Psi^*) + \int_R w_1 \psi_\rho^* + c_1 \mathcal{B}^* + \mathcal{F}, \qquad \boxed{\text{cs2}} \tag{101}$$

where $\mathcal{F}$ is defined by $(76)_3$ with $[\phi_0]_\Sigma = 1$ and

$$\hat{\mathcal{L}}_0^* = -\int_R L(1)\psi_\rho^*, \ \mathcal{A}^* = \int_R \psi_\rho^{*^2}, \ \Psi^* = -\int_R L(\gamma^*)\psi_\rho^*, \ \mathcal{B}^* = \int_R L(I)\psi_\rho^*.$$

By the evenness of h_i, it can be verified that

$$\int_R \int_R h_i(\rho - \rho')(\psi^*(\rho') - \psi^*(\rho))\psi_\rho^*(\rho) d\rho' d\rho = 0,$$

for $i = 0, 1, 2$. Therefore

$$\hat{\mathcal{L}}_0^* = -\int_R L(1)\psi_\rho^* = f_{0_T}(\tau_c, 0) - f_{0_T}(\tau_c, 1) = \hat{\mathcal{L}}_0.$$

If $\int_R \rho g(\rho) d\rho$ converges, then $\lim_{\rho\to\pm\infty} \int_\rho^{\pm\infty} \rho g(\xi) d\xi = 0$. This implies that as $\rho \to \pm\infty$,

$$\int_0^{\pm\rho} \rho g(\xi) d\xi = \rho \int_0^{\pm\infty} g(\xi) d\xi + o(1), \quad \int_0^{\pm\rho} \xi g(\xi) d\xi = \int_0^{\pm\infty} \xi g(\xi) d\xi + o(1).$$

By (96), (97) and $(58)_2$, we have

$$\hat{T}_1(0\pm) = v \int_0^{\pm\infty} \xi g(\xi) d\xi + c_2. \tag{102}$$

Replacing c_1 and c_2 with expressions obtained from (97) and (101), we may write the interface condition of T_1 as

$$\hat{T}_1(0\pm) - \hat{\mathcal{L}}_0^{-1}\mathcal{B}^*\hat{T}_{0_r}(0\pm) - \hat{\mathcal{L}}_0^{-1}\int_R w_1\psi_\rho^* - \hat{\mathcal{L}}_0^{-1}\mathcal{F}$$

$$= -v\left[-\int_0^{\pm\infty} \xi g(\xi) d\xi + \alpha\tau_c\hat{\mathcal{L}}_0^{-1}\mathcal{A}^* + \hat{\mathcal{L}}_0^{-1}\Psi^* - \hat{\mathcal{L}}_0^{-1}\mathcal{B}^*\int_0^{\pm\infty} g\right]. \qquad \boxed{\text{gtrn3}} \tag{103}$$

Equation (103) is our nonlocal version of the Gibbs-Thomson relation. The terms in (103) are generally analogous to corresponding ones in the local version (80), but are more complicated. The complication is due in part to the presence of the functions w_1 (92) and g (91). The other symbols in (103) are defined following (101).

6 Discussion

Our object has been to construct a framework analogous to classical irreversible thermodynamics in which highly nonequilibrium processes involving phase changes in an elastic solid can be modeled and studied. Although our construction is fairly general, the emphasis has been on the effects of nonlocal interactions. The state of the solid is specified by the temperature, strain tensor, and (possibly multicomponent) order parameter or phase variable. The inclusion of the latter means that the resulting models will be of phase-field type.

The aim has been to develop reasonable equations giving evolution laws for the state of the material. For this purpose, concepts analogous to the classical ones of Helmholtz free energy and entropy are used, as well as the material's internal energy, heat content, etc. Relations among these concepts are postulated, again in analogy with equilibrium relations in the classical case. Also an entropy principle is postulated, under which the entropy production is to be nonnegative. This principle leads to natural constitutive relations involving generalized forces and fluxes.

As a result of all this, evolution laws are derived. These laws are based on the postulated form for the Helmholtz free energy as a function of the global temperature of the solid, the global order parameter, and the strain tensor. Given such an assumed form, the evolution equations are determined, except for functions and parameters which do not affect the qualitative properties of these laws.

Possibly the most important information to be extracted from evolution laws for these materials is their implication regarding the dynamics of phase interfaces. We pursue this analysis in the case of two examples.

Our two examples are based on Helmholtz free energy densities of either local or nonlocal Ginzburg-Landau type. Free energy densities of this type consist of bulk plus interfacial free energy densities. We incorporate the elastic energy density in the bulk part. The interfacial contributions are traditionally represented in phase field theory by terms involving the gradients of order parameters. In our two examples, the interfacial energy density is embodied in either order parameter gradient terms or their nonlocal analogues. In both cases, there is a small interaction parameter ϵ which is a rough measure of the width of the phase interface. In the nonlocal example, it is also a measure of the distance involved in the nonlocal interaction.

The evolution equations are studied by a singular perturbation analysis based on the smallness of ϵ. This analysis reveals conditions such as a Stefan-like condition and a generalized Gibbs-Thomson condition relating the temperature, temperature gradient, and elastic strain at the interface to its velocity and curvature (these conditions involve various material properties such as latent heat, relaxation times, elastic coefficients, etc.). The interface conditions reduce to the more traditional ones when traditional assumptions are made, such as locality of interactions. In the case of the nonlocal analogue of the Ginzburg-Landau free energy density, other geometric properties of the interface besides the curvature play a role, namely the coefficients of the first and second fundamental forms, as well as their derivatives.

Many possible models are incorporated into the framework presented here. In fact, the Helmholtz free energy, in its dependence on the state variables, is quite arbitrary. We have, however, shown in our two examples how to relate this function and its parameters to some potentially measurable properties of the interface, such as the coefficients in the Gibbs-Thomson relation and the surface tension.

We hope that this framework may be useful in providing macroscopic models of the very complex dynamics of solid materials which change phase. However, its generality dictates that a great deal of material-specific information must be incorporated as well.

7 Appendix

In this appendix, we derive the the inner expansion of a typical term in the basic equations derived from a nonlocal free energy density such as that in Section 5, using the tools of coordinate transformations and ε-power expansions. Specifically, we consider

$$I(\mathbf{x};\varepsilon) = \int_{R^3} J^{\varepsilon}(\mathbf{x}-\mathbf{y}, T(\mathbf{x}), T(\mathbf{y}))(\phi(\mathbf{y}) - \phi(\mathbf{x}))d\mathbf{y}.$$

We begin by recalling definitions of local coordinates and stretched local coordinates near the phase interface surface $\Sigma(t,\varepsilon)$ (Sections 4 and 5).

Let $S(t;\varepsilon)$ be a sufficiently small open subset of $\Sigma(t;\varepsilon)$ and $\mathbf{p}(s_1, s_2)$ be the parameterization of $S(t;\varepsilon)$. Define $r = r(\mathbf{x}, t; \varepsilon)$ to be the signed distance from the point $\mathbf{x}$ to $S(t;\varepsilon)$ such that $r < 0$ if $\mathbf{x}$ is in the phase zero region, and $r \geq 0$ otherwise. The local coordinates of $\mathbf{x}$ near $S(t;\varepsilon)$ are given by (s_1, s_2, r) so that (55) holds, where in (55) the point $\mathbf{p}(s_1, s_2) \in S(t;\varepsilon)$ is the orthogonal projection of $\mathbf{x}$ on $S(t;\varepsilon)$ and $\mathbf{n}(s_1, s_2)$ is the unit normal vector at $\mathbf{p}(s_1, s_2) \in S(t;\varepsilon)$ pointing toward the phase one region. Let $M : (s_1, s_2, r) \to (x_1, x_2, x_3) = \mathbf{x}$ represent this change of coordinates. The transformation M is assumed to be smooth. We mention here that as usual, functions with independent variables as subscripts represent partial derivatives.

Let J_M be the Jacobian of the transformation M. Therefore $J_M = \det(\mathbf{p}_{s_1} + r\mathbf{n}_{s_1}, \mathbf{p}_{s_2} + r\mathbf{n}_{s_2}, \mathbf{n})$. Since $\mathbf{p}_{s_1} + r\mathbf{n}_{s_1} = (1 + rk_1)\mathbf{p}_{s_1}$ and $\mathbf{p}_{s_2} + r\mathbf{n}_{s_2} = (1 + rk_2)\mathbf{p}_{s_2}$, where k_1 and k_2 are the normal curvatures of the interface surface in the directions of $\mathbf{p}_{s_1}$ and $\mathbf{p}_{s_1}$, we have

$$J_M = (1 + rk_1)(1 + rk_2)\delta = (1 + r(2H) + r^2K)\delta, \qquad \boxed{\text{jaco}} \tag{104}$$

where H is the mean curvature, K is the Gaussian curvature and $\delta = |\det(\mathbf{p}_{s_1}, \mathbf{p}_{s_2}, \mathbf{n})|$.

We now assume that both $\mathbf{x}$ and $\mathbf{y}$ are in a close neighborhood of the phase interface surface where the local coordinates are defined. Thus there are triples (s_1, s_2, r) and (s_1', s_2', r') such that $\mathbf{x}(s_1, s_2, r) = \mathbf{p}(s_1, s_2) + r\mathbf{n}(s_1, s_2)$ and $\mathbf{y}(s_1, s_2, r) = \mathbf{p}(s_1', s_2') + r'\mathbf{n}(s_1', s_2')$. Let $\Delta\mathbf{s} = (s_1 - s_1', s_2 - s_2', r - r')$ and $\Delta\mathbf{s}^T$ be its transpose. By the Taylor expansion, we have

$$\mathbf{x} - \mathbf{y} = \nabla\mathbf{x} \cdot \Delta\mathbf{s} + \frac{1}{2}\Delta\mathbf{s}\Sigma\Delta\mathbf{s}^T + O(d^3), \qquad \boxed{\text{tay1}} \tag{105}$$

where $d = \sqrt{(s_1 - s_1')^2 + (s_2 - s_2')^2 + (r - r')^2}$ and

$$\nabla\mathbf{x} = (\mathbf{p}_{s_1} + r\mathbf{n}_{s_1}, \mathbf{p}_{s_2} + r\mathbf{n}_{s_2}, \mathbf{n}),$$

$$-\Sigma = \begin{pmatrix} \mathbf{p}_{s_1s_1} + r\mathbf{n}_{s_1s_1} & \mathbf{p}_{s_1s_2} + r\mathbf{n}_{s_1s_2} & \mathbf{n}_{s_1} \\ \mathbf{p}_{s_2s_1} + r\mathbf{n}_{s_2s_1} & \mathbf{p}_{s_2s_2} + r\mathbf{n}_{s_2s_2} & \mathbf{n}_{s_2} \\ \mathbf{n}_{s_1} & \mathbf{n}_{s_2} & 0 \end{pmatrix}. \qquad \boxed{\text{fstt}} \tag{106}$$

The vectors $(\mathbf{p}_{s_1}(s_1, s_2), \mathbf{p}_{s_2}(s_1, s_2), \mathbf{n}(s_1, s_2))$ form a reference frame tied to the the point represented by (s_1, s_2) on the surface $\Sigma(t;\varepsilon)$. Therefore

$$\begin{aligned} \mathbf{p}_{s_1s_1} &= \Gamma_{11}^1\mathbf{p}_{s_1} + \Gamma_{11}^2\mathbf{p}_{s_2} + L_1\mathbf{n}, \qquad & \mathbf{p}_{s_1s_2} &= \Gamma_{12}^1\mathbf{p}_{s_1} + \Gamma_{12}^2\mathbf{p}_{s_2} + L_2\mathbf{n}, \\ \mathbf{p}_{s_2s_1} &= \Gamma_{21}^1\mathbf{p}_{s_1} + \Gamma_{21}^2\mathbf{p}_{s_2} + L_2\mathbf{n}, \qquad & \mathbf{p}_{s_2s_2} &= \Gamma_{22}^1\mathbf{p}_{s_1} + \Gamma_{22}^2\mathbf{p}_{s_2} + L_3\mathbf{n}, \\ \mathbf{n}_{s_1} &= a_{11}\mathbf{p}_{s_1} + a_{21}\mathbf{p}_{s_2}, \qquad & \mathbf{n}_{s_2} &= a_{12}\mathbf{p}_{s_1} + a_{22}\mathbf{p}_{s_2}, \end{aligned} \qquad \boxed{\text{rel}} \tag{107}$$

where $a_{i,j}$, for $i,j=1,2$, Γ_{ij}^k, for $i,j,k=1,2$, and L_i, for $i=1,2,3$, can be determined. We note here that the a_{ij} are entries of the 2^{nd} fundamental form matrix of the surface $\Sigma(t,\varepsilon)$; Γ_{ij}^k are the Christoffel symbols (cf. [10]).

Let $\sigma=(\sigma_1,\sigma_2,\rho)=(\frac{s_1}{\varepsilon},\frac{s_2}{\varepsilon},\frac{r}{\varepsilon})$ and $\sigma'=(\sigma_1',\sigma_2',\rho')=(\frac{s_1'}{\varepsilon},\frac{s_2'}{\varepsilon},\frac{r'}{\varepsilon})$. By (106) and (107), we have

$$\nabla\mathbf{x}\cdot\Delta\mathbf{s}=\varepsilon[\mathbf{p}_{s_1}(\sigma_1-\sigma_1')+\mathbf{p}_{s_2}(\sigma_2-\sigma_2')+\mathbf{n}(\rho-\rho')]$$
$$+\varepsilon^2\rho[\mathbf{p}_{s_1}(a_{11}(\sigma_1-\sigma_1')+a_{12}(\sigma_2-\sigma_2'))+\mathbf{p}_{s_2}(a_{21}(\sigma_1-\sigma_1')+a_{22}(\sigma_2-\sigma_2'))],$$

and

$$\frac{1}{2}\Delta\mathbf{s}\Sigma\Delta\mathbf{s}^T=-\frac{\varepsilon^2}{2}(\sigma-\sigma')\mathbf{C}(\sigma-\sigma')^T+O(\varepsilon^3),$$

where, also by (107),

$$\mathbf{C}=\begin{pmatrix}\mathbf{p}_{s_1s_1} & \mathbf{p}_{s_1s_2} & \mathbf{n}_{s_1}\\ \mathbf{p}_{s_2s_1} & \mathbf{p}_{s_2s_2} & \mathbf{n}_{s_2}\\ \mathbf{n}_{s_1} & \mathbf{n}_{s_2} & 0\end{pmatrix}=\mathbf{p}_{s_1}C^1+\mathbf{p}_{s_2}C^2+\mathbf{n}\,C^3,$$

with

$$C^1=\begin{pmatrix}\Gamma_{11}^1 & \Gamma_{12}^1 & a_{11}\\ \Gamma_{21}^1 & \Gamma_{22}^1 & a_{12}\\ a_{11} & a_{12} & 0\end{pmatrix},$$

$$C^2=\begin{pmatrix}\Gamma_{11}^2 & \Gamma_{12}^2 & a_{21}\\ \Gamma_{21}^2 & \Gamma_{22}^2 & a_{22}\\ a_{21} & a_{22} & 0\end{pmatrix},\quad C^3=\begin{pmatrix}L_1 & L_2 & 0\\ L_2 & L_3 & 0\\ 0 & 0 & 0\end{pmatrix}.$$

As a result,

$$\begin{aligned}\frac{\mathbf{x}-\mathbf{y}}{\varepsilon} &= \mathbf{p}_{s_1}((\sigma_1-\sigma_1')+\varepsilon\mathcal{Q}_1(\sigma-\sigma')+O(\varepsilon^2))\\ &\quad+\mathbf{p}_{s_2}((\sigma_2-\sigma_2')+\varepsilon\mathcal{Q}_2(\sigma-\sigma')+O(\varepsilon^2))\\ &\quad+\mathbf{n}\,((\sigma_3-\sigma_3')+\varepsilon\mathcal{Q}_3(\sigma-\sigma')+O(\varepsilon^2)), \qquad \boxed{\text{xmyoe}}\end{aligned} \tag{108}$$

where

$$\begin{aligned}\mathcal{Q}_1(\sigma) &= -\frac{1}{2}\sigma C^1\sigma^T+a_{11}\sigma_1\rho+a_{12}\sigma_2\rho,\\ \mathcal{Q}_2(\sigma) &= -\frac{1}{2}\sigma C^2\sigma^T+a_{21}\sigma_1\rho+a_{22}\sigma_2\rho,\\ \mathcal{Q}_3(\sigma) &= -\frac{1}{2}\sigma C^3\sigma^T. \qquad \boxed{\text{qQ3}}\end{aligned} \tag{109}$$

Let $B(\mathbf{x})$ be a ball centered at $\mathbf{x}$ and contained in a neighborhood of $\Sigma(t;\varepsilon)$ where the local coordinates are defined; namely, $B(\mathbf{x})$ is contained in the range of the diffeomorphic transformation M. We split the integral that defines I into two integrals which are over

$B(\mathbf{x})$ and $B^c(\mathbf{x}) = R^3 \backslash B(\mathbf{x})$. By $(81)_1$, it follows that the integral over $B^c(\mathbf{x})$ is $O(\varepsilon^2)$, for all $T \in C_b(R^3)$. Hence,

$$I(\mathbf{x};\varepsilon) = \int_{B(\mathbf{x})} J^\varepsilon(\mathbf{x}-\mathbf{y}, T(\mathbf{x}), T(\mathbf{y}))(\phi(\mathbf{y}) - \phi(\mathbf{x}))d\mathbf{y} + O(\varepsilon^2). \qquad \boxed{\text{ixe}} \tag{110}$$

In the near field of the phase interface surface, field functions can be expressed in terms of stretched local coordinates and expanded to the second power of ε (cf. (57)). We also write field functions in terms of the $(\sigma_1, \sigma_2, \rho)$ coordinates:

$$\tilde{\mathcal{U}}(\sigma_1, \sigma_2, \rho) = \tilde{u}(s_1, s_2, \rho) = \hat{u}(s_1, s_2, r) = u(\mathbf{x}). \qquad \boxed{\text{TU}} \tag{111}$$

By (108) and the definitions of J^ε, for $\mathbf{y} \in B(\mathbf{x})$, the function $J^\varepsilon(\mathbf{x}-\mathbf{y}, T(\mathbf{x}), T(\mathbf{y}))$ is expressed in terms of $\sigma = (\sigma_1, \sigma_2, \rho)$ as

$$\begin{aligned} &\frac{1}{\varepsilon^3}[k(\sigma - \sigma', \tilde{\mathcal{T}}(\sigma), \tilde{\mathcal{T}}(\sigma')) \\ &+\varepsilon \sum_{l=1}^{3} k_{\sigma_l}(\sigma-\sigma', \tilde{\mathcal{T}}(\sigma), \tilde{\mathcal{T}}(\sigma'))\mathcal{Q}_l(\sigma-\sigma') + O(\varepsilon^2)], \end{aligned} \qquad \boxed{\text{JseK}} \tag{112}$$

where k is defined by (82) and $k_{\sigma_l} = \frac{\partial}{\partial \sigma_l}k$, for $l = 1, 2, 3$.

The phase interface surface $\Sigma(t;\varepsilon)$ depends on ε. All geometric quantities relating to it depend on ϵ and in general their dependence on ϵ is regular. However, for simplicity we consider only the lowest order terms in all cases. Therefore by (104) we have

$$J_M = \delta + \varepsilon\delta\rho 2H + O(\varepsilon^2). \qquad \boxed{\text{jaco1}} \tag{113}$$

Knowing $B(\mathbf{x})$ is contained in the range of M, we let

$$\sigma = \frac{1}{\varepsilon}M^{-1}(\mathbf{x}), \quad \mathcal{V} = \frac{1}{\varepsilon}M^{-1}(B(\mathbf{x})) = \{\frac{1}{\varepsilon}M^{-1}(\mathbf{y}) |\ \mathbf{y} \in B(\mathbf{x})\},$$

where M^{-1} is the inverse map of M. By the change of coordinates given by (113) and (112), the integral in (110) can be expressed in terms of σ as follows:

$$\begin{aligned} &\delta \int_{\sigma-\mathcal{V}} k(\sigma', \tilde{\mathcal{T}}(\sigma), \tilde{\mathcal{T}}(\sigma-\sigma'))(\tilde{\Phi}(\sigma-\sigma') - \tilde{\Phi}(\sigma))d\sigma' \\ &+2\varepsilon H\delta \int_{\sigma-\mathcal{V}} k(\sigma', \tilde{\mathcal{T}}(\sigma), \tilde{\mathcal{T}}(\sigma-\sigma'))(\tilde{\Phi}(\sigma-\sigma') - \tilde{\Phi}(\sigma))(\rho-\rho')d\sigma' \\ &+\varepsilon\delta \int_{\sigma-\mathcal{V}} \sum_{l=1}^{3} k_{\sigma_l}(\sigma', \tilde{\mathcal{T}}(\sigma), \tilde{\mathcal{T}}(\sigma-\sigma'))(\tilde{\Phi}(\sigma-\sigma') - \tilde{\Phi}(\sigma))\mathcal{Q}_l(\sigma')d\sigma'. \end{aligned} \qquad \boxed{\text{inint}} \tag{114}$$

We claim an error of $O(\varepsilon^2)$ is incurred when the range of integration in the above expressions is extended to R^3.

Let $\mathcal{V}^c = R^3 \backslash \mathcal{V}$. Thus the compliment of $\sigma - \mathcal{V}$ is $\sigma - \mathcal{V}^c$. Assume that $B'(\sigma) \subset \mathcal{V}$ is a ball centered at σ. Thus $B'(0) = \sigma' - B'(\sigma)$ is the ball with the same radius but centered at 0. Define $U : R^3 \to R^3$ by $U : (\sigma_1, \sigma_2, \rho) \to \mathbf{p}_{s_1}\sigma_1 + \mathbf{p}_{s_2}\sigma_2 + \mathbf{n}\rho$. The mapping U is nonsingular, i.e., det $U = |U| \neq 0$ with inverse U^{-1}. By using (81), we have

$$\begin{aligned} &\delta \left| \int_{\sigma - V^c} k(\sigma', \tilde{\mathcal{T}}(\sigma), \tilde{\mathcal{T}}(\sigma - \sigma'))(\tilde{\Phi}(\sigma - \sigma') - \tilde{\Phi}(\sigma))d\sigma' \right| \\ &\leq \varepsilon^2 \delta 2C \int_{B'^c(0)} |\mathbf{p}_{s_1}\sigma_1' + \mathbf{p}_{s_2}\sigma_2' + \mathbf{n}\rho'|^{-5} d\sigma_1' d\sigma_2' d\rho', \qquad \boxed{\text{e2ci}} \end{aligned} \tag{115}$$

where the integral in (115) is equal to $\|U\|^{-1} \int_{U^{-1}(B'^c(0))} |\sigma'|^{-5} d\sigma' < \infty$. Therefore the error incurred when the domain of the integral is extended to R^3 is only $O(\varepsilon^2)$. By using (81), the same statement can be made of all integrals in (114).

By (57) and (111), we have $\tilde{\mathcal{U}}(\sigma) = \tilde{u}_0(\rho) + \varepsilon \tilde{u}_1(\rho) + O(\varepsilon^2)$ and

$$\begin{aligned} \tilde{\mathcal{U}}(\sigma - \sigma') &= \tilde{u}_0(\rho - \rho') \\ &+ \varepsilon[\tilde{u}_1(\rho - \rho') - \sigma_1' \tilde{u}_{0_{s_1}}(\rho - \rho') - \sigma_2' \tilde{u}_{0_{s_2}}(\rho - \rho')] + O(\varepsilon^2). \end{aligned}$$

By switching the σ coordinates in which the field functions are expressed back to the stretched local coordinates and using the above relations, we conclude that the inner expansion of $I(\mathbf{x}, \varepsilon)$ is given by

$$\begin{aligned} \tilde{I}(\rho) = \delta \int_{R^3} & k(\sigma', \tilde{T}_0(\rho), \tilde{T}_0(\rho - \rho'))(\tilde{\phi}_0(\rho - \rho') - \tilde{\phi}_0(\rho))d\sigma' \\ & + \varepsilon \delta W(\rho) + O(\varepsilon^2). \qquad \boxed{\text{ieis1}} \end{aligned} \tag{116}$$

Here (suppressing the dependence of k and its derivatives on $\tilde{T}_0(\rho)$ and $\tilde{T}_0(\rho - \rho')$)

$$\begin{aligned} W(\rho) &= \tilde{T}_1(\rho) \int_{R^3} k_{T_1}(\sigma')(\tilde{\phi}_0(\rho - \rho') - \tilde{\phi}_0(\rho))d\sigma' \\ &+ \int_{R^3} k_{T_2}(\sigma')(\tilde{\phi}_0(\rho - \rho') - \tilde{\phi}_0(\rho))[\tilde{T}_1(\rho - \rho') - \sigma_1' \tilde{T}_{0_{s_1}}(\rho - \rho') - \sigma_2' \tilde{T}_{0_{s_2}}(\rho - \rho')]d\sigma' \\ &+ \int_{R^3} k(\sigma')[(\tilde{\phi}_1(\rho - \rho') - \tilde{\phi}_1(\rho)) - \sigma_1' \tilde{\phi}_{0_{s_1}}(\rho - \rho') - \sigma_2' \tilde{\phi}_{0_{s_2}}(\rho - \rho')]d\sigma' \\ &+ \sum_{l=1}^{3} \int_{R^3} k_{\sigma_l}(\sigma')(\tilde{\phi}_0(\rho - \rho') - \tilde{\phi}_0(\rho))(\rho - \rho')\mathcal{Q}_l(\sigma')d\sigma' \\ &+ 2H \int_{R^3} k(\sigma')(\tilde{\phi}_0(\rho - \rho') - \tilde{\phi}_0(\rho))(\rho - \rho')d\sigma' \qquad \boxed{\text{W1}} \end{aligned} \tag{117}$$

The inner expansions of all the other terms defined by integrals in the basic equations can be obtained the same way as shown here. After the expansions are made, of course, the inner basic equations of the various orders are obtained by equating terms involving the same order of ε.

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