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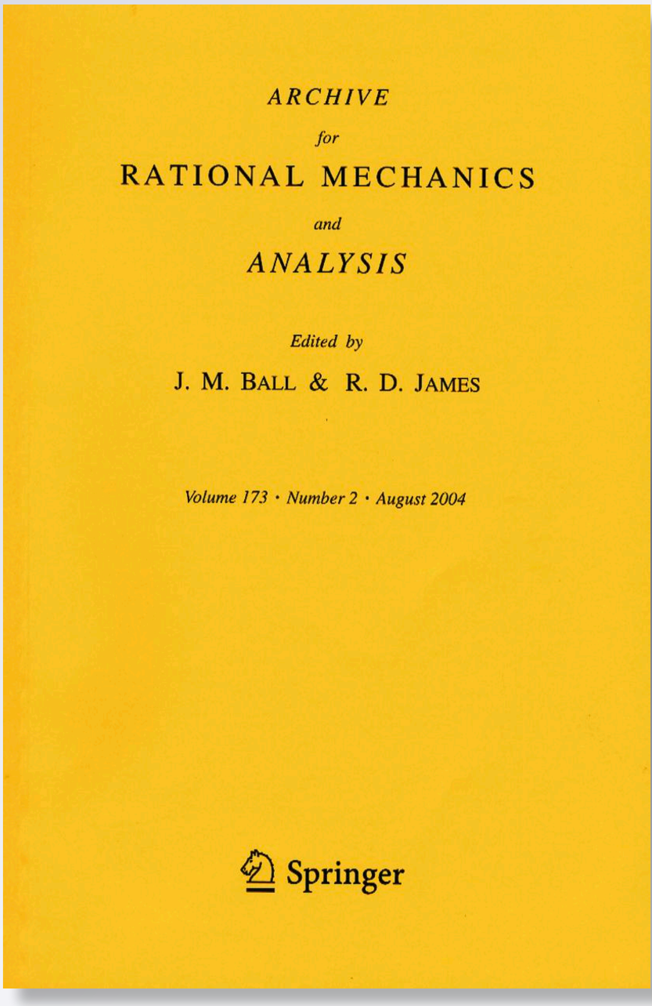

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Interface Conditions for a Phase Field Model with Anisotropic and Non-Local Interactions

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Abstract

An alternative formulation of the phase field method is utilized from an integral equation perspective. The technique allows one to derive macroscopic conditions at the interface from the microscopic potentials. Differential geometry and asymptotic analysis yield interface conditions, in arbitrary spatial dimension, for interactions that may include anisotropy as well as non-local potentials. The interface conditions can be expressed in various formulations, for example, in terms of the principal curvature directions of the interface, or the second order directional derivatives of the (signed) distance function and the Hessian of the surface tension.

1. Introduction

Phase boundaries have been studied in a mathematical context since 1831 when Lamé and Clapeyron [20] introduced a one-phase model for the freezing of the ground. A half-century later, Stefan [23] modified this to a two-phase problem. These original one-dimensional models were generalized to higher spatial dimensions, posing the mathematical problem of determining both the temperature, $T = T(x, t)$, and interface, Γ_t, for $x \in \Omega \subset \mathbb{R}^N$ and $t \in \mathbb{R}^+$, satisfying the system of equations

$$\rho\, c\, T_t = \operatorname{div}(K\nabla T) \quad \text{in} \quad \Omega\backslash\Gamma_t, \tag{1.1}$$

$$\rho\, l\, v = \mathbf{n}\cdot[K\nabla T]_+^- \quad \text{on} \quad \Gamma_t, \tag{1.2}$$

$$T = T_{\mathrm{E}} \quad \text{on} \quad \Gamma_t,$$

where v is the (normal) velocity of the interface, $\mathbf{n}$ the unit normal to the interface, $\mathbf{n}\cdot[K\nabla T]_+^-$ the sum of the exterior normal components of the energy flux of the two phases, K the thermal conductivity, ρ the density, c the specific heat per unit mass, T_{E} the equilibrium melting temperature, and l the latent heat. The Stefan model designates a dual role for the temperature since the phase is determined by the sign of $T - T_{\mathrm{E}}$.

The condition of melting temperature at the one-dimensional interface, that is $T = T_{\mathrm{E}}$, appeared to generalize trivially to higher dimensions. However, GIBBS' work [15] on fluid pressures suggested that the temperature at a curved interface in equilibrium should differ from T_{E} by a term proportional to the sum of principal curvatures, κ, and the surface tension, σ. Furthermore, heuristic materials science arguments suggested that an additional term proportional to the velocity of the interface should be present, leading to an interface condition

$$T - T_{\mathrm{E}} = -\frac{\sigma}{[s]_{\mathrm{E}}}\kappa - \beta v \quad \text{on} \quad \Gamma_t, \tag{1.3}$$

where $[s]_{\mathrm{E}}$ is the entropy difference between phases in equilibrium and β is a constant depending on the material. Following the works of GIBBS, WULFF [24] published a key result in 1901. This is essentially a prescription to draw equilibrium surfaces (with or without anisotropy). A half-century later Herring presented a derivation of an interface equilibrium relation [17] which relates the anisotropic surface tension and its derivatives to the temperature of the interface by

$$[s]_{\mathrm{E}}(T - T_{\mathrm{E}}) = -\kappa\{\bar{\sigma}(\theta) + \bar{\sigma}''(\theta)\}, \tag{1.4}$$

where $\bar{\sigma}(\theta)$ is the anisotropic surface tension with θ being the angle between a fixed axis and the normal to the interface (see also [18] for a modern derivation).

As a result of these discoveries, the sign of the temperature could no longer determine the phase, necessitating a key departure from the classical Stefan model. This led to the implementation of basic "order parameter" ideas, originally developed for critical phenomena (for example, in the region of the phase diagram where liquid and solid merge into a single phase). By coupling the temperature with the order parameter, φ, one can study a (microscopic) system of (phase field) equations such that the interface is given by the zero-level set of φ [4] (see also [7] for more discussion and references). One of the modern challenges has been to establish a connection between these macroscopic ideas and those of microscopic physics. Another has been to develop a set of computational methods that lead to efficient computation of the interface. Phase field models, based upon the idea of averaging local interactions, have provided a methodology whereby interface relations such as (1.3) can be derived, and solutions to systems such as (1.1)–(1.3) can be solved without tracking the interface. A formal derivation was first presented in [4]. A series of rigorous results followed (see [6] and references therein). These works rekindled a mathematical interest in motion by mean curvature in which the role of temperature is eliminated [9,13,14]. More recently, using a variation of the phase field model, CHEN ET AL. [10] proved that one can obtain convergence that is second order in interface thickness.

In the first work to study anisotropy from the phase field perspective, CAGINALP [5] started from a lattice Hamiltonian that led to an anisotropic phase field model whose interface satisfied

$$-u + \alpha(\theta)v + \kappa\{\bar{\sigma}(\theta) + \bar{\sigma}''(\theta)\} = 0, \tag{1.5}$$

where u is the scaled temperature, $\alpha(\theta)$ is a positive function, $\mathbf{n} = \langle \cos\theta, \sin\theta \rangle$ is the unit normal and $\bar{\sigma}(\theta)$ is the interfacial energy density for interfaces with normal $\langle \cos\theta, \sin\theta \rangle$. Following this idea we consider a microscopic lattice system involving a set of "spins", denoted by a real value ϕ_k for each lattice point k, and interactions of strength J_{kl} between these spins. In statistical mechanics, the Hamiltonian (essentially the internal energy) of this physical system is described by

$$H_{\text{interaction}}[\phi] = \sum_{k,l} \tfrac{1}{4}(\phi_k - \phi_l)^2 J_{kl}.$$

The free energy, which is the internal energy minus entropy multiplied by temperature, is often approximated in statistical mechanics using a double well potential, denoted $W(\phi_k)$, which takes its minimum values on the bulk (that is, single phase) material. In particular, $\phi_k \simeq 1$ denotes the higher energy phase (liquid), while $\phi_k \simeq -1$ denotes the lower energy (solid). Using this concept, the free energy can be written as

$$F[\phi] = \sum_{k,l} \frac{1}{4} J_{kl}(\phi_k - \phi_l)^2 + \sum_k W(\phi_k) - \sum_k (T - T_{\mathrm{E}})S(\phi_k). \tag{1.6}$$

When passing to the continuum limit, the interaction strength must be scaled appropriately [5]. In the continuum limit if we replace the summation by integrals (and the physical quantities by their calligraphic letters) the interfacial excess free energy becomes

$$\mathcal{F}[\phi] = \int \frac{1}{4} J_\varepsilon(x-y)(\phi(x)-\phi(y))^2 \mathrm{d}x\,\mathrm{d}y + \int W(\phi(x))\mathrm{d}x - \int (T - T_{\mathrm{E}})S(\phi(x))\mathrm{d}x,$$

where $J_\varepsilon(z) = \varepsilon^{-N} J(\varepsilon^{-1} z)$ and ε is an atomic length scale.

The phase field equation is coupled with the temperature with a basic conservation law, for example,

$$\frac{\partial}{\partial t}\left(u + \frac{\ell}{2}\phi\right) = \operatorname{div}(D(\phi)\nabla u), \tag{1.7}$$

where ℓ and D are related to the latent heat and the heat diffusion, respectively. Other heat transport mechanisms are also possible [21].

The free energy (1.6) has been the starting point for a number of investigations of interface relations and anisotropy. In most cases the sum has been converted to Fourier space (denoted by q). In the earliest work, it was truncated after the q^2 term leading to a free energy of the form

$$\mathcal{F}[\phi] = \int \frac{1}{2} a(\nabla\phi(x))\mathrm{d}x + \int W(\phi(x))\mathrm{d}x - \int uS(\phi(x))\mathrm{d}x,$$

where a is a positive definite bilinear form. The truncation averages the detailed anisotropy, thereby necessitating higher order differential equations in order to address more detailed anisotropy (for example $\cos(n\theta)$ with n as a large positive integer). In [7] the truncation was carried out in two-dimensional space at arbitrarily large order, leading to a $2n$th order differential equation that was analyzed asymptotically to obtain the Gibbs–Thomson–Herring result (1.4) and its dynamic generalization (1.5).

In the current paper we develop a new approach to anisotropy by working directly on the convolution for non-local interactions without using the conversion into Fourier space and truncation which uses higher order differential operators to approximate non-local operators. This has a number of advantages, one of which is that one does not need to consider arbitrarily large order differential equations. Another issue that is avoided is the convergence of the Fourier series. Non-local phase-field systems in various isotropic settings have been studied in [2,3,12,16,19,22] (and references therein) in terms of existence, traveling waves, asymptotic limits and other features.

In terms of anisotropy, the different approaches have the same goal. Given a set of microscopic interactions, namely the J_{kl}, what is the resulting interface condition (for example, analogous to the Gibbs–Thomson–Herring condition)? Moreover, what is the resulting shape (for example, the Wulff shape)? The physically interesting question involves the understanding of how the microscopic interactions are communicated to the macroscopic shape. Anisotropy has been a focal point of interface phenomena for several reasons. A basic issue is that it provides an understanding for the mechanism whereby microscopic interactions lead to a macroscopic interface. Another is that surface tension is a stabilizing factor, while undercooling is destabilizing. Hence, anisotropy in microscopic interactions results in anisotropic surface tension that influences the direction of the growth of instabilities, as well as the growth rate (see discussion and references in [7]).

In this paper, we derive a phase field model from a free energy function comprising a linear combination of a local interaction term ($\int a(\nabla\phi(x))\mathrm{d}x$) and a non-local interaction term ($\int\int J_\varepsilon(x-y)[\phi(x)-\phi(y)]^2\mathrm{d}x\mathrm{d}y$). We demonstrate that the phase field model provides the following condition on the liquid–solid interface:

$$u+\alpha(\mathbf{n})v+\mathrm{Trace}(\nabla\mathbf{n}\ D^2\sigma(\mathbf{n}))=0, \tag{1.8}$$

where $\mathbf{n}$ is the unit normal of the interface, pointing from solid to liquid, and is extended by a constant along the normal lines, $D^2\sigma(\zeta)$ is the Hessian of $\sigma(\zeta)=|\zeta|\sigma\left(\frac{\zeta}{|\zeta|}\right)$ at $\zeta\in\mathbb{R}^N\setminus\{0\}$, and $\sigma(\mathbf{n})$, for $\mathbf{n}\in\mathbb{S}^{N-1}$, is the interfacial energy density of interfaces with unit normal $\mathbf{n}$. In particular, if we denote by $\kappa^1,\dots,\kappa^{N-1}$ the principal curvatures and $\tau_1,\dots,\tau_{N-1}$ the the principal curvature directions of the interface, then (1.8) can be written as

$$u+\alpha(\mathbf{n})v+\sum_{i=1}^{N-1}\kappa^i\sigma_{\tau_i\tau_i}(\mathbf{n})=0, \tag{1.9}$$

where $\sigma_{\tau_i\tau_i}(\zeta)$ is the second order directional derivative in the direction τ_i. If we represent the interface by the zero level set of a function Ψ with $\Psi>0$ in liquid and $\Psi<0$ in solid, then the interfacial condition (1.8) can be written as

$$\alpha\left(\frac{\nabla\Psi}{|\nabla\Psi|}\right)\frac{\Psi_t}{|\nabla\Psi|} = u + \operatorname{div}\left(\sigma_\zeta\left(\frac{\nabla\Psi}{|\nabla\Psi|}\right)\right) \quad \text{on} \quad \Gamma_t := \{x \mid \Psi(x,t) = 0\}. \tag{1.10}$$

In the two-dimensional case, (1.5) is equivalent to (1.8) with $\sigma(\rho\cos\theta, \rho\sin\theta) := \rho\bar{\sigma}(\theta)$.

2. The Phase Field Model

A phase field model describes the phase (liquid or solid) of an underlying material by a phase order parameter φ with $\varphi \sim 1$ for liquid and $\varphi \sim -1$ for solid. The temperature u is governed by the law of conservation of energy, which we shall not discuss in this paper. The dynamics of the phase order parameter are typically modeled by a gradient flow of a free energy functional.

In this paper, we consider the following free energy functional, for a given temperature field u,

$$\begin{aligned}\mathcal{F}[\phi] = &\int_\Omega \left\{\frac{\varepsilon\lambda}{2}a(\nabla\phi) + \frac{W(\phi)}{\varepsilon} - uG(\phi)\right\}\mathrm{d}x \\ &+ \frac{1-\lambda}{4\varepsilon}\iint_{\Omega^2} J_\varepsilon(x-y)|\phi(x)-\phi(y)|^2 \mathrm{d}x\,\mathrm{d}y.\end{aligned}$$

Here ε is a small positive parameter. Since the energy does not change when $J_\varepsilon(x)$ is replaced by $\frac{1}{2}[J_\varepsilon(x) + J_\varepsilon(-x)]$, J_ε can be assumed to be even. Also, for simplicity, we take $\Omega = \mathbb{R}^N$ $(N \geqq 2)$. We make the following assumptions:

1. $\lambda \in [0, 1]$ is a constant and $a(\zeta) = \zeta A \zeta^T$ where A is a semi-positive definite constant matrix;
2. $J_\varepsilon(x) = \varepsilon^{-N} J(\varepsilon^{-1}x)$ where $J \in C^1(\mathbb{R}^N)$ satisfies
$$J(x) = J(-x) \geqq 0\;\forall x \in \mathbb{R}^N, \quad \int_{\mathbb{R}^N} J(x)\mathrm{d}x = 1, \quad \int_{\mathbb{R}^N} |x|^3 J(x)\mathrm{d}x < \infty;$$
3. $W \in C^\infty([-1, 1])$, $0 = W(\pm1) < W(\phi)\;\forall\phi \neq \pm1$, $W''(\pm1) > 0$;
4. Either λA is positive definite or $W''(\phi) > \lambda - 1\;\forall\phi \in [-1, 1]$;
5. $G \in C^2([-1, 1])$, $G(1) - G(-1) = 1$, $G'(\pm1) = 0$.

The phase field equation for the phase order parameter is a gradient flow for the free energy. For a smooth ψ with compact support we can calculate the first variation of $\mathcal{F}$ in the direction ψ by

$$\begin{aligned}\left\langle\frac{\delta\mathcal{F}[\phi]}{\delta\phi}, \psi\right\rangle &:= \lim_{\delta\to0}\frac{\mathcal{F}[\phi+\delta\psi] - \mathcal{F}[\phi]}{\delta} \\ &= \int_{\mathbb{R}^N}\psi\left\{-\varepsilon\lambda A : D^2\phi + \frac{W'(\phi)}{\varepsilon} - uG'(\phi) - \frac{1-\lambda}{\varepsilon}[J_\varepsilon * \phi - \phi]\right\}\mathrm{d}x,\end{aligned}$$

where

$$J_\varepsilon * \phi(x) := \int_{\mathbb{R}^N} J_\varepsilon(x-y)\phi(y)\mathrm{d}y = \int_{\mathbb{R}^N} J(y)\phi(x-\varepsilon y)\mathrm{d}y.$$

Here $D^2\phi = (\phi_{x^i x^j})_{N\times N}$ and for $N \times N$ matrices $C = (c^{ij})_{N\times N}$ and $D = (d_{ij})_{N\times N}$,

$$C : D = \sum_{i,j=1}^{N} c^{ij} d_{ij} = \mathrm{Trace}(C^T D), \quad \text{so} \quad A : D^2\phi = \sum_{i,j=1}^{N} a^{ij}\phi_{x^i x^j}.$$

The phase field equation is taken as φ_t being proportional to $-\delta\mathcal{F}/\delta\phi$, that is,

$$\varepsilon^2\tau\varphi_t = \varepsilon^2\lambda A : D^2\varphi + (1-\lambda)(J_\varepsilon * \varphi - \varphi) - W'(\varphi) + \varepsilon u G'(\varphi), \tag{2.1}$$

where $\tau > 0$ is a scaled relaxation time. We are interested in the asymptotic behavior of the solution as $\varepsilon \searrow 0$, with fixed λ, τ and A. When necessary, we shall write the solution of (2.1) as $\varphi = \varphi_\varepsilon(x, t)$.

Remark 2.1. Traditionally [4], G is taken as $G(\varphi) = \varphi/2$. Here the assumption $G'(\pm 1) = 0$ provides a number of advantages over the traditional one. The condition $G'(\pm 1) = 0$ implies that both $\varphi \equiv 1$ and $\varphi \equiv -1$ are solutions of (2.1), so it ensures that any physically relevant solution of (2.1) satisfies $|\varphi| \leqq 1$. In addition, in a matched asymptotic expansion, the outer expansion is trivial: $\varphi^{\text{outer}} \equiv 1$ in the liquid region and $\varphi^{\text{ outer}} \equiv -1$ in the solid region.

In the sequel, we regard $x = (x^1, \ldots, x^N)^T$ as a column vector and $\nabla\phi = (\phi_{x_1}, \ldots, \phi_{x_N})$ as a row operator. Also, for vectors $c = (c_i)_{N\times 1}$ (or $(c_i)_{1\times N}$) and $d = (d_i)_{N\times 1}$ (or $(d_j)_{1\times N}$), we denote

$$c \otimes d = (c_i d_j)_{N\times N}, \quad \text{so} \quad A : \nabla\phi \otimes \nabla\phi = \nabla\phi A \nabla^T\phi = \sum_{i,j=1}^{N} \phi_{x_i} a^{ij} \phi_{x^j} = a(\nabla\phi).$$

Using convolution, we can write the free energy as

$$\mathcal{F}[\phi] = \int_{\mathbb{R}^N} \left\{ \frac{\lambda\varepsilon}{2} A : \nabla\phi \otimes \nabla\phi + \frac{1-\lambda}{2\varepsilon}\phi[\phi - J_\varepsilon * \phi] + \frac{W(\phi)}{\varepsilon} - uG(\phi) \right\} \mathrm{d}x. \tag{2.2}$$

3. Planar Interfaces and Interfacial Energy Density

In this section, we seek solutions of (2.1) that represent stationary planar interfaces at the melting temperature. For this purpose, we assume that $u \equiv 0$.

3.1. Stationary Solution with Planar Interfaces

Given a point $x_0 \in \mathbb{R}^N$ and a direction $\zeta \in \mathbb{R}^N \setminus \{0\}$, we seek a stationary solution of (2.1) such that $\varphi(x_0, t) = 0$ and all level sets of φ are hyperplanes perpendicular to ζ. This is equivalent to seeking a solution of the form

$$\varphi(x, t) = Q(\zeta, z), \quad z := \frac{(x - x_0)\cdot\zeta}{\varepsilon} \in \mathbb{R}.$$

Under this special form, we can calculate

$$\varepsilon^2 A : D^2\varphi(x,t) = a(\zeta)Q_{zz}(\zeta,z), \quad a(\zeta) := A : \zeta \otimes \zeta = \zeta^T A\zeta = |\sqrt{A}\,\zeta|^2.$$

Making the change of variables $y = \hat{z}\zeta + y'$ with $\hat{z} \in \mathbb{R}$ and $y' \perp \zeta$, we obtain $\mathrm{d}y = |\zeta|\mathrm{d}\hat{z}\mathrm{d}y'$, so that

$$\begin{aligned} J_\varepsilon * \varphi(x,t) &= \int_{\mathbb{R}^N} J(y)\varphi(x-\varepsilon y,t)\mathrm{d}y = \int_{\mathbb{R}^N} J(y)Q(\zeta, z - y\cdot\zeta)\mathrm{d}y \\ &= \int_{\mathbb{R}} Q(\zeta, z-\hat{z})\left(|\zeta|\int_{y'\perp\zeta} J(\hat{z}\zeta + y')\mathrm{d}y'\right)\mathrm{d}\hat{z} = j(\zeta) * Q(\zeta), \end{aligned}$$

where $j(\zeta) = j(\zeta,\cdot)$ is defined by

$$j(\zeta,z) := |\zeta|\int_{y'\perp\zeta} J(z\zeta + y')\mathrm{d}y' \quad \forall\, z \in \mathbb{R}.$$

Thus, for certain boundary conditions of interest, $u \equiv 0$, $\varphi(x,t) = Q(\zeta, (x-x_0)\cdot\zeta/\varepsilon)$ is a stationary solution of (2.1) if $Q(\zeta)$ solves the following boundary value problem of an autonomous integral–differential equation:

$$\begin{cases} \lambda\, a(\zeta)\, Q_{zz} + (1-\lambda)[j(\zeta) * Q - Q] - W'(Q) = 0 \quad \text{on} \quad \mathbb{R}, \\ \lim_{z\to\pm\infty} Q(\zeta,z) = \pm 1, \quad Q(\zeta,0) = 0. \end{cases} \tag{3.1}$$

For fixed $\zeta \in \mathbb{R}^N \setminus \{0\}$, it is easy to verify that

$$j(\zeta,z) = j(\zeta,-z) = j(-\zeta,z) \geqq 0\, \forall\, z \in \mathbb{R}, \quad \int_{\mathbb{R}} j(\zeta,z)\mathrm{d}z = 1,$$
$$\int_{\mathbb{R}} |z|^3 j(\zeta,z)\mathrm{d}z < \infty.$$

Also, when λA is positive definite, $\lambda a(\zeta) > 0$; when λA is not positive definite, $\lambda a(\zeta) \geqq 0$, but in this case we have assumed that the function $\phi \in [-1,1] \to (1-\lambda)\phi + W'(\phi)$ is increasing. Hence, from a general theory of Chen [8], we have the following:

Lemma 3.1. *For each* $\zeta \in \mathbb{R}^{N-1} \setminus \{0\}$, *problem* (3.1) *admits a unique solution. In addition, the solution is smooth, strictly monotonic, and globally asymptotically stable for the one-dimensional dynamics*

$$\begin{cases} \varphi_t = \lambda a(\zeta)\varphi_{zz} + (1-\lambda)[j(\zeta) * \varphi - \varphi] - W'(\varphi) \quad \text{on} \quad \mathbb{R}\times(0,\infty), \\ \varphi(\cdot,0) = \varphi_0(\cdot) \quad \text{on}\ \mathbb{R}\times\{0\}. \end{cases} \tag{3.2}$$

Here "globally asymptotically stable" means that there exist constants $c \in (0,1)$ and $\nu > 0$ such that if $\|\varphi_0\|_{L^\infty(\mathbb{R})} \leqq 1$, $\underline{\lim}_{z\to\infty}\varphi_0(z) \geqq c$, and $\overline{\lim}_{z\to-\infty}\varphi_0(z) \leqq -c$, then for some $z_0 \in \mathbb{R}$ and $K > 0$,

$$\|\varphi(\cdot,t) - Q(\zeta,\cdot - z_0)\|_{L^\infty(\mathbb{R})} \leqq K e^{-\nu t} \quad \forall\, t > 0.$$

3.2. Interfacial Energy Density

Notice that when $u \equiv 0$ and $\phi(x) = Q(\zeta, (x - x_0) \cdot \zeta/\varepsilon)$, the integrand in (2.2) is a positive constant on each hyperplane that is perpendicular to ζ, so the integral is unbounded. A relevant quantity is the integral along any line in the direction ζ, say, $\zeta\mathbb{R} := \{z\zeta \mid z \in \mathbb{R}\}$. Hence, we define

$$\sigma(\zeta) := \int_{\mathbb{R}} \left\{ \frac{\lambda a(\zeta)}{2} Q_z^2 + W(Q) + \frac{1-\lambda}{2} Q\,(Q - j(\zeta) * Q) \right\} \mathrm{d}z \Big|_{Q=Q(\zeta,\cdot)} \tag{3.3}$$

Clearly, $\sigma(\zeta)$ does not depend on ε and x_0. When $\zeta = \mathbf{n}$ is a unit vector, we call $\sigma(\mathbf{n})$ the *interfacial energy density* for interfaces with unit normal $\mathbf{n}$. If γ is a macroscopically observed solid–liquid interface, its total interfacial energy is defined as

$$\int_\gamma \sigma(\mathbf{n}(x)) H^{N-1}(\mathrm{d}x),$$

where $\mathbf{n}(x)$ is the unit normal of γ at $x \in \gamma$ (pointing from solid to liquid), and $H^{N-1}(\mathrm{d}x)$ is the surface element of γ. We call $\sigma : \mathbb{R}^{N-1} \setminus \{0\} \to (0, \infty)$ the naturally extended interfacial energy density, or simply the interfacial energy density function.

Remark 3.1. Since $j(\zeta, \cdot)$ is an even function, $Q(\zeta, \cdot)$ is an odd function; numerically it can be obtained by taking the limit, as $t \to \infty$, of a solution of (3.2) with odd initial data that approaches 1 as $z \to \infty$. For example, one can choose a small positive Δt and perform the following:

$$\begin{aligned} \phi_0(z) &= \tanh z \quad \forall\, z \in \mathbb{R}^n, \\ \phi_{k+1} &= \phi_k + \Delta t \{\lambda a(\zeta)\phi_k'' + (1-\lambda)[j(\zeta) * \phi_k - \phi_k] - W'(\phi_k)\}, \\ Q(\zeta) &= \lim_{k\to\infty} \phi_k, \\ \sigma(\zeta) &= \int_{\mathbb{R}} \left(W(Q) - \frac{1}{2}\, Q\, W'(Q) \right) \mathrm{d}z \Big|_{Q=Q(\zeta)}. \end{aligned} \tag{3.4}$$

Here the formula (3.4) is obtained from (3.3) by an integration by parts and a substitution of the integro-differential equation for $Q(\zeta)$.

In the sequel, $Q_\zeta = (Q_{\zeta^1}, \ldots, Q_{\zeta^N})$ is the gradient of $Q(\zeta, z)$ with respect to ζ. Also $D^2\sigma = (\sigma_{\zeta^k\zeta^l})_{N\times N}$ is the Hessian of $\sigma(\zeta)$. The following will be used later in deriving interfacial conditions for solutions of the phase field equation (2.1).

Lemma 3.2. *The interfacial energy density function σ has the following properties:*

1. *σ is even and homogeneous of degree one, that is*

$$\sigma(L\mathbf{n}) = |L|\sigma(\mathbf{n}) \quad \forall\, L \neq 0,\ \mathbf{n} \in \mathbb{S}^{N-1};$$

Consequently,

$$\zeta \cdot \nabla\sigma(\zeta) = \sigma(\zeta), \quad D^2\sigma(\zeta)\,\zeta = (0)_{N\times 1}, \quad \zeta^T D^2\sigma(\zeta) = (0)_{1\times N}. \tag{3.5}$$

2. *Using the abbreviation Q for $Q(\zeta, z)$ and $\hat{Q}$ for $Q(\zeta, z - y\cdot\zeta)$, we have*

$$D^2\sigma(\zeta) = \int_{\mathbb{R}} Q_z \Big(\lambda[AQ_z + 2A\zeta \otimes Q_\zeta] + (1-\lambda)\int_{\mathbb{R}^N} J(y)\Big(\frac{y\otimes y}{2}\hat{Q}_z - y\otimes \hat{Q}_\zeta\Big)\mathrm{d}y\Big)\,\mathrm{d}z.$$

Proof. (1) Since $j(\zeta, z)$ is even in z and in ζ and the solution of (3.1) is unique, it is easy to verify that $Q(-\zeta, z) = Q(\zeta, -z)$, so by (3.4), $\sigma(\zeta) = \sigma(-\zeta)$. Similarly, for $\mathbf{n} \in \mathbb{S}^{N-1}$ and $\zeta = L\,\mathbf{n}$ with $L > 0$, both $Q(\mathbf{n}, x\cdot\mathbf{n}/\varepsilon)$ and $Q(\zeta, x\cdot\zeta/\varepsilon)$ represent the same stationary solution of (2.1) with planar interfaces perpendicular to $\mathbf{n}$, so one can verify that $Q(\zeta, z) = Q(\mathbf{n}, z/L)$. It then follows from (3.4) that $\sigma(\zeta) = L\sigma(\mathbf{n})$. Thus, $\sigma(\cdot)$ is even and homogeneous of degree one.

Now differentiating $t\sigma(\zeta) = \sigma(t\zeta)$ with respect to t and setting $t = 1$, we have $\sigma(\zeta) = \zeta\cdot\nabla\sigma(\zeta)$. Differentiating this relation with respect to ζ^k we obtain $\sigma_{\zeta^k} = \sigma_{\zeta^k} + \zeta\cdot\nabla\sigma_{\zeta^k}$ so $\zeta\cdot\nabla\sigma_{\zeta^k} = 0$. This implies that $\zeta^T D^2\sigma(\zeta) = \mathbf{0}$, $D^2\sigma(\zeta)\,\zeta = \mathbf{0}$.

(2) Using the abbreviation Q for $Q(\zeta, z)$ and $\hat{Q}$ for $Q(\zeta, z - y\cdot\zeta)$ we can write (3.3) as

$$\sigma(\zeta) = \int_{\mathbb{R}} \left\{ \frac{\lambda a(\zeta)}{2} Q_z^2 + W(Q) + \frac{1-\lambda}{2} Q \int_{\mathbb{R}^N} J(y)[Q - \hat{Q}]\mathrm{d}y \right\} \mathrm{d}z. \quad (3.6)$$

Since $j(\zeta, \cdot)$ is an even function, denoting by $\langle\cdot,\cdot\rangle$ the $L^2(\mathbb{R})$ inner product, we have

$$\langle f,\ j(\zeta) * g\rangle = \int_{\mathbb{R}}\int_{\mathbb{R}} f(z) j(\zeta, z - \hat{z}) g(\hat{z}) \mathrm{d}z\,\mathrm{d}\hat{z} = \langle j(\zeta) * f,\ g\rangle.$$

Differentiating (3.6) with respect to ζ^k and using the above identity with $f = Q$ and $g = Q_{\zeta^k}$ we then obtain,

$$\frac{\partial\sigma(\zeta)}{\partial\zeta^k} = \int_{\mathbb{R}} \left\{\lambda a(\zeta) Q_z Q_{z\zeta^k} + W'(Q) Q_{\zeta^k} + (1-\lambda) Q_{\zeta^k}[Q - j(\zeta) * Q]\right\} \mathrm{d}z + \int_{\mathbb{R}} \left\{ \frac{\lambda a_{\zeta^k}(\zeta)}{2} Q_z^2 + \frac{1-\lambda}{2} Q \int_{\mathbb{R}^N} J(y) y^k Q_z(\zeta, z - y\cdot\zeta)\mathrm{d}y \right\} \mathrm{d}z.$$

Note that $a_{\zeta^k}(\zeta) = 2\sum_{i=1}^N a^{ki}\zeta_i =: 2(A\zeta)^k$. Also, the first integral equals, by integration by parts,

$$\int_{\mathbb{R}} Q_{\zeta^k} \left\{-\lambda a(\zeta) Q_{zz} + W'(Q) - (1-\lambda)[j(\zeta) * Q - Q]\right\} \mathrm{d}z = 0$$

by the integral–differential equation for $Q = Q(\zeta, z)$. Thus,

$$\frac{\partial\sigma(\zeta)}{\partial\zeta^k} = \int_{\mathbb{R}} \left\{ \lambda(A\zeta)^k Q_z^2 + \frac{1-\lambda}{2} Q \int_{\mathbb{R}^N} J(y) y^k Q_z(\zeta, z - y\cdot\zeta)\mathrm{d}y \right\} \mathrm{d}z.$$

Consequently, one more differentiation gives

$$\frac{\partial^2\sigma(\zeta)}{\partial\zeta^k\partial\zeta^l} = \int_{\mathbb{R}}\Big\{\lambda a^{kl} Q_z^2 + 2\lambda(A\zeta)^k Q_z Q_{\zeta^l}\Big\}\,\mathrm{d}z + \frac{1-\lambda}{2}\int_{\mathbb{R}} Q_{\zeta^l}\int_{\mathbb{R}^N} J(y)y^k \hat{Q}_z\,\mathrm{d}y\,\mathrm{d}z + \frac{1-\lambda}{2}\int_{\mathbb{R}} Q\int_{\mathbb{R}^N} J(y)y^k[\hat{Q}_{z\zeta^l} - y^l\hat{Q}_{zz}]\mathrm{d}y\,\mathrm{d}z.$$

Since $y^k J(y)$ is an odd function, we have

$$\int_{\mathbb{R}} Q_{\zeta^l}\int_{\mathbb{R}^N} J(y)y^k\hat{Q}_z\,\mathrm{d}y\mathrm{d}z = -\int_{\mathbb{R}} Q_z\int_{\mathbb{R}^N} J(y)y^k\hat{Q}_{\zeta^l}\,\mathrm{d}y\mathrm{d}z.$$

Also, integrating by parts in z we have

$$\int_{\mathbb{R}} Q\int_{\mathbb{R}^N} J(y)y^k[\hat{Q}_{z\zeta^l} - y^l\hat{Q}_{zz}]\mathrm{d}y\mathrm{d}z = -\int_{\mathbb{R}} Q_z\int_{\mathbb{R}^N} J(y)y^k[\hat{Q}_{\zeta^l} - y^l\hat{Q}_z]\mathrm{d}y\mathrm{d}z.$$

Substituting the last two identities into the expression of $\sigma_{\zeta^k\zeta^l}$ we then obtain the second assertion of the lemma. This completes the proof. □

3.3. A Solvability Condition

For $\zeta\in\mathbb{R}^N\setminus\{0\}$, consider the linear operator $\mathcal{L}^\zeta$ defined by

$$\mathcal{L}^\zeta\phi = \lambda a(\zeta)\phi_{zz} + (1-\lambda)[j(\zeta)*\phi - \phi] - W''(Q(\zeta))\phi.$$

Lemma 3.3. *Let $\zeta\in\mathbb{R}^N\setminus\{0\}$ and $Q = Q(\zeta,\cdot)$. Then*

$$\mathcal{L}^\zeta Q_z \equiv 0,\quad \mathcal{L}^\zeta Q_\zeta = -2\lambda(A\zeta)Q_{zz} + (1-\lambda)\int_{\mathbb{R}^N} J(y)yQ_z(\zeta, z-y\cdot\zeta)\mathrm{d}y. \tag{3.7}$$

In addition, for every $m\in\mathbb{R}$ and bounded f satisfying $f(\pm\infty) = 0$, the equation

$$\mathcal{L}^\zeta\phi = f \quad on \quad \mathbb{R},\quad \phi(\pm\infty) = 0,\quad \phi(0) = m \tag{3.8}$$

has a unique solution if and only if

$$\int_{\mathbb{R}} Q_z(\zeta,\, z)f(z)dz = 0. \tag{3.9}$$

Proof. (1) The first assertion (3.7) follows by differentiating (3.1) with respect to z and ζ and using $a(\zeta)_\zeta = 2A\zeta$ and

$$\frac{\partial}{\partial\zeta}j(\zeta)*Q = \frac{\partial}{\partial\zeta}\int_{\mathbb{R}^N} J(y)Q(\zeta, z-y\cdot\zeta)\mathrm{d}y = j*Q_\zeta - \int_{\mathbb{R}^N} J(y)yQ_z(\zeta, z-y\cdot\zeta)\mathrm{d}y.$$

(2) Since $j(\zeta, \cdot)$ is even, one can check that $\mathcal{L}^\zeta$ is self-adjoint in the sense that

$$\langle \mathcal{L}^\zeta \phi,\ \psi \rangle = \langle \phi,\ \mathcal{L}^\zeta \psi \rangle \quad \forall\, \phi, \psi \in C_0^\infty(\mathbb{R}).$$

Also, 0 is an eigenvalue of $\mathcal{L}^\zeta$ with eigenvector $Q_z(\zeta, \cdot)$. Since $W''(\pm 1) > 0$ and $Q_z(\zeta, \cdot) > 0$ on $\mathbb{R}$, one can show that 0 is a simple eigenvalue and the remaining spectrum of $\mathcal{L}^\zeta$ lies on the half-plane $\{\mu \in \mathbb{C} \mid Re(\mu) < -\mu_0\}$ for some positive real number $\mu_0 \leqq \min\{W''(1), W''(-1)\}$. The assertion then follows from the Fredholm alternative, for which we omit further technical details. When (3.9) holds, the equation $\mathcal{L}^\zeta \phi = f$ admits infinitely many solutions, each of which can be written as $\phi(z) = \phi_{\text{sp}}(z) + c Q_z(\zeta, z)$, where c is an arbitrary constant and ϕ_{sp} is a special solution. Since $Q_z(\zeta, 0) > 0$, when the extra condition $\phi(0) = m$ is imposed, the constant c is uniquely determined so the solution is unique. □

4. Some Differential Geometry

In studying free boundary problems, quite often one needs local representations of free boundaries. Here we briefly present a key technique used in formal asymptotic expansions from a differential geometry perspective.

4.1. Local Coordinates

Let $\Gamma = \cup_{0 \leqq t \leqq T} (\Gamma_t \times \{t\}) \subset \mathbb{R}^N \times [0, T]$ be a smooth N-dimensional manifold, where $[0, T]$ is a time interval of interest. Fixing an arbitrary point on Γ, we can parameterize Γ near that point by a local chart, denoted by

$$X_0(s', t) \in \Gamma_t, \quad s' = (s^1, \ldots, s^{N-1}) \in \mathbb{R}^{N-1}.$$

Fixing an orientation, we denote by $\mathbf{n}(s', t)$ the unit normal of Γ_t at $X_0(s', t)$ and define

$$X(s, t) := X_0(s', t) + s^N \mathbf{n}(s', t), \quad s = (s', s^N) = (s^1, \ldots, s^N) \in \mathbb{R}^N.$$

Then locally $x = X(s, t)$ is a diffeomorphism. We denote by $s = S(x, t) = (S'(x, t), S^N(x, t))$ the inverse of $x = X(s, t)$ so that

$$x = X_0(S'(x, t), t) + S^N(x, t)\, \mathbf{n}(S'(x, t), t). \tag{4.1}$$

4.2. Curvature and Normal Velocity

(1) It is easy to see that

$$h(x, t) := S^N(x, t) \text{ is the } \textit{signed distance} \text{ from } x \text{ to } \Gamma_t.$$

In addition, differentiating the identity (4.1) with respect to x we have

$$\delta^{ij} = \frac{\partial x^i}{\partial x^j} = \frac{\partial X^i(S(x, t), t)}{\partial x^j} = \sum_{k=1}^{N-1} \left(X^i_{0 s^k} + s^N \mathbf{n}^i_{s^k} \right) S^k_{x^j} + \mathbf{n}^i S^N_{x^j}.$$

Thus,

$$\mathbf{n}^j = \sum_{i=1}^{N} \mathbf{n}^i \delta^{ij} = \sum_{k=1}^{N-1} \left(\mathbf{n} \cdot X_{0s^k} + s^N \mathbf{n} \cdot \mathbf{n}_{s^k} \right) S^k_{x^j} + \mathbf{n} \cdot \mathbf{n} S^N_{x^j} = S^N_{x^j}.$$

Here we have used the fact that X_{0s^k} is a tangent vector of Γ_t, so it is perpendicular to $\mathbf{n}$. Hence,

$$\nabla S^N(x,t) = \mathbf{n}(s',t).$$

This equation explains that the normal $\mathbf{n}$ of the interface, originally defined on Γ_t, can be extended to a neighborhood of Γ_t (by a constant along normal lines), so that

$$\nabla \mathbf{n} := \nabla \mathbf{n}(S'(x,t),t) = D^2 S^N(x,t).$$

It is easy to see that $\mathbf{n}$ is an eigenvector of $\nabla \mathbf{n}$ with eigenvalue zero. Let $\{\mathbf{n}, \tau_1, \ldots, \tau_{N-1}\}$ be an orthonormal eigenbasis of $\nabla \mathbf{n}$ with corresponding eigenvalues $\{0, \kappa^1, \ldots, \kappa^{N-1}\}$. Restricting x to the point $X_0(s',t)$, the eigenvalues $\{\kappa^1, \ldots, \kappa^{N-1}\}$ are called *principal curvatures* of Γ_t at $X_0(s',t)$, and $\{\tau_1, \ldots, \tau_{N-1}\}$ the corresponding *principal directions*. It then follows by the decomposition of a symmetric matrix that

$$\nabla \mathbf{n}(S'(x,t),t)\Big|_{x=X_0(s',t)} = D^2 S^N(X_0(s',t),t) = \sum_{i=1}^{N-1} \kappa^i \tau_i \otimes \tau_i. \tag{4.2}$$

(2) Next, differentiating (4.1) with respect to t gives

$$\mathbf{0} = \frac{\partial x}{\partial t} = X_{0t} + \sum_{k=1}^{N-1} (X_{0s^k} + s^N \mathbf{n}_{s^k}) S^k_t + \mathbf{n} S^N_t + S^N \mathbf{n}_t.$$

Taking the inner product with $\mathbf{n}$ we obtain $0 = X_{0t} \cdot \mathbf{n} + S^N_t$, so that

$$S^N_t(x,t) = -X_{0t}(s',t) \cdot \mathbf{n}(s',t) = -v(X_0(s',t),t),$$

where $v(X_0(s',t),t) := X_{0t}(s',t) \cdot \mathbf{n}(s',t)$ is called the *normal velocity* of Γ_t at $X_0(s',t)$ in the normal direction $\mathbf{n}(s',t)$. Here again, $S^N_t(x,t)$ is constant along the normal lines.

4.3. The Stretched Variable

Let $\varphi = \varphi_\varepsilon$ be a solution of (2.1) and $\Gamma^\varepsilon_t := \{x \mid \varphi_\varepsilon(x,t) = 0\}$ be the zero level set of φ_ε. With respect to the ε-independent reference manifold Γ_t, we represent Γ^ε_t locally as

$$X_\varepsilon(s',t) := X_0(s',t) + \varepsilon\, H_\varepsilon(s',t)\mathbf{n}(s',t) \in \Gamma^\varepsilon_t,$$

where $\varepsilon H_\varepsilon$ admits an expansion $\varepsilon H_\varepsilon(s',t) = \varepsilon h_1(s',t) + \varepsilon^2 h_2(s',t) + \cdots$. In this context, h_0 can be regarded as the unknown X_0. The location of the interface Γ^ε_t

is then uniquely determined by the coefficients $X_0, h_1, h_2, \ldots,$ of the asymptotic ε power series expansion of X_ε.

We introduce the stretched variable

$$z = Z(x,t) := \frac{S^N(x,t) - \varepsilon\, H_\varepsilon(S'(x,t),t)}{\varepsilon} = \frac{s^N}{\varepsilon} - H_\varepsilon(s',t). \tag{4.3}$$

We call (z, s', t) the local coordinates in which Γ_t^ε is represented by $z = 0$.

Remark 4.1. In the case $u \equiv 0$, the phase field equation (2.1) (with $\lambda = 1$) becomes the well-studied Allen–Cahn equation [1]. It is known that $\varphi_\varepsilon(x,t) = Q(\mathbf{n}_\varepsilon, d_\varepsilon(x,t)/\varepsilon) + O(\varepsilon^2)$ where $d_\varepsilon(x,t)$ is the signed distance from x to the interface Γ_t^ε, with normal $\mathbf{n}_\varepsilon$. This fact leads to a common practice (for example [11]) in which $\hat{z} := d_\varepsilon/\varepsilon$ is defined as the stretched variable and the local variables $(\hat{s}', \hat{z}, t)$ are the inverse of

$$x = X_\varepsilon(\hat{s}', t) + \varepsilon\, \hat{z}\, \mathbf{n}_\varepsilon(\hat{s}', t).$$

Comparing with this ε-dependent local chart, our chart $x = X_0(s',t) + \varepsilon[z + H_\varepsilon(s',t)]\mathbf{n}(s',t)$ has advantages and disadvantages. The obvious advantage is that $s' = S'(x,t)$ does not depend on ε. The disadvantage is that $Q(\mathbf{n}(s',t), z)$ is only an $O(\varepsilon)$ approximation of $\varphi_\varepsilon(x,t)$. Using

$$\begin{aligned} \mathbf{n}_\varepsilon &= \mathbf{n} - \varepsilon \nabla H_\varepsilon(S'(x,t),t) + O(\varepsilon^2), \\ Q(\mathbf{n}_\varepsilon, z) &= Q(\mathbf{n}, z) - \varepsilon \nabla H_\varepsilon(s',t) \cdot Q_\zeta(\mathbf{n}, z) + O(\varepsilon^2), \end{aligned}$$

we can eliminate this disadvantage by subtracting the quantity $\varepsilon \nabla H_\varepsilon \cdot Q_\zeta$ from our asymptotic expansion.

4.4. *Smooth Function Expanded in ε Power Series*

The transformation from (z, s', t) to (x, t) can be expressed as

$$x = X_0(s',t) + \varepsilon\, [z + H_\varepsilon(s',t)]\, \mathbf{n}(s',t).$$

A smooth function $f(x,t)$ for x near Γ_t can be expressed in (z, s', t) via the Taylor expansion

$$\begin{aligned} f(x,t) &= f(X_0,t) + \varepsilon(z + H_\varepsilon)(\mathbf{n}\cdot\nabla) f(X_0,t) \\ &\quad + \frac{\varepsilon^2 (z + H_\varepsilon)^2}{2} (\mathbf{n} \otimes \mathbf{n} : \nabla \otimes \nabla) f(X_0,t) + \cdots, \end{aligned}$$

where X_0 and H_ε are short for $X_0(s',t)$ and $H_\varepsilon(s',t)$. In particular,

$$\begin{cases} S_t^N(x,t) = -v(X_0,t), \quad \nabla S^N(x,t) = \mathbf{n}(s',t), \\ S_t^k(x,t) = S_t^k(X_0,t) + \varepsilon[z + H_\varepsilon](\mathbf{n}\cdot\nabla)\nabla S_t^k(X_0,t) + \cdots, \\ \nabla S^k(x,t) = \nabla S^k(X_0,t) + \varepsilon[z + H_\varepsilon](\mathbf{n}\cdot\nabla)\nabla S^k(X_0,t) + \cdots, \\ D^2 S^k(x,t) = D^2 S^k(X_0,t) + \varepsilon[z + H_\varepsilon](\mathbf{n}\cdot\nabla) D^2 S^k(X_0,t) + \cdots. \end{cases} \tag{4.4}$$

4.5. Chain Rule

As a function of (x, t), relevant derivatives of Z defined by the second equation in (4.3) are

$$Z_t = \varepsilon^{-1}\, S^N_t(x,t) - \partial_t H_\varepsilon(S'(x,t),t) = -\varepsilon^{-1}\, v(X_0,t) - \partial_t H_\varepsilon(s',t),$$
$$\nabla Z = \varepsilon^{-1}\mathbf{n}(s',t) - \nabla H_\varepsilon(s',t), \quad D^2 Z = \varepsilon^{-1}\nabla\mathbf{n} - D^2 H_\varepsilon(s',t).$$

In the sequel, for a function $F(z, s', t)$, we shall use $\tilde\nabla$, $\tilde\partial_t$, and $\tilde D^2$ to denote the corresponding partial derivatives with respect to t and x, with z considered as a constant:

$$\tilde\nabla F(z,s',t) := \sum_{k=1}^{N-1} F_{s^k}(z,s',t)\nabla S^k(x,t)\Big|_{x=X_0(s',t)+\varepsilon[z+H_\varepsilon(s',t)]\mathbf{n}(s',t)},$$
$$\tilde\partial_t F(z,s',t) := \sum_{k=1}^{N-1} F_{s^k}(z,s',t) S^k_t(x,t)\Big|_{x=X_0+\varepsilon[z+H_\varepsilon]\mathbf{n}} + F_t(z,s',t),$$
$$\tilde D^2 F(z,s',t) = \sum_{k,l=1}^{N-1} F_{s^k s^l}\nabla S^k\otimes\nabla S^l + \sum_{k=1}^{N-1} F_{s^k} D^2 S^k\Big|_{x=X_0+\varepsilon[z+H_\varepsilon]\mathbf{n}}.$$

Here in the (z, s', t) variable, the expansions in (4.4) are needed for the right-hand side. When $F(z, s', t)$ does not depend on z, the operators $\tilde\nabla$, $\tilde\partial_t$, $\tilde D^2$ are identical to ∂_t, ∇, and D^2, respectively.

Let $F(z, s', t) = f(x, t)$ with x evaluated at $x = X_0(s', t) + \varepsilon[z + H_\varepsilon(s', t)]\,\mathbf{n}(s', t)$. Then

$$f_t(x,t) = -F_z(z,s',t)[\varepsilon^{-1}\, v(X_0,t) + \partial_t H_\varepsilon(s;,t)] + \tilde\partial_t F(z,s',t),$$
$$\nabla f(x,t) = \varepsilon^{-1} F_z(z,s',t)\mathbf{n}(s',t) - F_z(z,s',t)\nabla H_\varepsilon(s',t) + \tilde\nabla F(z,s',t),$$
$$D^2 f(x,t) = \varepsilon^{-2}\mathbf{n}\otimes\mathbf{n}\, F_{zz} + \varepsilon^{-1}\Big\{F_z\nabla\mathbf{n} - F_{zz}[\mathbf{n}\otimes\nabla H_\varepsilon + \nabla H_\varepsilon\otimes\mathbf{n}]$$
$$+[\mathbf{n}\otimes\tilde\nabla F_z + \tilde\nabla F_z\otimes\mathbf{n}]\Big\} + \tilde D^2 F - F_z D^2 H_\varepsilon + F_{zz}\nabla H_\varepsilon\otimes\nabla H_\varepsilon$$
$$-[\nabla H_\varepsilon\otimes\tilde\nabla F_z + \tilde\nabla F_z\otimes\nabla H_\varepsilon].$$

4.6. The Convolution in the Stretched Variable

With $f(x, t) = F(z, s', t)$ where $z = Z(x, t)$ and $s' = S'(x, t)$ we have

$$f(x-\varepsilon y,t) = F(Z(x-\varepsilon y), S'(x-\varepsilon y), t),$$
$$Z(x-\varepsilon y,t) = \frac{S^N(x-\varepsilon y,t) - \varepsilon H_\varepsilon(S'(x-\varepsilon y,t),t)}{\varepsilon}.$$

Using the Taylor's expansion and $\nabla S^N = \mathbf{n}$, $D^2 S^N = \nabla\mathbf{n}$, we derive that

$$Z(x-\varepsilon y,t) = Z(x,t) - y\cdot\mathbf{n}(s',t) + \varepsilon\left(y\cdot\nabla H_\varepsilon + \frac{y\otimes y}{2} : \nabla\mathbf{n}\right)$$
$$-\frac{\varepsilon^2}{2} y\otimes y : D^2 H_\varepsilon + \cdots.$$

Here we keep track of only those $O(\varepsilon^2)$ terms that depend on $D^2 H_\varepsilon$. Thus, with $z := Z(x,t)$ and $s' := S'(x,t)$ one has

$$f(x-\varepsilon y,t) = F(z-y\cdot\mathbf{n},s',t) - \varepsilon y\cdot\tilde\nabla F(z-y\cdot\mathbf{n},s',t) + F_z(z-y\cdot\mathbf{n},s',t) \left\{\varepsilon\left(y\cdot\nabla H_\varepsilon + \frac{y\otimes y}{2} : \nabla\mathbf{n}\right) - \frac{\varepsilon^2}{2} y\otimes y : D^2 H_\varepsilon\right\} + \cdots.$$

Hence, abbreviating $F(z-y\cdot\mathbf{n},s',t)$ as $\hat F$, we have

$$J_\varepsilon * f(x,t) = j(\mathbf{n}) * F + \varepsilon\int_{\mathbb{R}^N} J(y)\left(\left[y\cdot\nabla H_\varepsilon + \frac{y\otimes y}{2} : \nabla\mathbf{n}\right]\hat F_z - y\cdot\tilde\nabla\hat F\right)\mathrm{d}y - \frac{\varepsilon^2 D^2 H_\varepsilon}{2} : \int_{\mathbb{R}^N} y\otimes y\hat F_z\,\mathrm{d}y + \cdots.$$

5. Asymptotic Expansion for the Phase Field Equation

Let $\varphi = \varphi_\varepsilon$ be a solution of (2.1) and $\Gamma_t^\varepsilon := \{x \mid \varphi_\varepsilon(x,t) = 0\}$ be the zero level set of φ_ε. Let Γ_t be the limit, as $\varepsilon \searrow 0$, of Γ_t^ε. We call Γ_t the macroscopically observed liquid–solid interface. We would like to derive macroscopically observable interfacial conditions from the microscopic model, that is, the phase field equation (2.1) for $\varphi = \varphi_\varepsilon(x,t)$.

5.1. The Expansion

Using the local coordinates (z,s',t) introduced in the previous section, we write

$$\varphi_\varepsilon(x,t) = \Phi(z,s',t) \quad\text{with}\quad x = X_0(s',t) + \varepsilon[z + H_\varepsilon(s',t)]\,\mathbf{n}(s',t).$$

Under the local coordinates (z,s',t), the differential equation (2.1) can be written as (using basic identities in Sections 4.4 and 4.5)

$$\begin{aligned}0 &= \lambda\, a(\mathbf{n})\,\Phi_{zz} - W'(\Phi) + (1-\lambda)[j(\mathbf{n}) * \Phi - \Phi] + \varepsilon\left\{\tau\, v\,\Phi_z + u\, G'(\Phi)\right\}\\ &\quad + \varepsilon\lambda A : \left\{\Phi_z\nabla\mathbf{n} - 2\Phi_{zz}\mathbf{n}\otimes\nabla H_\varepsilon + 2\mathbf{n}\otimes\tilde\nabla\Phi_z\right\}\\ &\quad + \varepsilon(1-\lambda)\int_{\mathbb{R}^N} J(y)\left(\left[y\cdot\nabla H_\varepsilon + \frac{y\otimes y}{2} : \nabla\mathbf{n}\right]\hat\Phi_z - y\cdot\tilde\nabla\hat\Phi\right)\mathrm{d}y\\ &\quad + \varepsilon^2\left\{\tau\Phi_z\partial_t H_\varepsilon - D^2 H_\varepsilon : \left[\lambda A\Phi_z + \frac{1-\lambda}{2}\int_{\mathbb{R}^N} y\otimes y J(y)\hat\Phi_z\,\mathrm{d}y\right]\right\}\\ &\quad + \cdots, \end{aligned} \tag{5.1}$$

where $v = v(X_0(s',t),t)$, $u = u(x,t)|_{x=X_0(s',t)+\varepsilon[z+H_\varepsilon(s',t)]}$, $\Phi = \Phi(z,s',t)$, $\hat\Phi = \Phi(z-y\cdot\mathbf{n},s',t)$, and "$\cdots$" are $O(\varepsilon^2)$ terms that are not relevant to our final conclusion.

We assume the asymptotic expansion

$$\Phi(z, s', t) \sim \Phi_0(z, s', t) + \varepsilon\Phi_1(z, s', t) + \varepsilon^2\Phi_2(z, s', t) + \cdots, \tag{5.2}$$

$$H_\varepsilon(s', t) \sim h_1(s', t) + \varepsilon h_2(s', t) + \varepsilon^2 h_3(s', t) + \cdots, \tag{5.3}$$

where $\Phi_0, \Phi_1, \Phi_2, \ldots, h_1, h_2, \ldots,$ are smooth functions that do not depend on ε.

The outer expansion yields the simple solutions $\varphi^{\text{outer}}(x) \equiv \pm 1$, so the matching condition becomes $\Phi(\pm\infty, s', t) = \pm 1$. Also, since the zero level set of $\varphi_\varepsilon = \Phi$ is characterized by $z = 0$, we need $\Phi(0, s', t) = 0$. Hence, we impose

$$\Phi_0(\pm\infty, s', t) = \pm 1, \quad \Phi_0(0, s', t) = 0, \tag{5.4}$$

$$\Phi_i(\pm\infty, s', t) = 0, \quad \Phi_i(0, s', t) = 0 \; \forall i = 1, \cdots. \tag{5.5}$$

5.2. The Zeroth Order Expansion

Substituting (5.2) into (5.1), expanding both sides in ε power, and equating the leading order coefficients we obtain the equation

$$\lambda\, a(\mathbf{n})\, \Phi_{0zz} + (1 - \lambda)[j(\mathbf{n}) * \Phi_0 - \Phi_0] - W'(\Phi_0) = 0.$$

With the boundary conditions in (5.4), the solution is uniquely given by

$$\Phi_0(z, s', t) = Q(\mathbf{n}(s', t), z). \tag{5.6}$$

Note that $\tilde{\nabla}$ is the partial derivative with respect to x with z regarded as a constant. Hence

$$\begin{aligned} \tilde{\nabla}\Phi_0 &= \tilde{\nabla} Q(\mathbf{n}(s', t), z) = \sum_{k=1}^{N} Q_{\zeta^k}(\mathbf{n}, z) \nabla \mathbf{n}^k(S'(x, t), t) \\ &= \sum_{k=1}^{N} \nabla S^N_{x_k} Q_{\zeta^k} = (\nabla \mathbf{n}) Q_\zeta, \\ y \cdot \tilde{\nabla}\Phi_0 &= \nabla\mathbf{n} : y \otimes Q_\zeta, \quad A : \mathbf{n} \otimes \tilde{\nabla}\Phi_{0z} = \nabla\mathbf{n} : (A\mathbf{n}) \otimes Q_{z\zeta}. \end{aligned} \tag{5.7}$$

5.3. The Default Correction

As mentioned in Remark 4.1, in the definition $z = (S^N - \varepsilon H_\varepsilon)/\varepsilon$, the quantity $S^N(x, t) - \varepsilon H(S'(x, t), t)$ is not exactly the distance function from x to the zero level set, Γ^ε_t, of $\varphi_\varepsilon(\cdot, t)$. This deficiency leads to certain default first order expansion terms. Here we eliminate them by expanding the solution as

$$\Phi(z, s', t) = Q(\mathbf{n}(s', t), z) - \varepsilon Q_\zeta(\mathbf{n}(s', t), z) \cdot \nabla H_\varepsilon(s', t) + \varepsilon\hat{\Phi}, \tag{5.8}$$

$$\hat{\Phi}(z, s', t) \sim \hat{\Phi}_1(z, s', t) + \varepsilon\hat{\Phi}_2(z, s', t) + \cdots. \tag{5.9}$$

Since $Q(\zeta, 0) = 0$, we have $Q_\zeta(\zeta, 0) = \mathbf{0}$. Hence, the boundary condition (5.5) is equivalent to

$$\hat{\Phi}_i(\pm\infty, s', t) = 0, \quad \hat{\Phi}_i(0, s', t) = 0 \quad \forall i = 1, 2, \cdots.$$

Using (3.7) we see that, abbreviating $Q(\mathbf{n}(s',t),z)$ as Q and $Q(\mathbf{n}(s',t),z-y\cdot\mathbf{n}(s',t))$ as $\hat{Q}$,

$$\nabla H_\varepsilon \cdot \mathcal{L}^{\mathbf{n}} Q_\zeta = \nabla H_\varepsilon \cdot \left\{ -2A\mathbf{n}Q_{zz} + (1-\lambda)\int_{\mathbb{R}^N} J(y)y\hat{Q}_z\,\mathrm{d}y \right\}. \tag{5.10}$$

Now substituting (5.7), (5.8), and (5.10) into (5.1) and keeping track of the D^2H_ε term, we derive that (5.1) is equivalent to

$$-\mathcal{L}^{\mathbf{n}}\hat{\Phi} = \tau v Q_z + uG'(Q) + \nabla\mathbf{n} : B + \varepsilon\left(\tau Q_z \partial_t H_\varepsilon - D^2H_\varepsilon : B\right) + \cdots \tag{5.11}$$

where

$$B := \lambda[AQ_z + 2A\mathbf{n}\otimes Q_{z\zeta}] + (1-\lambda)\int_{\mathbb{R}^N} J(y)\left\{\frac{y\otimes y}{2}\hat{Q}_z - y\otimes\hat{Q}_\zeta\right\}\mathrm{d}y.$$

5.4. The First Order Equation

The first order equation of (5.11) reads

$$-\mathcal{L}^{\mathbf{n}}\hat{\Phi}_1 = \tau\, v(X_0,t)\, Q_z + u(X_0,t)\, G'(Q) + \nabla\mathbf{n}(X_0,t) : B,$$

where $X_0 = X_0(s',t)$ is a generic point on Γ_t. The solvability condition (3.9) requires that the following interfacial condition be satisfied on Γ:

$$\begin{aligned} 0 &= \tau v(X_0,t)\int_{\mathbb{R}} Q_z^2\,\mathrm{d}z + u(X_0,t)\int_{\mathbb{R}} G'(Q)Q_z\,\mathrm{d}z \\ &\quad + \nabla\mathbf{n}(X_0,t) : \int_{\mathbb{R}} B(z,s',t)Q_z\,\mathrm{d}z. \end{aligned}$$

Using Lemma 3.2(2) and $\int_{\mathbb{R}} G'(Q)Q_z dz = G(1) - G(-1) = 1$, this condition can be written as

$$u(X_0,t) + \alpha(\mathbf{n})v(X_0,t) + \nabla\mathbf{n} : D^2\sigma(\mathbf{n}) = 0, \tag{5.12}$$

where $\mathbf{n} = \mathbf{n}(X_0,t)$, $\alpha(\mathbf{n}) = \tau\int_{\mathbb{R}} Q_z(\mathbf{n},z)^2\mathrm{d}z$, and $X_0 = X_0(s',t)$ is a generic point on the limit interface Γ_t. This is exactly the equation (1.8). Note that if we use (4.2), then we have

$$\nabla\mathbf{n} : D^2\sigma(\mathbf{n}) = \sum_{i=1}^{N-1}\kappa^i\tau_i\otimes\tau_i : D^2\sigma(\mathbf{n}) = \sum_{i=1}^{N-1}\kappa^i\sigma_{\tau_i\tau_i}(\mathbf{n}).$$

Here the direction τ_i in the second order directional derivative $\sigma_{\tau_i\tau_i}$ is assumed to be constant in the differentiation. Consequently, the interfacial condition (5.12) can be written as (1.9).

Assume that this interfacial condition is satisfied. Then there is a unique solution $\hat{\Phi}_1$.

5.5. High Order Expansions

The equation for $\hat{\Phi}_{k+1}$, $k \geqq 1$, can be written as

$$-\mathcal{L}^{\mathbf{n}}\hat{\Phi}_{k+1} = \tau Q_z \partial_t^\Gamma h_k - \nabla^\Gamma \otimes \nabla^\Gamma h_k : B - C \cdot \nabla^\Gamma h_k - \hat{C} : \nabla^\Gamma h_1 \otimes \nabla^\Gamma h_k \\ -Dh_k - E_k,$$

where ∂_t^Γ, ∇^Γ, and $\nabla^\Gamma \otimes \nabla^\Gamma$ are the restrictions of ∂_t, ∇, and D^2 on Γ, respectively; that is,

$$\partial_t^\Gamma h(s', t) := \sum_{i=1}^{N-1} h_{s^i}(s', t) S_t^i(X_0, t) + h_t(s', t),$$

$$\nabla^\Gamma h(s', t) := \sum_{i=1}^{N-1} h_{s^i}(s', t) \nabla S^i(X_0, t),$$

$$\nabla^\Gamma \otimes \nabla^\Gamma h(s', t) := \sum_{i,j=1}^{N-1} h_{s^i s^j}(s', t) \nabla S^i(X_0, t) \otimes \nabla S^j(X_0, t) \\ + \sum_{i=1}^{N-1} h_{s^i}(s', t) D^2 S^i(X_0, t),$$

where $X_0 = X_0(s', t)$. Also, C, $\hat{C}$, D are functions depending only on Q and X_0, whereas E_k depends only on lower order expansions Φ_0, $\hat{\Phi}_1, \ldots, \hat{\Phi}_k$, X_0, $h_1, \ldots, h_{k-1}$. The solvability condition (3.9) for $\hat{\Phi}_{k+1}$ can be written as

$$\mathcal{L}^\Gamma h_k(s', t) = e_k(s', t), \tag{5.13}$$

where

$$\mathcal{L}^\Gamma := \alpha(\mathbf{n})\partial_t^\Gamma - D^2\sigma(\mathbf{n}) : \nabla^\Gamma \otimes \nabla^\Gamma - c(s', t) \cdot \nabla^\Gamma + d(s', t).$$

Here one can verify that $\int_{\mathbb{R}} Q_z \hat{C}(z, s', t) dz = 0$, so there is no $\nabla^\Gamma h_1 \otimes \nabla^\Gamma$ term.

When the matrix $D^2\sigma(\mathbf{n})$ is positive definite on the tangent space $\{\tau \mid \tau \perp \mathbf{n}\}$, for every $\mathbf{n} \in \mathbb{S}^{N-1}$, (5.13) is a parabolic linear equation defined on the manifold Γ. If we impose appropriate initial and boundary conditions, say, $h_k(s', 0) \equiv 0$ and Γ_t has no boundary, we can solve the parabolic equation to obtain a unique h_k, from which, we obtain a unique $\hat{\Phi}_{k+1}$. The induction can proceed to arbitrary high order expansions.

We summarize our derivation as follows:

Theorem 1. *The solution $\varphi = \varphi_\varepsilon(x, t)$ of (2.1) admits a formal asymptotic expansion only if the interface condition (5.12) is satisfied on the limit interface.*

Remark 5.1. In general, $h_1 \not\equiv 0$. In [10], for the case of $\lambda = 1$, a special non-linearity of W and G was selected so that the solution of the resulting system of the phase field equations gives $h_1 \equiv 0$. This means that the zero level set of φ_ε is within an $O(\varepsilon^2)$ distance from the limit interface.

6. Special Representation of the Interfacial Condition

6.1. The Two-dimensional Case

In the two-dimensional case, we can express the normal as $\mathbf{n} = (\cos\theta, \sin\theta)$ and the tangent as $\tau = (-\sin\theta, \cos\theta)$. Using polar coordinates and the homogeneity of σ we can express σ as

$$\sigma(\rho\cos\theta, \rho\sin\theta) = \rho\,\bar{\sigma}(\theta).$$

Consequently,

$$\nabla\sigma(\zeta) = [\sigma_{\zeta^1}\ \sigma_{\zeta^2}] = [\cos\theta\ \ \sin\theta]\bar{\sigma}(\theta) + [-\sin\theta\ \ \cos\theta]\,\bar{\sigma}'(\theta),$$

$$D^2\sigma(\zeta) = \begin{bmatrix} \sigma_{\zeta^1\zeta^1} & \sigma_{\zeta^2\zeta^1} \\ \sigma_{\zeta^1\zeta^2} & \sigma_{\zeta^2\zeta^2} \end{bmatrix} = \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix} [-\sin\theta\ \ \cos\theta]\,\frac{\bar{\sigma}(\theta) + \bar{\sigma}''(\theta)}{\rho},$$

$$\tau\otimes\tau : D^2\sigma(\mathbf{n}) = \tau^T D^2\sigma(\mathbf{n})\tau = \bar{\sigma}(\theta) + \bar{\sigma}''(\theta).$$

Thus, in the two-dimensional case, (1.9) can be written as (1.5).

6.2. Interfacial Condition Using the Distance Function

Let $h(x,t)$ be the signed distance from x to Γ_t, positive in the liquid region and negative in the solid region. Then $h(x,t) = S^N(x,t)$, $\nabla h(x,t) = \mathbf{n}$, and $D^2h = \nabla\mathbf{n}$. Also, $v = -h_t$. Hence, the interfacial condition (1.9) can be expressed as

$$\alpha(\nabla h)h_t = u + \sum_{i,j=1}^{N} \sigma_{\zeta^i\zeta^j}(\nabla h)h_{x^i x^j} \quad \text{on } \Gamma = \{h = 0\}. \tag{6.1}$$

This equation is valid only on Γ. Off the set, the governing equation for h is $|\nabla h| = 1$ (see, for example, [6]).

6.3. Interfacial Condition Using Level Sets

Suppose the interface Γ is represented by the non-degenerate zero level set of a function Ψ, that is $\Gamma_t = \{x \mid \Psi(x,t) = 0\}$ with $\nabla\Psi\cdot\mathbf{n} > 0$ on Γ_t. Then there exists a positive function C such that in a small neighborhood of Γ,

$$h(x,t) = C(x,t)\Psi(x,t).$$

Consequently,

$$h_t = C\Psi_t + C_t\Psi, \quad \nabla h = C\nabla\Psi + \Psi\nabla C,$$

$$D^2h = CD^2\Psi + \nabla C\otimes\nabla\Psi + \nabla\Psi\otimes\nabla C + \Psi D^2C.$$

Thus, on Γ_t,

$$h = \Psi = 0, \quad \nabla h = C \nabla \Psi, \quad C = \frac{1}{|\nabla \Psi|},$$

$$h_t = C\Psi_t = \frac{\Psi_t}{|\nabla \Psi|}, \quad D^2 h = \frac{D^2 \Psi}{|\nabla \Psi|} + \nabla C \otimes \nabla \Psi + \nabla \Psi \otimes \nabla C.$$

Since (3.5) implies that $\nabla \Psi \; D^2 \sigma(\mathbf{n}) = \mathbf{0}$ and $D^2 \sigma(\mathbf{n}) \; \nabla^T \Psi = \mathbf{0}$, we then obtain, on Γ,

$$\begin{aligned} \nabla \mathbf{n} : D^2 \sigma(\mathbf{n}) &= D^2 h : D^2 \sigma(\mathbf{n}) = \frac{D^2 \Psi}{|\nabla \Psi|} : D^2 \sigma(\mathbf{n}) = D \left(\frac{\nabla \Psi}{|\nabla \Psi|} \right) : D^2 \sigma\,(\mathbf{n}) \\ &= \sum_{i,j=1}^{N} \sigma_{\zeta^i \zeta^j} \left(\tfrac{\nabla \Psi}{|\nabla \Psi|} \right) \frac{\partial}{\partial x^i} \left(\frac{\Psi_{x^j}}{|\nabla \Psi|} \right) \\ &= \sum_{i=1}^{N} \frac{\partial}{\partial x_i} \sigma_{\zeta^i} \left(\tfrac{\nabla \Psi}{|\nabla \Psi|} \right) = \operatorname{div} \left(\sigma_\zeta \left(\frac{\nabla \Psi}{|\nabla \Psi|} \right) \right). \end{aligned}$$

Finally, recalling that the normal velocity of the interface is given by $v = -h_t = -\Psi_t / |\nabla \Psi|$, the interfacial condition (1.8) thus can be written as (1.10). Unlike (6.1), equation (1.10) can be regarded as valid in the whole space, whose viscosity solutions have been well-studied; see, for example, EVANS ET AL. [13] and CHEN ET AL. [9].

6.4. A Three-dimensional Example

Assume, for positive constants a, b, c, that the anisotropy is given by

$$\sigma(\zeta) = \frac{a(\zeta^1)^2 + b(\zeta^2)^2 + c(\zeta^3)^2}{|\zeta|} \quad \forall \zeta = (\zeta^1, \zeta^2, \zeta^3)^T \in \mathbb{R}^3 \setminus \{0\}.$$

Then

$$\begin{aligned} \nabla \sigma(\zeta) &= \frac{[2a\zeta^1 \; 2b\zeta^2 \; 2c\zeta^3]}{|\zeta|} - \frac{\zeta^T \; \sigma}{|\zeta|^2}, \\ D^2 \sigma(\zeta) &= \frac{\operatorname{diag}(2a, 2b, 2c)}{|\zeta|} - \frac{\sigma I}{|\zeta|^2} + \frac{3\sigma}{|\zeta|^2} \zeta \otimes \zeta \\ &\quad - \frac{2}{|\zeta|^3} \left\{ [a\zeta^1 \; b\zeta^2 \; c\zeta^3] \otimes \zeta + \zeta \otimes [a\zeta^1 \; b\zeta^2 c\zeta^3] \right\}. \end{aligned}$$

Now let $h(x, t) = S^N(x, t)$ be the signed distance from x to the interface Γ_t. Then $\mathbf{n} = \nabla h$ and $\nabla \mathbf{n} = D^2 h$. Using $\mathbf{n}^T D^2 h = (0)_{1 \times N}$ and $D^2 h \; \mathbf{n} = (0)_{N \times 1}$ we obtain

$$\nabla \mathbf{n} : D^2 \sigma(\mathbf{n}) = 2a h_{x^1 x^1} + 2b h_{x^2 x^2} + 2c h_{x^3 x^3} - (a h_{x^1}^2 + b h_{x^2}^2 + c h_{x^3}^2) \Delta h.$$

The operator on the right-hand side is elliptic for every $\mathbf{n} = \nabla h \in \mathbb{S}^{N-1}$ if and only if

$$2 \min\{a, b, c\} > \max\{a, b, c\}.$$

7. The Wulff shape—a Numerical Example

We consider a special two-dimensional case where J is given in the polar coordinates by

$$J(x, y) = \bar{J}(r, \theta) = J_0(r) + \delta \cos(n\theta) J_1(r), \quad r = \sqrt{x^2 + y^2}, \quad \tan\theta = \frac{y}{x},$$

where n is an even positive integer. For $\mathbf{n} = (\cos\theta, \sin\theta)$ we write $j(\mathbf{n})$ and $\sigma(\mathbf{n})$ as $\bar{j}(\theta)$ and $\bar{\sigma}(\theta)$, respectively. Then

$$\begin{aligned}
\bar{j}(\theta, z) &= \int_{-\infty}^{\infty} J\left(z\langle\cos\theta, \sin\theta\rangle + \ell\langle-\sin\theta, \cos\theta\rangle\right) \mathrm{d}\ell \\
&= \int_{-\infty}^{\infty} \bar{J}\left(\sqrt{z^2 + \ell^2},\ \theta + \arctan\frac{\ell}{z}\right) \mathrm{d}\ell \\
&= \hat{j}(\delta \cos n\theta, z),
\end{aligned}$$

where

$$\begin{aligned}
\hat{j}(h, z) &= j_0(z) + h j_n(z), \\
j_0(z) &= 2\int_0^{\infty} J_0(\sqrt{z^2 + \ell^2}) \mathrm{d}\ell, \\
j_n(z) &= 2\int_0^{\infty} J_1(\sqrt{z^2 + \ell^2}) \cos\left(n \arctan\frac{\ell}{z}\right) \mathrm{d}\ell.
\end{aligned}$$

As an illustration, we choose the following:

$$n = 6, \quad J_0(r) = \frac{e^{-r^2}}{\pi}, \quad J_1(r) = -\frac{r^6 e^{3-2r^2}}{27\pi}.$$

Then

$$j_0(z) = \frac{e^{-z^2}}{\sqrt{\pi}}, \quad j_6(z) = \frac{e^{3-2z^2}(15 - 180z^2 + 240z^4 - 64z^6)}{1728\sqrt{2\pi}}.$$

The function $\hat{j}(h, \cdot) := j_0(\cdot) + h j_6(\cdot)$ is shown in Fig. 1a. It is easy to verify that

$$\begin{aligned}
J(x, y) \geqq 0 \quad \forall (x, y) \in \mathbb{R}^2 \quad &\Longleftrightarrow \quad |\delta| \leqq 1, \\
\bar{j}(\theta, z) = \hat{j}(\delta \cos n\theta, z) \geqq 0 \quad \forall \theta \in [0, 2\pi], z \in \mathbb{R} \quad &\Longleftrightarrow \quad |\delta| \leqq 6.15285\cdots.
\end{aligned}$$

For each $h \in [-12, 12]$, we denote by $\hat{Q}(h, \cdot)$ the solution Q of (3.1) with

$$\lambda = 0, \quad j(\zeta, z) = \hat{j}(h, z), \quad W(q) = \frac{(1 - q^2)^2}{4}.$$

Then (3.1) can be written as

$$\hat{j}(h) * \hat{Q}(h) = \hat{Q}^3(h).$$

Numerically, we compute the solution by the iteration scheme

$$Q_0(z) = \tanh(z), \quad Q_{k+1} = \sqrt[3]{\hat{j}(h) * Q_k}, \quad \hat{Q}(h, \cdot) = \lim_{k\to\infty} Q_k(\cdot).$$

The solution $\hat{Q}(h, \cdot)$ is shown in Fig. 1b. For $h \in [11, 12]$, we find that $\hat{Q}(h, \cdot)$ is not monotonic; this is caused in part by the fact that $\hat{j}(h, \cdot)$ is not positive when

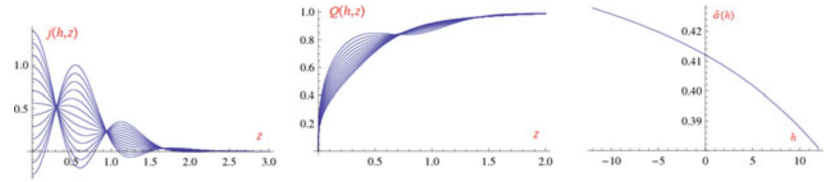

Fig. 1. **a** The function $\hat{j}(h, \cdot) := j_0(\cdot) + hj_6(\cdot)$, $h = -12, -10, \ldots, 12$; **b** the odd function $\hat{Q}(h, \cdot)$, $h = -12, -10, \ldots, 12$; **c** the function $\hat{\sigma}(\cdot)$

$h \geqq 6.15\cdots$. The corresponding surface energy density, plotted in Fig. 1c, is calculated by

$$\hat{\sigma}(h) = \int_{\mathbb{R}} \left(W(Q) - \tfrac{1}{2}QW'(Q)\right) \mathrm{d}z = \frac{1}{4}\int_{\mathbb{R}} \left(1 - \hat{Q}^4(h, z)\right) \mathrm{d}z.$$

Now for fixed δ, denoting $\mathbf{n} = (\cos\theta, \sin\theta)$ we have

$$Q(\mathbf{n}, z) = \hat{Q}(\delta\cos(6\theta), z), \quad \sigma(\mathbf{n}) = \bar{\sigma}(\theta) = \hat{\sigma}(\delta\cos(6\theta)).$$

From the plot of $\hat{\sigma}(\cdot)$ in Fig. 1c, we see that

$$\hat{\sigma}(h) \approx 0.412062 - 0.00177\, h - 0.0000500\, h^2.$$

Thus,

$$\begin{aligned}
\bar{\sigma}(\theta) &\approx 0.412062 - 0.00177\,\delta\cos(6\theta) - 0.0000500\,\delta^2\cos^2(6\theta),\\
\bar{\sigma}'(\theta) &\approx \delta[0.0106 + 0.000600\,\delta\cos(6\theta)]\sin(6\theta),\\
\bar{\sigma}''(\theta) &\approx \delta[0.0639\ \cos(6\theta) + 0.00360\,\delta\cos(12\theta)].
\end{aligned}$$

For $\delta = 1, 8$ and 12, the functions $\bar{\sigma}(\theta) = \hat{\sigma}(\delta\cos(6\theta))$ and $\bar{\sigma}(\theta) + \bar{\sigma}''(\theta)$ are plotted in Fig. 2. Numerically, we find that $\bar{\sigma}(\theta) + \bar{\sigma}''(\theta) > 0$ for all $\theta \in [0, 2\pi]$ when $|\delta| < 9.78\cdots$.

The *Wulff shape* [24] is the shape of a solid under the undercooling temperature $u \equiv -1$. From (1.5), the Wulff shape can be computed in terms the surface energy density as follows. Denote the boundary of the Wulff shape by $x = X(\theta)$, where $\theta \in [0, 2\pi]$ and $\langle\cos\theta, \sin\theta\rangle$ is the unit normal at $X(\theta)$. Then, with respect to the arc length parameter s, we have

$$\frac{\mathrm{d}X}{\mathrm{d}\theta} = \frac{\mathrm{d}X}{\mathrm{d}s}\frac{\mathrm{d}s}{\mathrm{d}\theta} = \langle -\sin\theta,\ \cos\theta\rangle\frac{\mathrm{d}s}{\mathrm{d}\theta}, \quad \frac{\mathrm{d}\theta}{\mathrm{d}s} = \kappa = \frac{1}{\bar{\sigma}(\theta) + \bar{\sigma}''(\theta)}.$$

It then follows that

$$\frac{\mathrm{d}X(\theta)}{\mathrm{d}\theta} = [\bar{\sigma}(\theta) + \bar{\sigma}''(\theta)]\langle -\sin\theta,\ \cos\theta\rangle.$$

After integration, we obtain the function for the boundary of the Wulff shape:

$$X(\theta) = \bar{\sigma}(\theta)\langle\cos\theta,\ \sin\theta\rangle + \bar{\sigma}'(\theta)\langle -\sin\theta,\ \cos\theta\rangle, \quad \theta \in [0, 2\pi].$$

For $\delta = 1, 8, 12$, the Wulff shapes are given in the third row in Fig. 2. When $\delta \in [9.79, 12]$, the function $\bar{\sigma} + \bar{\sigma}''$ is not positive; the corresponding Wulff shape is close to a hexagon with "ears" at the vertices.

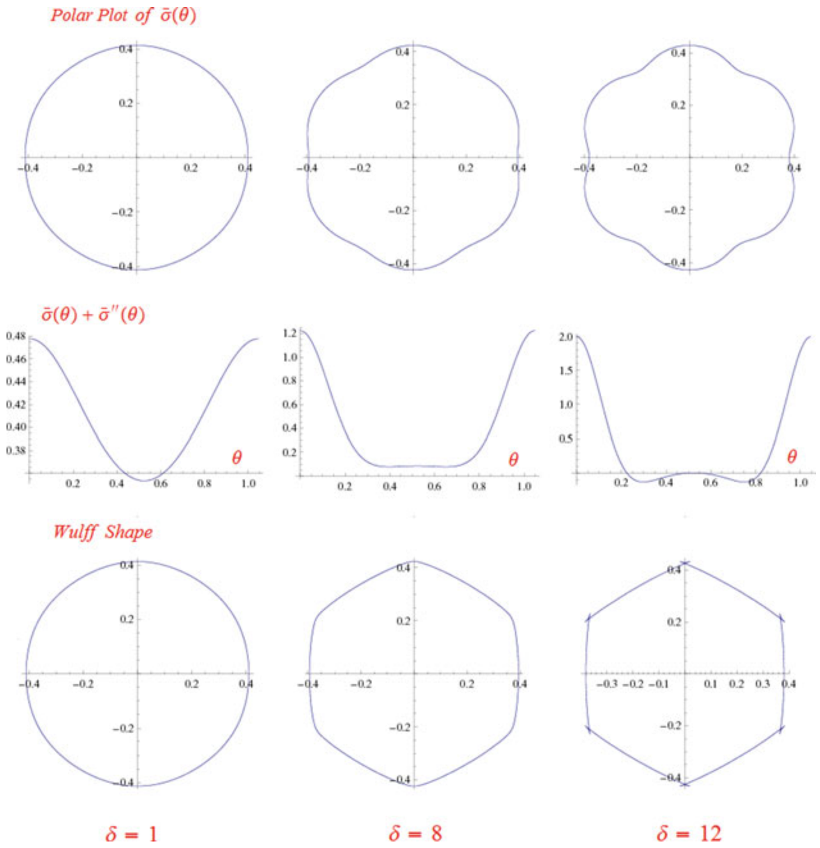

Fig. 2. *First row* the function $\bar{\sigma}(\theta)$ with θ axis represented by the unit *circle* and $\bar{\sigma}(\theta)$ the distance to the origin; *second row* the function $\bar{\sigma}(\theta) + \bar{\sigma}''(\theta)$ in one period ($[0, \pi/3]$); *last row* the Wulff shapes

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