Triple Junction Motion for Allen-Cahn/Cahn-Hilliard Systems

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Abstract

Long time asymptotics are developed here for an Allen-Cahn/Cahn-Hilliard system derived recently by Cahn & Novick-Cohen [11] as a diffuse interface model for simultaneous order-disorder and phase separation. Proximity to a deep quench limit is assumed, and spatial scales are chosen to model Krzanowski instabilities in which droplets of a minor disordered phase bounded by interphase boundaries (IPB) of high curvature coagulate along a slowly curved antiphase boundaries (APB) separating two ordered variants. The limiting motion couples motion by mean curvature of the APBs with motion by minus the surface Laplacian of the IPBs on the same time scale. Quasi-static surface diffusion of the chemical potential occurs along APBs. The framework outlined here should also be suitable for describing sintering of small grains and thermal grain boundary grooving in polycrystalline films.

KEYWORDS: triple-junction motion, motion by mean curvature, motion by minus the surface Laplacian of mean curvature, surface diffusion, geometric motion, phase transitions, Allen-Cahn/Cahn-Hilliard equations, diffuse interface models, Krzanowski instabilities, sintering, grain boundary grooving in polycrystalline films.

1 Introduction.

The Allen-Cahn/Cahn-Hilliard system:

$$u_t = 4\epsilon^2 \nabla \cdot Q(u, v) \nabla \frac{\delta F}{\delta u}, \tag{1.1}$$

$$v_t = -\frac{1}{4} Q(u, v) \frac{\delta F}{\delta v}, \tag{1.2}$$

where

$$F = \int_\Omega \Big\{ \frac{\Theta}{2}\{(u+v)\ln(u+v)+(u-v)\ln(u-v)+(1-(u+v))\ln(1-(u+v))+(1-(u-v))\ln(1-(u-v))\}$$

$$+ \alpha u(1-u) - \beta v^2 + \frac{1}{2}\epsilon^2\{|\nabla u|^2 + |\nabla v|^2\}\Big\} dx \tag{1.3}$$

is taken to be defined on a smooth bounded domain $\Omega \subset R^n$, $n = 1, 2,$ or 3. Neumann boundary conditions are prescribed for u where u is a conserved order parameter, typically a concentration, no-flux boundary for the mass flux $j = -Q\nabla\frac{\delta F}{\delta u}$ where $Q = Q(u, v)$ is the mobility and $\mu = \frac{\delta F}{\delta u}$ is the chemical potential, and Neumann boundary conditions for v where v is a non-conserved order parameter. Here Θ represents the temperature. This system of equations can be viewed as a simplest prototype system which can exhibit simultaneous ordering and phase separation.

While a system similar in form to (1.1)-(1.3) with constant mobility Q and with a quartic polynomial for the free energy F has been proposed by Eguchi, et. al. [19], a systematic derivation of the Allen-Cahn/Cahn-Hilliard system has been given in Cahn & Novick-Cohen [11] based on energetic exchange probabilities for an Fe-Al binary alloy system on a large but finite BCC lattice. In their derivation, the conserved and non-conserved order parameters u and v may be defined roughly as

$$u(n) = \frac{1}{16}\sum_{a\in A}\{c(n+a) + c(n)\} \text{ and } v(n) = \frac{1}{16}\sum_{a\in A}\{c(n+a) - c(n)\}$$

where $c(n)$ represents the probability of finding an Fe atom at site n of a given lattice segment and A represents the set of nearest neighbors. The system (1.1)-(1.3) may then be obtained either by taking respectively conserved and non-conserved gradient flow for u and v from a quasi-continuum limit of a discretely defined free energy, or by further averaging the values of u and v over a larger number of lattice neighbors and then taking a quasi-continuum limit in the discrete dynamic equations. See also the discussions in Chen [15] and Chen & Khachaturyan [16]. An advantage of the derivation given in [11] is that the relative size of the mobilities for the concentration equation (1.1) and the order parameter equation (1.2) is predicted; in the derivation given in *e.g.* [19] this is not the case.

Certain characteristics of the Allen-Cahn/Cahn-Hilliard system are easily ascertained. For $0 < \alpha < \beta$, linear stability analysis about a uniform homogeneous state indicates the onset of an initial order-disorder instability. Under these conditions, it can be shown that at low temperatures there exist two pairs of minimizers of the free energy with differing energies [11, §2]. The pair with lower free energy can be approximated by $(u, v) = (\frac{1}{2}, \pm\frac{1}{2})$, and the other pair corresponds roughly to $(u, v) = (0, 0)$ and $(1, 0)$. Since the mean mass $\bar{u} = \frac{1}{|\Omega|}\int_\Omega u\, dx$ is conserved under the evolution of the (1.1)-(1.3) and since the Allen-Cahn/Cahn-Hilliard system corresponds to gradient flow in $H^{-1}(\Omega)\times L^2(\Omega)$, if the mean concentration differs initially from $\frac{1}{2}$ then the system can be expected to evolve at late times towards a configuration which is largely dominated by smoothly bounded regions containing any of three equal depth minimizers of the free energy obtainable by a tie-line construction. Combining the description of the early time behavior with the characteristics of late

time behavior, it follows that conditional spinodal decomposition must occur, see Allen & Cahn [2].

It is possible to envision a generalization of (1.1)-(1.3) involving n Allen-Cahn equations coupled with m Cahn-Hilliard equations. Such a generalisation which also accounts for the underlying lattice structure has been outlined in [11], see also Cahn, McFadden, and Novick-Cohen [12]. Recently, studies of systems of Cahn-Hilliard equations, known also as Morral-Cahn [29] systems, have appeared, see for example Alt & Pawlow [4], Eyre [20], Elliott & Luckhaus [22], Elliott & Garcke [21], Garcke and Novick-Cohen [23] and Bronsard, Garcke, and Stoth [7].

Questions of existence, uniqueness, regularity, and the existence of inertial sets have been addressed for the Allen-Cahn/Cahn-Hilliard system for the constant mobility case and with quartic polynomial free energy F in Brochet, Hilhorst, and Novick-Cohen [6]. One should hope to prove global existence and regularity of solutions $(u,\, v)$ for the Allen-Cahn/Cahn-Hilliard system as given in (1.1)-(1.3) for initial data in $H^2(\Omega) \times L^2(\Omega)$. Such solutions should be uniformly restricted to the domain

$$0 < u + v < 1 \text{ and } 0 < u - v < 1.$$

As noted, during late times the system should to be dominated by a finite number of regions in which one of three minimizing phases prevail, and these regions can be expected to be separated by thin interfacial regions. Since the system contains three types of minimizers, clearly the possibility of "triple-junctions" or small transitional domains connecting the three types of minimizers arises. The majority of this paper is devoted to formal asymptotics appropriate for the description of this late time behavior and in particular for the description of the triple-junction motion. We outline these formal asymptotics in a fair amount of detail, as we see them to differ significantly from the triple-junction asymptotics given in the Allen-Cahn context [8].

It is useful to comment on the behavior which can be expected to occur. Note first that the Allen-Cahn/Cahn-Hilliard system encompasses both the Allen-Cahn and the Cahn-Hilliard equations, since taking the concentration u to be identically equal to $\frac{1}{2}$, the system reduces to a Allen-Cahn equation, and by taking the non-conserved order parameter v is taken to be identically equal to zero, the system is governed by a Cahn-Hilliard equation. Along interfaces separating the minimizers $(\frac{1}{2},\, \pm\frac{1}{2})$ known as ordered variants, the concentration should be roughly equal to $\frac{1}{2}$ and hence in the neighborhood of such an interface, known as an antiphase boundary or APB, the system should be approximately governed by the Allen-Cahn equation. In accordance with the known behavior for Allen-Cahn equations [33], on a time scale $\tau = t$ such an interface should move by motion by mean curvature. Along interfaces known as interphase boundaries (or IPB's) which separate ordered variants and the minimizers $(0,\, 0)$ or $(1,\, 0)$ known as disordered phases, both equations should be important though the slower behavior of the Cahn-Hilliard equation may be expected to dominate. As formal asymptotics [32] rigorously justified in [1], [17], [36] indicate, on an appropriate time scale which is ϵ times slower that the Allen-Cahn time scale for motion by mean curvature, the Cahn-Hilliard equation evolves as a (non-local) Mullins-Sekerka type boundary problem. Similar predictions have also been given recently by Giacomin and Lebowitz [25],[27] for a Cahn-Hilliard like equation with non-local, derivable via Kawasaki lattice dynamics [26]. It has been shown by Cahn, Elliott, and Novick-Cohen [9] that if the Cahn-Hilliard equation is considered

with a mobility which vanishes in the pure phases $u = 0$ and $u = 1$ and with a free energy taken to be of the form given by (1.3) with $v \equiv 0$, then on the even slower time scale $\tau = \epsilon^2 t$, formal asymptotics indicate that the interface moves by minus the surface Laplacian of the mean curvature. Here, assuming similarly that the mobility vanishes in all three pure phases, we could expect to obtain that the IPBs move by motion by minus the surface Laplacian of the mean curvature. The difficulty which presents itself immediately is that in each of the previous analogue problems, the limiting motion of interest occurs on different time scales. This difficulty is addressed shortly.

Previous work on triple-junctions given in the context of a system of Allen-Cahn equations [8] dictates a balance of forces or "Young's law" (see Young [39]) to govern the angles at which the three interfaces meet at the triple junction. Since the coupling of motion by minus the surface Laplacian of the mean curvature requires a coupling of higher order, additional conditions occur at the triple-junction, and not surprisingly an extra condition arises which is based on a balance of mass flux, a condition which is not to be expected for a system of Allen-Cahn equations which is not mass conservative. In forthcoming work [23], both Young's law and a balance of mass flux law arise at triple-junctions which occur when studying systems of Cahn-Hilliard equations with a degenerate mobility matrix. In a short note [13], it is shown that if the curvature of the APB's is taken to be $\mathcal{O}(\epsilon)$ and the curvature of the IPB's is taken to be $\mathcal{O}(1)$, then the resulting behavior leads to motion by mean curvature coupled to motion by minus the surface Laplacian of the mean curvature, but these two motions do not occur on the same time scale. See Fig. 1.i.

In the present paper, long time asymptotics are considered employing scaling assumptions chosen to model the Krzanowski instability [3] near the deep quench limit when the disordered phase is taken to constitute a minor phase, in which small droplets of the minor phase coagulate along smooth slowly varying antiphase boundaries and detach at points of high curvature. In order to capture this behavior, the curvature of the interphase boundaries bounding the droplets of the disordered phase is assumed to be asymptotically large ($\mathcal{O}(\epsilon^{-1/2})$), and the curvature of the antiphase boundaries is taken to be asymptotically small ($\mathcal{O}(\epsilon^{3/2})$). Furthermore a time scale $\tau = \epsilon^{7/2} t$ is assumed. By considering our system as a perturbation of the zero temperature limit, it is easily checked that the free energy as defined gives rise to complete wetting. The discussions which follow, however, do not preclude the non-complete wetting case which can arise from an alternative (non-quadratic) zero-temperature free energy limit. Under these assumptions we demonstrate that the limiting behavior then does indeed couple motion by mean curvature with motion by minus the Laplacian of the mean curvature on the same time scale. At triple-junctions, the limiting behavior is governed by Youngs law, a mass flux balance, and a condition on the sum of mean curvatures which is implied by the continuity of the chemical potential. Both APBs and IPBs meet the external boundary at 90°, and a no-flux through the external boundary condition arises. Along APBs, the chemical potential obeys a null surface Laplacian condition which can be construed as quasi-static surface diffusion. Since ABP's and IPB's cannot spontaneously detach from the external boundary (unless they detach in pairs) and since an APB or IPB cannot spontaneously detach from a triple-junction, a kinetic or "persistence" condition [23] follows in both instances. See Fig. 1.ii.

For the limiting motion, the volume of the disordered phase is conserved, as is the volume of the union of each of the ordered phases. If the sum is taken over the length of all interfaces, weighting

Figure 1.i: The limiting motion when the curvature of APBs is assumed to be $\mathcal{O}(\epsilon)$ and the curvature of IPBs is assumed to be $\mathcal{O}(1)$, see [13].

Figure 1.ii: The limiting equations of motion under the assumption that the curvature of APBs is $\mathcal{O}(\epsilon^{3/2})$ and that the curvature of IPBs is $\mathcal{O}(\epsilon^{-1/2})$, see text.

each APB or IPB segment by its respective surface energy per unit length (surface tension), then this weighted sum is a non-increasing function of time and acts as a Liapunov functional for the system. See equation (7.54). In this sense the behavior obtained is to be compared with surface diffusion (SD) and surface aggregation limited kinetics (SALK) [14], both of which are mass conservative and perimeter decreasing, and can be described as gradient flows [37]. Other equations of motion for interfaces in a volume conservative framework have been prescribed either on phenomenological grounds as in the early work by Mullins [30] in the context of thermal grain boundary grooving or as in the more recent work by Wong, et.al. [38] in the context of the dynamics of solid thin films, or via a constituitive approach as formulated by Davi and Gurtin [18] in the context of surface diffusion.

While the Allen–Cahn/Cahn–Hilliard system of equations and the accompanying limiting equations of motion were constructed in [11] with the Krzanowski instability in mind, this setting should also be appropriate for the consideration of other microstructural dynamics such as

i) grain boundary grooving of polycrystalline films,

or

ii) sintering of small grains.

In the context of the evolution of film microstructure (for a recent review, see Srolovitz and Goldiner [34]), our equations may be appropriate for describing thermal pitting [24] and grooving [30], [35], if the main mechanism of variation of the upper surface of the polycrystalline film is via surface diffusion, and if the main mechanism of alteration of the grain boundary groove is by quasi-static diffusion and surface minimization. A similar discussion might be appropriate in considering the sintering of small grains, where after an initial transient period exterior boundaries might act effectively like highly curved IPBs and the internal boundaries might act as APBs with lesser curvature, see [5]. While it may be possible to prescribe sharp interface models to describe the dynamics for these phenomena on physical and phenomenological grounds as described above, the ability to embed these sharp interface models in a diffuse interface theory is desirable as it permits a numerical context in which to run these models past possible topological changes. It also lends a coherent framework in which to determine conditions at triple-junctions and external boundaries based on a unified set of scaling assumptions.

The outline of this paper is as follows. In §1, the underlying assumptions for our analysis are carefully prescribed. The assumptions concerning the asymptotic behavior of the outer solutions dominated by one of the three minimizers are given in §2 and are shown to be self-consistent. In §3, the asymptotics for the inner solutions governing the behavior within APBs and IPBs is outlined. Youngs law, the balance of mass flux, and the condition on the sum of curvatures are derived in §4. The limiting conditions satisfied at intersections of APBs and IPBs with external boundaries are given in §5. In §6 the limiting equations are summarized and the proof is given that the area of the disordered phase is conserved and that the surface energy weighted perimeter is a non-increasing function of time. A short discussion is given in §7.

2 Preliminaries.

In this paper we work with a system of Allen-Cahn/Cahn-Hilliard equations, written below as:

$$u_t = 4\epsilon^2 \nabla \cdot Q(u,\, v)\nabla\mu, \tag{2.1}$$

$$v_t = -\frac{1}{4} Q(u,\, v)\frac{\delta F}{\delta v}, \tag{2.2}$$

where

$$\mu = \frac{\delta F}{\delta u}, \tag{2.3}$$

and where the free energy F is given by

$$F = \int_\Omega \Big\{ \frac{\Theta}{2}\{(u+v)\ln(u+v)+(u-v)\ln(u-v)+(1-(u+v))\ln(1-(u+v))+(1-(u-v))\ln(1-(u-v))\}$$

$$+ \alpha u(1-u) - \beta v^2 + \frac{1}{2}\epsilon^2\{|\nabla u|^2 + |\nabla v|^2\}\Big\}\, dx. \tag{2.4}$$

The mobility is taken to vanish in the "pure" phases; i.e., at either of the ordered variants or at a disorderd phases composed entirely of either of the two components of the binary system. This assumption generalises the mobility

$$M(u) = u(1-u),$$

considered in the original derivation of Cahn and Hilliard [10]. For simplicity we take

$$Q(u,v) = \tilde{Q}\, \Pi_{i=1}^4 \Big((u + v - w_1^i)^2 + (u - v - w_2^i)^2 \Big)^{1/2}, \tag{2.5}$$

where $w_j^i = [i+j]_{mod 2}$. The arguments presented should be readily extendable to somewhat more general forms of mobility. We remark also that the free energy prescribed in (2.4) corresponds to that of a system in which the external boundary is inert. To consider the case of non-inert boundaries, additional terms should be included in the free energy.

The free energy given in (2.4) has two minimizers known as ordered phase variants located transcendentally close ($\mathcal{O}(e^{-c/\Theta})$) to $(u,\, v) = (\frac{1}{2},\, \pm\frac{1}{2})$ and given implicitely by

$$u = \frac{1}{2}, \quad 2\beta v = \Theta\Big\{\ln\Big(\frac{1}{2} + v\Big) + \ln\Big(\frac{1}{2} - v\Big)\Big\}, \tag{2.6}$$

as well as two minima located transcendentally close to $(u,\, v) = (0,\, 0)$ and $(u,\, v) = (1,\, 0)$ known as disordered phases which satisfy

$$-\alpha(1-2u) = \Theta\{\ln(u) - \ln(1-u)\}, \quad v = 0. \tag{2.7}$$

If

$$0 < \alpha < \beta,$$

then the free energy of the minima given by (2.6) is lower than that of the pair of minima given by (2.7). Moreover, if the mean concentration of the system

$$\bar{u} = \frac{1}{|\Omega|}\int_{\Omega} u(x,\, t)\, dx$$

is not equal to $\frac{1}{2}$ then a tie line construction shows there to be three equal depth minima consisting of the pair of minima given in (2.6) and one of the two minima from (2.7). Without loss of generality, we assume these minima to be located transcendentally close to

$$\Big(\frac{1}{2},\, -\frac{1}{2}\Big),\, \Big(\frac{1}{2},\, +\frac{1}{2}\Big),\, (1,\, 0). \tag{2.8}$$

We shall assume throughout that $\Theta \propto \epsilon^{1/2}$.

In undertaking our asymptotic analysis, the time scale $\tau = \epsilon^{7/2}t$ is introduced and the Allen-Cahn/Cahn-Hilliard system is written as

$$\epsilon^{5/2}u_t = 4\epsilon\, \nabla \cdot Q(u,\, v)\nabla\mu, \tag{2.9}$$

$$\epsilon^{7/2}v_t = -\frac{1}{4}Q(u,\, v)[F_v(u,\, v) - \epsilon^2 \triangle v], \tag{2.10}$$

$$\mu = F_u(u,\, v) - \epsilon^2 \triangle v. \tag{2.11}$$

In addition, the system is assumed to be initially composed of internal sub-domains dominated by one of the three minimizers of the free energy. As we wish to model the Krzanowski instability, the mean concentration is be assumed to be close to $\bar{u}$; i.e., the disordered phase is taken to be a minor phase. For simplicity, it is possible to imagine the system to initially contain precisely three internal domains: two large sub-domains containing ordered phase variants, and a smaller internal domain containing the disordered phase. Thin interfacial partitions with width of order ϵ are assumed to separate these three sub-domains. Partitions between ordered variants and the disordered phase are known as interphase boundaries (IPBs), whereas partitions between two differing ordered variants are known as antiphase boundaries (APBs). Away from the interfacial partitions, the solution is assumed to be transcendentally close to one of the minimizing configurations. More precisely, in such regions the solution is taken to be given by an the outer solution satisfying

$$u = u_i^0 + T.S.T., \quad v = v_i^0 + T.S.T., \tag{2.12}$$

where $(u_i^0,\, v_i^0)$ corresponds to one of the three minimizers of (2.8), and

$$\mu = \mu_i^0 + \epsilon^{1/2}\mu_i^{1/2} + \mathcal{O}(\epsilon), \quad j = 4\, Q(u,\, v)\nabla\mu = T.S.T., \tag{2.13}$$

where $i = 1, 2$ refers to the two ordered phase variants and $i = 3$ refers to the disordered phase. We shall assume that these features of the initial configuration maintain themselves throughout the evolution of the system. The behavior of the outer solution is described in greater detail in §3. Since the internal domains containing ordered phase variants are assumed to be large, it is

reasonable to assume that the curvature of the antiphase boundaries is small. More specifically, we assume that

$$\mathcal{K}_{antiphase} = \epsilon^{3/2}\mathcal{K}^{3/2} + \mathcal{O}(\epsilon^2).$$

Similarly, as the disordered phase is assumed to be a minor phase, we assume the curvature of the antiphase boundaries to be large, or more explicitely that

$$\mathcal{K}_{interphase} = \epsilon^{-1/2}\mathcal{K}^{-1/2} + \mathcal{K}^0 + \mathcal{O}(\epsilon^{1/2}).$$

Intuitively, the reason for employing the $\epsilon^{1/2}$ scaling is to distinguish the characteristic radius of the disordered domains from the characteristic width ($\mathcal{O}(\epsilon)$) of the interfacial partitions. This also explains the necessity of the $\epsilon^{1/2}$-expansions employed in (2.12)–(2.13). We apologise to the reader in advance for the clumsiness of the expansions in $\epsilon^{1/2}$ which appear throughout, but we believe it most appropriate to employ the characteristic interfacial partition width ϵ as the predominant variable. We remark that in a recent note [13], a similar initial three phase configuration was considered, but the disordered phase was not assumed to be a minor phase, and hence according the curvature of the antiphase boundaries was assumed to satisfy

$$\mathcal{K}_{antiphase} = \epsilon\mathcal{K}^1 + \mathcal{O}(\epsilon^2),$$

and the curvature of the interphase boundaries was taken to satisfy

$$\mathcal{K}_{interphase} = \mathcal{K}^0 + \epsilon\mathcal{K}^1 + \mathcal{O}(\epsilon^2).$$

Within the framework of that asymptotic analysis, all expansions were made in terms of ϵ, and there was no necessity for introducing the half powers. The effects of the two different sets of assumptions is critical, as the scaling employed in the present paper leads to motion on similar time scales along both the interphase and antiphase boundaries, whereas the scaling introduced in [13] lead to fast evolution of interphase boundaries and slow evolution of antiphase boundaries. The present set of scaling assumptions is seemingly more appropriate for modeling the Krzanowski instability. For simplicity, the three interfacial regions are assumed to meet at a unique triple junction located at some internal point within the domain Ω. A description of the behavior of the solution within the interfacial partitions is given in §4 within the framework of inner solutions. In the proximity of the triple-junctions and points of contact of the interfacial partitions with the exterior of the domain, additional expansions must be made which are presented respectively in §5 and §6.

3 Outer Solution.

In this section, we outline our assumptions on the form of the outer solution, and we show that these assumptions are consistent with the equations (2.9)-(2.11). In particular, we assume that the outer solution,

$$u(x,\, t) = u_0^i + (\epsilon^{1/2}u^{1/2} + \epsilon u^1 + \epsilon^{3/2}u^{3/2} + \mathcal{O}(\epsilon^2))e^{-c/\epsilon^{1/2}}, \tag{3.1}$$

$$v(x,\,t) = v_0^i + (\epsilon^{1/2}v^{1/2} + \epsilon v^1 + \epsilon^{3/2}v^{3/2} + \mathcal{O}(\epsilon^2))e^{-c/\epsilon^{1/2}}, \tag{3.2}$$

$$\mu(x,\,t) = \epsilon^{1/2}\mu^{1/2} + \epsilon\mu^1 + \epsilon^2\mu^2 + \mathcal{O}(\epsilon^3), \tag{3.3}$$

$$j = (j^0 + \epsilon^{1/2}j^{1/2} + \epsilon j^1 + \epsilon^{3/2}j^{3/2} + \mathcal{O}(\epsilon^2))e^{-c/\epsilon^{1/2}}. \tag{3.4}$$

where the pairs $\{u_0^i,\, v_0^i\}$ denote the (three) minimizers of the constrained free energy described in §2, and where the notation $T.S.T.$ indicates transcendentally small terms; i.e., $\mathcal{O}(e^{-c/\epsilon^{1/2}})$ where c is the same coefficient as appears in the expression for u_0 and v_0.

With this in mind, we write equations (2.9)-(2.11) as

$$\epsilon^{7/2}v_t = -\tfrac{1}{4}Q(u,\,v)\mu_v, \tag{3.5}$$

$$\epsilon^{5/2}u_t = 4\epsilon\,\nabla\cdot Q(u,\,v)\nabla\mu_u, \tag{3.6}$$

where

$$\mu_v \equiv F_v(u,\,v) - \epsilon^2\triangle u, \quad \mu_u \equiv F_u(u,\,v) - \epsilon^2\triangle v. \tag{3.7}$$

Furthermore, we define

$$j = -Q(u,\,v)\nabla\mu_u. \tag{3.8}$$

(In the sections which follow, we shall refrain from using the μ_u, μ_v notation, and shall revert to using a single chemical potential: $\mu = \mu_u$.)

We now show that these assumptions are consistent. Let us assume that both μ_u and μ_v have expansions of the form given in (3.3). From the assumptions on u and v given in (3.1) and (3.2) and noting that $Q(u,\,v)$ has regular roots at the pure phases, it follows that

$$Q(u,\,v) = \mathcal{O}(e^{-c/\epsilon^{1/2}}).$$

Therefore, employing these two estimates, (3.6) and (3.5) are seen to be consistent with the expansions (3.1) and (3.2). Similarly, in the context of equation (3.8), the assumptions (3.1)-(3.4) are seen to be self-consistent.

We now check that the assumptions on the expansions for u and v and for μ_u and μ_v are consistent with equations (3.7) and (3.7). Note first that u^0 and v^0 obviously solve the equations

$$F_u(u^0,\,v^0) = 0 \quad F_v(u^0,\,v^0) = 0.$$

Linearizing, $u^{1/2}$ and $v^{1/2}$ are given as the solutions to

$$\mu_u^{1/2} = F_{uu}(u^0,\,v^0)u^{1/2} + F_{uv}(u^0,\,v^0)v^{1/2},$$

$$\mu_v^{1/2} = F_{uv}(u^0,\,v^0)u^{1/2} + F_{vv}(u^0,\,v^0)v^{1/2}.$$

It is easy to check by solving for $u^{1/2}$ and $v^{1/2}$ and noting the form of u^0 and v^0 and the structure of F, that the assumed form of expansions are self-consistent within this framework. Proceeding to the equations for u^1 and v^1:

$$\mu_u^1 = F_{uu}(u^0,\,v^0)u^1 + F_{uv}(u^0,\,v^0)v^1 + F_{uuu}(u^0,\,v^0)(u^{1/2})^2 + 2F_{uuv}(u^0,\,v^0)u^{1/2}v^{1/2} + F_{uvv}(u^0,\,v^0)(v^{1/2})^2,$$

$$\mu_v^1 = F_{uv}(u^0,\,v^0)u^1 + F_{vv}(u^0,\,v^0)v^1 + F_{uuv}(u^0,\,v^0)(u^{1/2})^2 + 2F_{uvv}(u^0,\,v^0)u^{1/2}v^{1/2} + F_{vvv}(u^0,\,v^0)(v^{1/2})^2,$$

similar considerations again yield self-consistency. Higher order self-consistency may be readily demonstrated by induction.

4 The inner solution.

4.1 The inner solution for antiphase boundaries.

We recall from §2 that along antiphase boundaries, it has been assumed that

$$\mathcal{K} = \epsilon^{3/2}\mathcal{K}^{3/2} + \epsilon^2\mathcal{K}^2 + \mathcal{O}(\epsilon^{5/2}). \tag{4.1}$$

Similarly, we set

$$u(x,\, t) = U(\rho,\, s,\, t) = U^0 + \epsilon^{1/2}U^{1/2} + \epsilon U^1 + \mathcal{O}(\epsilon^{3/2})$$
$$v(x,\, t) = V(\rho,\, s,\, t) = V^0 + \epsilon^{1/2}V^{1/2} + \epsilon V^1 + \mathcal{O}(\epsilon^{3/2})$$

and

$$W = W^0 + \epsilon^{1/2}W^{1/2} + \mathcal{O}(\epsilon),$$

where $W = W(s,\, t)$ represents the normal velocity. The analysis of the equations which arise for the evolution of the inner solution of the antiphase boundaries at the various different asymptotic levels is given below.

At $\mathcal{O}(\epsilon^{-1})$

$$0 = 4(Q(U^0,\, V^0)\mu^0_\rho)_\rho,$$

which integrated yields

$$Q(U^0,\, V^0)\mu^0_\rho = b(s,\, t). \tag{4.2}$$

Matching of the fluxes within the interfacial region with the fluxes in the outer region and noting that $Q(U^0,\, V^0)\mu^0_\rho = n \cdot j^{-1}$, it follows that

$$b(s,\, t) = 0.$$

Assuming $Q(U^0,\, V^0)$ to be non-vanishing almost everywhere within the inner region, which is reasonable since by matching considerations the inner solution must connect values which are transcendentally close to the roots of $Q(U,\, V)$, we conclude from (4.2) that

$$\mu^0_\rho = 0,$$

and hence,

$$\mu^0 = c(s,\, t). \tag{4.3}$$

At $\mathcal{O}(\epsilon^{-1/2})$, using (4.3)

$$0 = 4(Q(U^0,\, V^0)\mu^{1/2}_\rho)_\rho.$$

Following the same steps as in the $\mathcal{O}(\epsilon^{-1})$ analysis,

$$\mu^{1/2} = d(s,\, t). \tag{4.4}$$

At $\mathcal{O}(1)$ employing (4.3) and (4.4),

$$0 = 4(Q(U^0,\, V^0)\mu^1_\rho)_\rho \tag{4.5}$$

$$\mu^0 = F_U(U^0, V^0) - U^0_{\rho\rho} \tag{4.6}$$

$$0 = -\frac{1}{4}Q(U^0, V^0)[F_V(U^0, V^0) - V^0_{\rho\rho}]. \tag{4.7}$$

From (4.6)-(4.7) assuming $Q(U^0, V^0)$ to be non-vanishing almost everywhere in the inner region, a heteroclinic orbit connecting equilibrium points which are transcendentally close to $(\frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, -\frac{1}{2})$ exists only if

$$\mu^0 = 0.$$

With this in mind, we set $\mu^0 = 0$ and assume U^0 and V^0 to correspond to the heteroclinic orbit given by the equations

$$0 = F_U(U^0, V^0) - U^0_{\rho\rho} \tag{4.8}$$

$$0 = F_V(U^0, V^0) - V^0_{\rho\rho}. \tag{4.9}$$

Integrating (4.5), noting that $Q(U^0, V^0)\mu^1_\rho = n \cdot j^0$, and matching with the fluxes in the outer solution yields

$$\mu^1 = e(s, t),$$

where $e(s, t) = \mathcal{O}(e^{-c/\epsilon^{1/2}})$.

At $\mathcal{O}(\epsilon^{1/2})$,

$$0 = 4(Q(U^0, V^0)\mu^{3/2}_\rho)_\rho \tag{4.10}$$

$$\mu^{1/2} = F_{UU}U^{1/2} + F_{UV}V^{1/2} - U^{1/2}_{\rho\rho} \tag{4.11}$$

$$0 = -\frac{1}{4}Q(U^0, V^0)[F_{UV}U^{1/2} + F_{VV}V^{1/2} - V^{1/2}_{\rho\rho}]. \tag{4.12}$$

Again, (4.10) leads to the conclusion that

$$Q(U^0, V^0)\mu^{3/2}_\rho = f(s, t) \tag{4.13}$$

where $f(s, t)$ is $T.S.T.$. By considering the boundary conditions at $+\infty$ and $-\infty$ and the definition of the free energy F, it follows from (4.8) and (4.9) that U^0 is symmetric and V^0 is anti-symmetric. These considerations allow us to conclude from (4.11) and (4.12) that the null adjoint condition imposes no constraint on $\mu^{1/2}$, $U^{1/2}$, and $V^{1/2}$, and that $U^{1/2}$ is a symmetric function and $V^{1/2}$ is an anti-symmetric function.

At $\mathcal{O}(\epsilon)$,

$$0 = 4\Big[Q(U^0, V^0)\mu^2_\rho + (Q_U(U^0, V^0)U^{1/2} + Q_V(U^0, V^0)V^{1/2})\mu^{3/2}_\rho)_\rho\Big] \tag{4.14}$$

$$\mu^1 = F_{UU}U^1 + F_{UV}V^1 - U^1_{\rho\rho} + F_{UUU}(U^{1/2})^2 + 2F_{UUV}U^{1/2}V^{1/2} + F_{UVV}(V^{1/2})^2 \tag{4.15}$$

$$0 = -\frac{1}{4}Q(U^0, V^0)[F_{UV}U^1 + F_{VV}V^1 - V^1_{\rho\rho} + F_{VUU}(U^{1/2})^2 + 2F_{VUV}U^{1/2}V^{1/2} + F_{VVV}(V^{1/2})^2]. \tag{4.16}$$

Integrating (4.14) and matching with the outer solution

$$0 = 4\Big[Q(U^0, V^0)\mu^2_\rho + (Q_U(U^0, V^0)U^{1/2} + Q_V(U^0, V^0)V^{1/2})\mu^{3/2}_\rho\Big] + g(s, t), \tag{4.17}$$

where $g(s,\,t)$ is $T.S.T.$. From equations (4.15)-(4.16), since $F_{UUU} = F_{UVV}$ is symmetric and $F_{UUV} = F_{VVV}$ is anti-symmetric no new condition is imposed on μ^1, U^1, and V^1 by the null adjoint condition, and it is easy to ascertain that U^1 is symmetric and V^1 is anti-symmetric.

At $\mathcal{O}(\epsilon^{3/2})$

$$-W^0 U^0_\rho = 4\Big[(Q(U^0,\,V^0)\mu_\rho^{5/2} + (Q_U(U^0,V^0)U^{1/2} + Q_V(U^0,V^0)V^{1/2})\mu_\rho^2$$

$$+(Q_U(U^0,V^0)U^1 + Q_V(U^0,V^0)V^1)\mu_\rho^{3/2} + (Q_{UU}(U^0,V^0)(U^{1/2})^2 + 2Q_{UV}(U^0,V^0)U^{1/2}V^{1/2}$$

$$+ Q_{VV}(U^0,V^0)(V^{1/2})^2)\mu_\rho^{3/2}\Big]_\rho + 4Q(U^0,\,V^0)\triangle_s\mu^{1/2} \tag{4.18}$$

$$\mu^{3/2} = F_{UU}U^{3/2} + F_{UV}V^{3/2} - U^{3/2}_{\rho\rho} + F_{UUU}U^1U^{1/2} + F_{UUV}(U^1V^{1/2} + U^{1/2}V^1) + F_{UVV}V^1V^{1/2}$$

$$+ \frac{1}{6}F_{UUUU}(U^{1/2})^3 + \frac{1}{2}F_{UUUV}(U^{1/2})^2V^{1/2} + \frac{1}{2}F_{UUVV}U^{1/2}(V^{1/2})^2 + \frac{1}{6}F_{UVVV}(V^{1/2})^3 \tag{4.19}$$

$$0 = -\frac{1}{4}Q(U^0,\,V^0)\Big[F_{VU}U^{3/2} + F_{VV}V^{3/2} - V^{3/2}_{\rho\rho} + F_{VUU}U^1U^{1/2} + F_{VUV}(U^1V^{1/2} + U^{1/2}V^1) +$$

$$F_{VVV}V^1V^{1/2} + \frac{1}{6}F_{VUUU}(U^{1/2})^3 + \frac{1}{2}F_{VUUV}(U^{1/2})^2V^{1/2} +$$

$$\frac{1}{2}F_{UVVV}U^{1/2}(V^{1/2})^2 + \frac{1}{6}F_{VVVV}(V^{1/2})^3\Big]. \tag{4.20}$$

Imposition of the null-adjoint condition on (4.19)-(4.20) and symmetry considerations yield that

$$f(s,\,t) = 0. \tag{4.21}$$

Integrating equation (4.18) between $-\epsilon^{-1/4}$ and $\epsilon^{-1/4}$ and matching the fluxes $n\cdot j^1$ with the associated fluxes in the outer solution, gives to leading order

$$-W^0[U^0]^\infty_{-\infty} = 4\int_{-\infty}^{\infty} Q(U^0,\,V^0)\,dx\;\triangle_s\mu^{1/2} = 0,$$

which reduces by virtue of the symmetry of the functions U^0 and $U^{1/2}$ and the positivity of $Q(U^0,\,V^0)$ to the condition

$$\triangle_s d(s,\,t) = h(s,\,t) \tag{4.22}$$

where $h(s,\,t)$ is $T.S.T.$. Returning to (4.17) and using (4.21),

$$\mu^2 = \frac{1}{4}\int_{-\infty}^{\rho}\frac{g(s,\,t)}{Q(U^0,\,V^0)}\,d\tilde{\rho} + k(s,\,t). \tag{4.23}$$

Using (4.22) in (4.18) and integrating, an implicit formula for $\mu^{5/2}$ is obtained

$$-W^0[U^0]^\rho_{-\infty} = 4\Big[Q(U^0,\,V^0)\mu_\rho^{5/2} + (Q_U(U^0,\,V^0)U^{1/2} + Q_V(U^0,\,V^0)V^{1/2})\mu_\rho^2\Big] + l(s,\,t) \tag{4.24}$$

where $l(s,\,t)$ is $T.S.T.$. By (4.19) and (4.20), $U^{3/2}$ is symmetric and $V^{3/2}$ is anti-symmetric.

At $\mathcal{O}(\epsilon^2)$

$$-W^0 U^{1/2}_\rho - W^{1/2} U^0_\rho = 4\Big[Q(U^0,\, V^0)\mu^3_\rho + (Q_U U^{1/2} + Q_V V^{1/2})\mu^{5/2}_\rho$$

$$+(Q_U U^1 + Q_V V^1)\mu^2_\rho + (Q_{UU}(U^{1/2})^2 + 2Q_{UV}U^{1/2}V^{1/2} + Q_{VV}(V^{1/2})^2)\mu^2_\rho\Big]_\rho$$

$$+ 4Q(U^0,\, V^0)\triangle_s \mu^1 + 4(Q_U(U^0,\, V^0)U^{1/2} + Q_V(U^0,\, V^0)V^{1/2})\triangle_s \mu^{1/2} \tag{4.25}$$

and

$$\mu^2 = F_{UU}U^2 + F_{UV}V^2 - U^2_{\rho\rho} + \text{ symmetric terms in } U^i, V^i,\, i = 0, \ldots, \frac{3}{2}. \tag{4.26}$$

$$0 = -\frac{1}{4}Q(U^0,\, V^0)\Big[F_{VU}U^2 + F_{VV}V^2 - V^2_{\rho\rho} + \text{ anti-symmetric terms in } U^i, V^i,\, i = 0, \ldots, \frac{3}{2}\Big]. \tag{4.27}$$

Integrating (4.25) over the interval $(-\epsilon^{-1/4},\, \epsilon^{-1/4})$ and applying symmetry considerations yields

$$\triangle_s e(s,\, t) = m(s,\, t)$$

where $m(s,\, t)$ is $T.S.T.$. Applying the null-adjoint condition (4.26)-(4.27) gives

$$\int_{-\infty}^{\infty} \mu^2 U^0_\rho \, d\rho = 0.$$

Noting by (4.13) and (4.14) that

$$4\int_{-\infty}^{\infty} \mu^2 U^0_\rho \, d\rho = \int_{-\infty}^{\infty} U^0_\rho \int_{-\infty}^{\rho} \frac{g(s,\, t)}{Q(U^0,\, V^0)}\, d\tilde{\rho},$$

and integrating by parts

$$\int_{-\infty}^{\infty} U^0_\rho \int_{-\infty}^{\rho} \frac{g(s,\, t)}{Q(U^0,\, V^0)}\, d\tilde{\rho} = -g(s,\, t)\int_{-\infty}^{\infty} \frac{U^0(\rho) - U^0(\infty)}{Q(U^0,\, V^0)}\, d\rho = T.S.T.,$$

hence $g(s,\, t) = 0$.

At $\mathcal{O}(\epsilon^{5/2})$, it suffices to consider the relevant asymptotic expansions for (2.9) and (2.10),

$$\mu^{5/2} = F_{UU}U^{5/2} + F_{UV}V^{5/2} - U^{5/2}_{\rho\rho} - \mathcal{K}_{3/2}U^0_\rho + \text{ symmetric terms in } U^i, V^i,\, i = 0, \ldots, 2,$$

$$-W^0 V^0_\rho = -\frac{1}{4}Q(U^0,\, V^0)[F_{UV}U^{5/2} + F_{VV}V^{5/2} - V^{5/2}_{\rho\rho} - \mathcal{K}^{3/2}V^0_\rho$$

$$+ \text{ anti-symmetric terms in } U^i, V^i,\, i = 0, \ldots, 2].$$

By the null-adjoint condition and symmetry considerations, to leading order

$$0 = W^0\left[\int_{-\infty}^{\infty} \frac{4(V^0_\rho)^2}{Q(U^0,\, V^0)}\, d\rho + \int_{-\infty}^{\infty} \frac{U^0(\rho) - U^0(-\infty)}{Q(U^0, V^0)}\, d\rho\right] + \mathcal{K}^{3/2}\int_{-\infty}^{\infty} \{(U^0_\rho)^2 + (V^0_\rho)^2\}\, d\rho. \tag{4.28}$$

4.2 The inner solution for interphase boundaries.

Proceeding as in the case of antiphase boundaries, but with the assumption now that

$$\mathcal{K} = \epsilon^{-1/2}\mathcal{K}^{-1/2} + \mathcal{K}^0 + \epsilon^{1/2}\mathcal{K}^{1/2} + \epsilon\mathcal{K} + \epsilon^{3/2}\mathcal{K}^{3/2} + \mathcal{O}(\epsilon^2),$$

similar expansions are assumed for U, V, and W as in §4.1, and the equations of evolution at the various asymptotic levels are found.

At $\mathcal{O}(\epsilon^{-1})$,

$$0 = 4(Q(U^0, V^0)\mu^0_\rho)_\rho,$$

which integrated yields

$$Q(U^0, V^0)\mu^0_\rho = b(s, t).$$

Matching the mass flux in the inner region with the mass flux in the outer region, gives $b(s, \tau) = 0$. Assuming as in §4.1 that $Q(U^0, V^0)$ is non-vanishing almost everywhere in the inner region then yields that $\mu^0_\rho = 0$, or integrating

$$\mu^0 = c(s, t). \tag{4.29}$$

At $\mathcal{O}(\epsilon^{-1/2})$, using (4.29)

$$0 = 4(Q(U^0, V^0)\mu^{1/2}_\rho)_\rho.$$

Following the steps of the $\mathcal{O}(\epsilon^{-1})$ analysis, we obtain here similarly

$$\mu^{1/2} = d(s, t). \tag{4.30}$$

At $\mathcal{O}(1)$, by (4.29) and (4.30)

$$0 = 4(Q(U^0, V^0)\mu^1_\rho)_\rho \tag{4.31}$$

$$\mu^0 = F_U(U^0, V^0) - U^0_{\rho\rho} \tag{4.32}$$

$$0 = -\frac{1}{4}Q(U^0, V^0)[F_V(U^0, V^0) - V^0_{\rho\rho}]. \tag{4.33}$$

From (4.31), by integrating and matching with the fluxes of the outer solution

$$n \cdot j^0 = Q(U^0, V^0)\mu^1_\rho = e(s, t),$$

where $e(s, t)$ is $\mathcal{O}(e^{-c/\epsilon^{1/2}})$. Noting that $Q(U^0, V^0)$ is also $T.S.T.$ in the limit $\rho \to \pm\infty$ and matching the chemical potential with the chemical potential in the outer region yields that $e(s, t) = 0$. Assuming that $Q(U^0, V^0)$ does not vanish almost everywhere in the inner region, (4.32)-(4.33) reduce to

$$\mu^0 = F_U(U^0, V^0) - U^0_{\rho\rho} \tag{4.34}$$

$$0 = F_V(U^0, V^0) - V^0_{\rho\rho}. \tag{4.35}$$

Matching the chemical potential with the chemical potential in the outer region,

$$\mu^0 = c(s, t) = 0, \tag{4.36}$$

and (4.34)-(4.35) determine the heteroclinic orbit prescribed by $(U^0,\, V^0)$.

At $\mathcal{O}(\epsilon^{1/2})$,

$$0 = 4(Q(U^0,\, V^0)\mu_\rho^{3/2})_\rho \tag{4.37}$$

$$\mu^{1/2} = F_{UU}U^{1/2} + F_{UV}V^{1/2} - U_{\rho\rho}^{1/2} - \mathcal{K}^{-1/2}U_\rho^0 \tag{4.38}$$

$$0 = -\frac{1}{4}Q(U^0,\, V^0)[F_{UV}U^{1/2} + F_{VV}V^{1/2} - V_{\rho\rho}^{1/2} - \mathcal{K}^{-1/2}V_\rho^0]. \tag{4.39}$$

From (4.37),

$$Q(U^0,\, V^0)\mu_\rho^{3/2} = f(s,\, t)$$

where $f(s,\, t)$ is $T.S.T.$. From (4.38) and (4.39) and the null-adjoint condition,

$$\mu^{1/2} = -\frac{\mathcal{K}^{-1/2}}{[U^0]_-^+}\int_{-\infty}^{\infty}\{(U_\rho^0)^2 + (V_\rho^0)^2\}\, d\rho. \tag{4.40}$$

At $\mathcal{O}(\epsilon)$,

$$0 = 4\Big[Q(U^0,\, V^0)\mu_\rho^2 + (Q_U(U^0,\, V^0)U^{1/2} + Q_V(U^0,\, V^0)V^{1/2})\mu_\rho^{3/2}\Big]_\rho. \tag{4.41}$$

Integrating (4.41) and matching the fluxes with the outer region

$$Q(U^0,\, V^0)\mu_\rho^2 + (Q_U(U^0,\, V^0)U^{1/2} + Q_V(U^0,\, V^0)V^{1/2})\mu_\rho^{3/2} = h(s,\, t) \tag{4.42}$$

where $h(s,\, t)$ is $T.S.T.$.

At $\mathcal{O}(\epsilon^{3/2})$, from (4.36)

$$-W^0U_\rho^0 = 4(n\cdot j^{3/2})_\rho + 4Q(U^0,\, V^0)\,\triangle_s\mu^{1/2}. \tag{4.43}$$

Integrating (4.43) between $-\epsilon^{-1/4}$ and $\epsilon^{1/4}$ and matching with the outer solution, and using (4.40)

$$W^0 = -\frac{4\triangle_s\mathcal{K}^{-1/2}}{([U^0]_-^+)^2}\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} Q(U^0,\, V^0)\, d\rho\cdot\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}}\{(U_\rho^0)^2 + (V_\rho^0)^2\}\, d\rho + T.S.T., \tag{4.44}$$

which to lowest order may be written

$$W^0 = -\frac{4\triangle_s\mathcal{K}^{-1/2}}{\{[U^0]_-^+\}^2}\int_{-\infty}^{\infty} Q(U^0,\, V^0)\, d\rho\cdot\int_{-\infty}^{\infty}\{(U_\rho^0)^2 + (V_\rho^0)^2\}\, d\rho. \tag{4.45}$$

5 Triple-junction conditions.

5.1 Youngs law.

In this section, Young's law is derived $\mathcal{O}(\epsilon^{1/2})$ accuracy. Our analysis here follows closely the analysis presented in [8]. The stretched variable

$$\eta = \frac{x - m(t)}{\epsilon}$$

is introduced, where $m(t)$ denotes the location of the triple-junction. The index i refers to one of the three interfaces Γ_i which meet at the triple-junction. For convenience, we denote the antiphase boundary by Γ_1 and the interphase boundaries which meet at the triple-junction by Γ_2 and Γ_3. An isosceles triangle R_ϵ with base length proportional to ϵ^β, $1/2 < \beta < 1$ is constructed at the triple-junction, such that its base is orthogonal to Γ_i, $i = 1, 2,$ or 3. Here we set $\eta_i = (\xi_i, \zeta_i)$, where ξ_i is orthogonal to Γ_i and ζ_i is tangent to Γ_i. See Fig. 5.i. In terms of this notation, equations (2.10)-(2.11) may be written as

$$\mu = F_U(U, V) - \triangle_\eta U$$
$$\epsilon^{7/2} V_t = -\tfrac{1}{4} Q(U, V)[F_V(U, V) - \triangle_\eta V].$$

Figure 5.i: The T_ϵ construction used at the triple-junction.

Noting that

$$\epsilon^{7/2} V_t = -\epsilon^{5/2} \nabla_\eta V \cdot m'(t) + \epsilon^{7/2} \frac{\partial V}{\partial t},$$

the above equations may be written as

$$\mu = F_U(U,V) - \triangle_\eta U \tag{5.1}$$

$$0 = -\tfrac{1}{4}Q(U,V)[F_V(U,V) - \triangle_\eta V] + \mathcal{O}(\epsilon^2). \tag{5.2}$$

Examining equation (5.2), clearly either $Q(U,V)$ must vanish or else $F_V(U,V) - \triangle_\eta V = 0$. However, since the roots of $Q(U,V)$ lie at the points $(\frac{1}{2}, \pm\frac{1}{2})$, $(1,0)$, $(0,0)$ and since the solution in the transitional region contained in the triangle under consideration must connect the minimizers of $F(U,V)$ which lie transcendentally close to points at which $Q(U,V)$ vanishes, we may assume that $Q(U,V) \neq 0$ almost everywhere within this transition region, and hence (5.1)-(5.2) may be written as

$$\begin{pmatrix} \mu \\ 0 \end{pmatrix} = \nabla_U F(U) - \triangle_\eta U + \mathcal{O}(\epsilon^2), \tag{5.3}$$

where $U = \begin{pmatrix} U \\ V \end{pmatrix}$. Following the expansions employed in §4, set

$$U = U^0 + \epsilon^{1/2}U^{1/2} + \epsilon U^1 + \epsilon^{3/2}U^{3/2} + \mathcal{O}(\epsilon^2)$$

$$V = V^0 + \epsilon^{1/2}V^{1/2} + \epsilon V^1 + \epsilon^{3/2}V^{3/2} + \mathcal{O}(\epsilon^2)$$

$$\mu = \epsilon^{1/2}\mu^{1/2} + \epsilon\mu^1 + \epsilon^{3/2}\mu^{3/2} + \mathcal{O}(\epsilon^2)$$

and

$$W = W^0 + \epsilon^{1/2}W^{1/2} + \epsilon W^1 + \epsilon^{3/2}W^{3/2} + \mathcal{O}(\epsilon^2).$$

To obtain Young's law, we multiply (5.3) by $\partial_{\xi_1} U$ and integrate over the triangle T_ϵ

$$\int_{T_\epsilon} \partial_{\xi_1} U \cdot \begin{pmatrix} \mu \\ 0 \end{pmatrix} dA = \int_{T_\epsilon} [\partial_{\xi_1} U \cdot \nabla_U F(U) - \partial_{\xi_1} U \cdot \triangle_{\eta_1} U]\, dA + \mathcal{O}(\epsilon^{2(1+\beta)}),$$

which, following [8] may be written as

$$\int_{T_\epsilon} \partial_{\xi_1} U \cdot \begin{pmatrix} \mu \\ 0 \end{pmatrix} dA = \int_{T_\epsilon} \partial_{\xi_1} [F(U) + \frac{1}{2}|\partial_{\zeta_1} U|^2 - \frac{1}{2}|\partial_{\xi_1} U|^2]\, dA - \int_{T_\epsilon} \partial_{\zeta_1}(\partial_{\xi_1} U \cdot \partial_{\zeta_1} U)\, dA. \tag{5.4}$$

Noting that

$$\int_{T_\epsilon} \partial_{\xi_1} U \cdot \begin{pmatrix} \mu \\ 0 \end{pmatrix} dA = \epsilon^{1/2} \int_{T_\epsilon} [\partial_{\xi_1} U^0]\mu^{1/2}\, dA + \mathcal{O}(\epsilon^{(1+2\beta)}),$$

it follows by writing (5.4) schematically as $I = II$ and employing Gauss's theorem that

$$0 = \mathcal{J} \equiv II - I = \epsilon \int_{\partial T_\epsilon} [F(U) - \mu U + \frac{1}{2}|\partial_{\zeta_1} U|^2 - \frac{1}{2}|\partial_{\xi_1} U|^2]\, \nu_1\, ds - \epsilon \int_{\partial T_\epsilon} [\partial_{\xi_1} U \cdot \partial_{\zeta_1} U]\, \nu_2\, ds + \mathcal{O}(\epsilon^{1+2\beta}),$$

where $\nu = (\nu_1, \nu_2)$ is the unit exterior normal to T_ϵ and ds indicates counterclockwise integration around the periphery of the triangle T_ϵ. From here, following the discussion in [8], it is possible to conclude that

$$0 = 2\cos\gamma_2 \int_{-\infty}^{\infty} F(U(\xi_2), V(\xi_2))\, d\xi_2$$

$$+ 2\cos\gamma_3 \int_{-\infty}^{\infty} F(U(\xi_3),\, V(\xi_3))\, d\xi_3 + o(1). \tag{5.5}$$

Introducing the notation

$$E_i = \int_{-\infty}^{\infty} F(U(\xi_i),\, V(\xi_i))\, d\xi_i,$$

(5.5) may be written as

$$0 = \cos\gamma_2 E_2 + \cos\gamma_3 E_3 + o(1). \tag{5.6}$$

Rotating the axes and undertaking the same analysis again,

$$0 = \cos\gamma_3 E_3 + \cos\gamma_1 E_1 + o(1), \tag{5.7}$$

and

$$0 = \cos\gamma_1 E_1 + \cos\gamma_2 E_2 + o(1). \tag{5.8}$$

Since E_2 and E_3 both represent interfacial energies for IPBs, clearly

$$E_2 = E_3$$

from which it follows that

$$\gamma_2 + \gamma_3 = \pi. \tag{5.9}$$

A special case to consider is the completely wetting case in which

$$E_2 = E_3 = \frac{1}{2} E_1,$$

which by (5.6)-(5.8) implies

$$\gamma_1 = \frac{3\pi}{2} \text{ and } \gamma_2 = \gamma_3 = \frac{\pi}{2}.$$

5.2 The balance of fluxes.

In this subsection, equation (2.9) and the construction presented in §5.1 are employed to derive a "balance of flux" or "mass balance" condition at the triple-junction. Thus the stretched coordinates,

$$\eta = \frac{x - m(t)}{\epsilon}$$

are introduced, where $m(t)$ denotes the location of the triple-junction, and $\eta = (\xi_i,\, \zeta_i)$ where ζ_i is tangent to Γ_i, ξ_i is perpendicular to Γ_i, and T_ϵ is an isosceles triangle whose sides are proportional to ϵ^β, $1/2 < \beta < 1$ and whose base is perpendicular to Γ_1 where Γ_1 corresponds to the APB separating the two ordered variants. Thus, in the present construction the isosceles triangle has a fixed orientation relative to the three phases which meet at the triple-junction. Here θ is the angle at base of the isosceles triangle, and recall that by (5.9)

$$\gamma_3 = \pi - \gamma_2, \tag{5.10}$$

where $\gamma_3(\gamma_2)$ is the angle between Γ_3 (Γ_2) and the ξ_1-axis. See Fig. 5.i.

Within the triple-junction region, a solution is sought of the form

$$U = U^0(\eta_1,\, t) + \epsilon^{1/2} U^{1/2}(\eta_1,\, t) + \mathcal{O}(\epsilon),$$

$$V = V^0(\eta_1,\, t) + \epsilon^{1/2} V^{1/2}(\eta_1,\, t) + \mathcal{O}(\epsilon),$$

$$\mu = \epsilon^{1/2} \mu^{1/2}(\eta_1,\, t) + \mathcal{O}(\epsilon),$$

and we write (2.9) as

$$-\epsilon^{3/2}\, m'(t) \cdot \nabla_{\eta_1} U = -\nabla_{\eta_1} \cdot j + \mathcal{O}(\epsilon^2), \tag{5.11}$$

where, in accordance with the behavior of the normal velocities seen in §5, it is assumed that $m'(t) = \mathcal{O}(1)$.

Integrating (5.11) over the isosceles triangle T_ϵ

$$-\epsilon^{3/2}\, m'(t) \cdot \int_{T_\epsilon} \nabla_{\eta_1} U \, dA = -\int_{T_\epsilon} \nabla_{\eta_1} \cdot j \, dA + \mathcal{O}(\epsilon^{2(1+\beta)}),$$

and using Gauss' theorem and the divergence theorem,

$$-\epsilon^{5/2}\, m'(t) \cdot \int_{\partial T_\epsilon} \nu U \, ds = -\epsilon \int_{\partial T_\epsilon} \nu \cdot j \, ds + \mathcal{O}(\epsilon^{2(1+\beta)}), \tag{5.12}$$

where $\nu = (\nu_1,\, \nu_2)$ is the unit exterior normal to T_ϵ. Let us parametrize the contributions to these integrals by expressing them in terms of the $(\xi_1,\, \zeta_1)$ coordinates. Denoting the integral on the l.h.s. of (5.12) as I and the integral on the r.h.s. of (5.12) as II, each of these integrals is evaluated by examining the contributions over the three sides ∂T_{bottom}, ∂T_{left}, and ∂T_{right} of the triangle T_ϵ.

The integral II is treated first. Using the above construction it is easy to check that

$$\int_{\partial T_{bottom}} \nu \cdot j \, ds = \int_{A_1}^{A_2} \hat{e}_{\zeta_1} \cdot j \, ds, \tag{5.13}$$

$$\int_{\partial T_{right}} \nu \cdot j \, ds = \int_{A_2}^{A_3} \left[-\frac{\cos(\gamma_2 + \theta)}{\sin(\gamma_2 + \theta)}\, \hat{e}_{\xi_2} \cdot j + \hat{e}_{\zeta_2} \cdot j \right] ds, \tag{5.14}$$

$$\int_{\partial T_{left}} \nu \cdot j \, ds = \int_{A_3}^{A_1} \left[\frac{\cos(\gamma_3 - \theta)}{\sin(\gamma_3 - \theta)}\, \hat{e}_{\xi_3} \cdot j + \hat{e}_{\zeta_3} \cdot j \right] ds, \tag{5.15}$$

where for $i = 1, 2, 3$, A_i is the vertex of the triangle T_ϵ opposite the angle θ_i. Noting now that since it was shown in §4 that both for APB and for IPB interfaces Γ_i, $\mu^{1/2}$, μ^1, and $\mu^{3/2}$ are all functions of s and t only,

$$j = -Q(U^0,\, V^0) \nabla \mu = -\epsilon^{1/2} Q(U^0,\, V^0) \mu_s^{1/2}(0+,\, t) \hat{e}_{\xi_i} + \mathcal{O}(\epsilon^1), \tag{5.16}$$

it follows from (5.13)-(5.15) that

$$\lim_{\epsilon \to 0} \int_{\partial T_{bottom}} \nu \cdot j \, ds = -\epsilon^{3/2} \frac{\partial}{\partial s_1} \mu_1^{1/2}(0+,\, t) \int_{-\infty}^{\infty} Q(U^0(\xi_1),\, V^0(\xi_1))\, d\xi_1 + \mathcal{O}(\epsilon^{(1+\beta)}), \tag{5.17}$$

$$\lim_{R\to\infty}\int_{\partial T_{right}} \nu\cdot j\, ds = -\epsilon^{3/2}\frac{\partial}{\partial s_2}\mu_2^{1/2}(0+,\,t)\int_{-\infty}^{\infty} Q(U^0(\xi_2),\,V^0(\xi_2))\,d\xi_2 + \mathcal{O}(\epsilon^{(1+\beta)}), \tag{5.18}$$

and

$$\lim_{R\to\infty}\int_{\partial T_{left}} \nu\cdot j\, ds = -\epsilon^{3/2}\frac{\partial}{\partial s_3}\mu_3^{1/2}(0+,\,t)\int_{-\infty}^{\infty} Q(U^0(\xi_3),\,V^0(\xi_3))\,d\xi_3 + \mathcal{O}(\epsilon^{(1+\beta)}), \tag{5.19}$$

where by the subscript i, it is implied that $\mu_i^{1/2}$ has been obtained by matching the transition layer solutions with the "outer" transition layer around the Γ_i interface and s_i corresponds to an arc-length parametrization along the Γ_i interface. Defining,

$$M^0_{APB} = \int_{-\infty}^{\infty} Q(U^0(\xi_1),\,V^0(\xi_1))\,d\xi_1$$

and

$$M^0_{IPB} = \int_{-\infty}^{\infty} Q(U^0(\xi_2),\,V^0(\xi_2))\,d\xi_2 = \int_{-\infty}^{\infty} Q(U^0(\xi_3),\,V^0(\xi_3))\,d\xi_3,$$

$$II = \epsilon^{5/2}M^0_{APB}\frac{\partial}{\partial s_1}\mu_1^{1/2}(0+,\,t) + \epsilon^{5/2}M^0_{IPB}\left[\frac{\partial}{\partial s_2}\mu_2^{1/2}(0+,\,t) + \frac{\partial}{\partial s_3}\mu_3^{1/2}(0+,\,t)\right] + o(\epsilon^{5/2}). \tag{5.20}$$

Returning now to the integral I, we evaluate the contributions to I from each of the sides of the isosceles triangle T_ϵ. Using the same parametrization as before

$$I = -\epsilon^{5/2}m'\cdot\int_{\partial R_\epsilon}\nu U^0\, ds$$

$$= -\epsilon^{5/2}m'\cdot\int_{\partial R_{bottom}}\nu U^0\, ds - \epsilon^{5/2}m'\cdot\int_{\partial R_{right}}\nu U^0\, ds - \epsilon^{5/2}m'\cdot\int_{\partial R_{left}}\nu U^0\, ds + o(\epsilon^{5/2}). \tag{5.21}$$

Noting that all contributions to I are $\mathcal{O}(\epsilon^{5/2+\beta})$, and returning and noting that $II = \mathcal{O}(\epsilon^{5/2})$, we see that $I = o(II)$. Hence to lowest order the balance of fluxes at the triple junction may be expressed as

$$0 = M^0_{APB}\frac{\partial}{\partial s_1}\mu_1^{1/2}(0+,\,t) + M^0_{IPB}\left[\frac{\partial}{\partial s_2}\mu_2^{1/2}(0+,\,t) + \frac{\partial}{\partial s_3}\mu_3^{1/2}(0+,\,t)\right]. \tag{5.22}$$

5.3 Continuity of the chemical potential.

Under the assumption that the chemical potential is continuous at the triple-junction, it is possible to demonstrate that the sum of the curvatures of the two interphase boundaries which meet at the triple-junction should vanish. This is accomplished as follows. Recall that by equation (4.40)

$$\mu^{1/2}[U^0(+\infty) - U^0(-\infty)] = -\mathcal{K}^{-1/2}\int_{-\infty}^{\infty}\{(U^0_\rho)^2 + (V^0_\rho)^2\}\,d\rho.$$

Thus, summing together the two equations of this sort which arise along the interphase boundaries which meet at a triple-junction, and noting that the energy per unit length along each interface

are identical by construction and that the rôles of $U^0(+\infty)$ and $U^0(-\infty)$ are exchanged as we pass from one IPB to the other, it is readily seen that

$$\sum_{i=1}^{2} \mathcal{K}_i^{-1/2} = 0 \tag{5.23}$$

where $\mathcal{K}_i^{-1/2}$, $i = 2, 3$ denote the mean curvatures of the two IPB's. Note further that continuity of the chemical potential yields that

$$d(0+, t) = \mu^{1/2}(0+, t)$$

where $\mu^{1/2}(0+, t)$ is determined by (4.40).

6 Conditions at junctions with the external boundary.

In this section conditions are developed which must hold at points of intersection of APBs and IPBs with the external boundary of the domain, $\partial\Omega$. As was the case with the conditions at the triple-junction, it is convenient to look for Neumann type conditions and balance of flux conditions separately.

6.1 The Neumann type condition.

The analysis here follows closely the analysis undertaken in §5.1. See also the discussion in [31]. Let

$$\eta = \frac{x - m(t)}{\epsilon}, \tag{6.24}$$

where $m(t)$ is the point of intersection of an interface Γ (either an APB or an IBP) with the external boundary, and set

$$\eta = (\xi, \zeta),$$

where ξ is the component of η which is tangent to the interface at the point $m(t)$ and ζ is the component of the vector η which is normal to the interface at the point $m(t)$, and a rectangle R_ϵ of fixed proportions and with sides proportional to ϵ^β where $1/2 < \beta < 1$ is constructed with the point $m(t)$ at the center of its lower side. The sides of the rectangle R_ϵ are denoted respectively by ∂R_{bottom}, ∂R_{left}, ∂R_{top}, and ∂R_{right}, see Fig. 6.i.

Following the discussion in §4, let us rewrite the second and third equations of the scaled Allen-Cahn/Cahn-Hilliard system (2.10)-(2.11) as

$$\begin{pmatrix} \mu \\ 0 \end{pmatrix} = \nabla_U F(U) - \triangle_\eta U + \mathcal{O}(\epsilon^2), \tag{6.25}$$

Figure 6.i: The R_ϵ construction used at points of intersection of APBs and IPBs with the external boundary.

where $U = \begin{pmatrix} U \\ V \end{pmatrix}$. In accordance with the behavior of the inner solutions, it is assumed that within the transitional region,

$$U = U^0 + \epsilon^{1/2} U^{1/2} + \epsilon U^1 + \epsilon^{3/2} U^{3/2} + \mathcal{O}(\epsilon^2)$$
$$V = V^0 + \epsilon^{1/2} V^{1/2} + \epsilon V^1 + \epsilon^{3/2} V^{3/2} + \mathcal{O}(\epsilon^2)$$

and

$$\mu = \epsilon^{1/2}\mu^{1/2} + \epsilon\mu + \epsilon^{3/2}\mu^{3/2} + \mathcal{O}(\epsilon^2).$$

To proceed, multiply (6.25) by $\partial_{\tau_\eta} U$, where τ denotes the unit vector which is tangent to $\partial\Omega$ at the point $m(t)$ and τ_η denotes a variable which is parallel to τ and scaled as η, and integrate over the rectangle R_ϵ.

$$\int_{R_\epsilon} \partial_{\tau_\eta} U \cdot \begin{pmatrix} \mu \\ 0 \end{pmatrix} dA = \int_{R_\epsilon} \partial_{\tau_\eta} U \cdot [\nabla_U F(U) - \triangle_\eta U]\, dA + \mathcal{O}(\epsilon^{2(1+\beta)}). \tag{6.26}$$

Noting that

$$\mu = \epsilon^{1/2}\mu^{1/2}(s,\, t) + \epsilon\mu^1(s,\, t) + \mathcal{O}(\epsilon^{3/2}) = \mu(0+, t) + \mathcal{O}(\epsilon^{3/2}),$$

it follows that

$$\int_{R_\epsilon} \partial_{\tau_\eta} U \cdot \begin{pmatrix} \mu \\ 0 \end{pmatrix} dA = \int_{R_\epsilon} \partial_{\tau_\eta}(\mu U)\, dA + \mathcal{O}(\epsilon^{3/2+2\beta}).$$

Hence (6.26) may be written as

$$0 = \mathcal{J} \equiv \int_{R_\epsilon} \partial_{\tau_\eta} U \cdot [\nabla_U (F(U) - \mu U) - \triangle_\eta U]\, dA + \mathcal{O}(\epsilon^{3/2+2\beta}). \tag{6.27}$$

The treatment of the integral $\mathcal{J}$ is similar to the asymptotic analysis which appears in §5.1. Thus we write $\mathcal{J}$ as

$$\mathcal{J} = \int_{R_\epsilon} \partial_{\tau_\eta} \Big[F(U) + \mu U + \frac{1}{2} |\partial_{\tau_\eta} U|^2 - \frac{1}{2} |\partial_{n_\eta} U|^2 \Big]\, dA - \int_{R_\epsilon} \partial_{n_\eta} (\partial_{\tau_\eta} U \cdot \partial_{n_\eta} U)\, dA + \mathcal{O}(\epsilon^{3/2+2\beta}),$$

where n denotes the unit exterior normal to $\partial\Omega$ at $m(t)$ and n_η denotes a variable parallel to n and varying on the η-scale. By Gauss' theorem

$$\mathcal{J} = \epsilon \int_{\partial R_\epsilon} \Big[F(U) - \mu U + \frac{1}{2} |\partial_{\tau_\eta} U|^2 - \frac{1}{2} |\partial_{n_\eta} U|^2 \Big] \tau \cdot \nu\, ds - \epsilon \int_{\partial R_\epsilon} \Big[\partial_{\tau_\eta} U \cdot \partial_{n_\eta} U \Big] n \cdot \nu\, ds + \mathcal{O}(\epsilon^{3/2+2\beta}), \tag{6.28}$$

where $\nu = (\nu_1, \nu_2)$ denotes the outward unit normal to ∂R_ϵ. All contributions to these integrals along the boundary ∂R_ϵ vanish except in an $(-\alpha, \alpha)$ neighborhood of the point, taken to be unique, where Γ intersects ∂R_{top} and ∂R_{bottom}. For simplicity, α is taken to be proportional to ϵ^β. Other contributions are $\mathcal{O}(\epsilon^{1/2+\beta})$ as we are essentially in the outer region where $\partial_\xi U = \partial_\zeta U = 0$ and $F(U) - \mu U = a_i(t) + \mathcal{O}(\epsilon^2)$ where $a_i(t) = \mathcal{O}(\epsilon^{1/2})$ and the value of $a_i(t)$ depends on whether it corresponds to one of the two ordered variants, or to the disordered phase. Moreover, since $\tau \cdot \nu = 0$ along ∂R_{top} and ∂R_{bottom}, only the second integral in $\mathcal{J}$ as written above is non-vanishing. In this remaining integral, let us denote the two non-vanishing components as

$$\mathcal{J} = \mathcal{J}_{top} + \mathcal{J}_{bottom}.$$

Since the Neumann boundary conditions imply that $\partial_n U = 0$ along $\partial\Omega$, the contribution $\mathcal{J}_{bottom}$ vanishes leaving only the contribution to $\mathcal{J}_{top}$ to evaluate.

To this end, note that along ∂R_{top}

$$\nu = \cos\theta\ \hat{e}_\xi + \sin\theta\ \hat{e}_\zeta,$$

and $\nu = -n$ along ∂R_{top}. Furthermore,

$$\partial_{n_\eta} U = -\cos\theta\ U_\xi - \sin\theta\ U_\zeta,$$

$$\partial_{\tau_\eta} U = \sin\theta\ U_\xi - \cos\theta\ U_\zeta.$$

Hence, changing variables by setting $ds = -\epsilon \sin\theta\, d\xi$,

$$\mathcal{J} = \epsilon^2 \int_{-\alpha/\epsilon}^{\alpha/\epsilon} \Big[-\frac{1}{2} \sin 2\theta\, |U_\xi|^2 + \cos 2\theta\ U_\xi \cdot U_\zeta + \frac{1}{2} \sin 2\theta\, |U_\zeta|^2 \Big] \sin\theta\, d\xi + \mathcal{O}(\epsilon^{3/2+\beta}).$$

To evaluate this term, note that it follows from §4 that U is of the form

$$U = U^0(\xi) + \mathcal{O}(\epsilon^{1/2}).$$

Similarly,

$$\theta(\epsilon) = \theta^0 + \mathcal{O}(\epsilon^{1/2}). \tag{6.29}$$

Therefore,

$$\mathcal{J} = \frac{1}{2}\epsilon^2 \sin 2\theta^0 \sin\theta^0 \int_{-\infty}^{\infty} |U_\xi^0|^2 \, d\xi + \mathcal{O}(\epsilon^{1/2+\beta}). \tag{6.30}$$

Since the integral in (6.30) may be assumed to be non-vanishing and since both u and v satisfy Neumann boundary conditions along the external boundary, we obtain from (6.30) that

$$\theta = \frac{1}{2}\pi + \mathcal{O}(\epsilon^{\beta-1/2}). \tag{6.31}$$

Hence to lowest order

$$\theta = \frac{1}{2}\pi. \tag{6.32}$$

6.2 The flux condition.

At this point we reintroduce the rectangle R_ϵ and the variable $\eta = (\xi, \zeta)$ constructed in §6.1, and write equation (2.8) as

$$-\epsilon^{3/2}\, m'(t) \cdot \nabla_\eta U = -\nabla_\eta \cdot j + \mathcal{O}(\epsilon^2). \tag{6.33}$$

Similarly, we set

$$U = U^0 + \epsilon^{1/2} U^{1/2} + \mathcal{O}(\epsilon)$$
$$V = V^0 + \epsilon^{1/2} V^{1/2} + \mathcal{O}(\epsilon),$$

and

$$\mu = \epsilon^{1/2}\mu^{1/2} + \mathcal{O}(\epsilon).$$

In accordance with the behavior of the normal velocity of the IPB and APB interfaces, it is assumed that $m'(t) = \mathcal{O}(1)$. Integrating equation (6.33) over the rectangle R_ϵ,

$$-\epsilon^{3/2}\, m'(t) \cdot \int_{R_\epsilon} \nabla_\eta U \, dA = \int_{R_\epsilon} \nabla_\eta \cdot j \, dA + \mathcal{O}(\epsilon^{2(1+\beta)}). \tag{6.34}$$

By Gauss' theorem and the divergence theorem, (6.34) becomes

$$-\epsilon^{5/2}\, m'(t) \cdot \int_{\partial R_\epsilon} \nu U^0 \, ds = \epsilon \int_{\partial R_\epsilon} \nu \cdot j \, ds + \mathcal{O}(\epsilon^{2(1+\beta)}) \tag{6.35}$$

where as in §6.1, ν denote the unit exterior normal to R_ϵ. Denoting the l.h.s. of (6.35) by I and the r.h.s. of (6.35) by II, we evaluate the various contributions. To this end, we set

$$II = \int_{\partial R_{bottom}} + \int_{\partial R_{left}} + \int_{\partial R_{top}} + \int_{\partial R_{right}}.$$

By the no flux boundary condition

$$\int_{\partial R_{bottom}} \nu \cdot j \, ds = 0.$$

Similarly, the terms

$$\int_{\partial R_{left}} \nu \cdot j \, ds \quad \text{and} \quad \int_{\partial R_{right}} \nu \cdot j \, ds$$

are vanishingly small as $\epsilon \to 0$ since these correspond to contributions evaluated in the outer region where $j = T.S.T.$. Looking lastly at the remaining contribution which arises from ∂R_{top}, clearly away from an interval of width 2α around the point where Γ intersects the top section of the rectangle, the rectangle is in the outer region where the flux is transcendentally small and hence there is no non-neglible contribution. Using the notation $\nu = (\cos\theta, \sin\theta)$ and $ds = \epsilon \sin\theta d\xi$ introduced in §6.1 and recalling that

$$j = Q(U^0, V^0)\nabla\mu = \epsilon^{1/2} Q(U^0(\xi), V^0(\xi))\mu_s^{1/2}(0+, t)\hat{e}_\xi + \mathcal{O}(\epsilon),$$

it follows that

$$II = \epsilon^{5/2} \sin^2\theta \mu_s^{1/2}(0+, t) \int_{-\alpha/\epsilon}^{\alpha/\epsilon} Q(U^0(\xi), V^0(\xi))\, d\xi + \mathcal{O}(\epsilon^{(2+\beta)}).$$

Since by (6.31),

$$\cos\theta = \mathcal{O}(\epsilon^{1/2}) \text{ and } \quad \sin\theta = 1 + \mathcal{O}(\epsilon^{1/2}),$$

we find now that

$$II = \epsilon^{5/2} \mu_s^{1/2}(0+, t) \int_{-\alpha/\epsilon}^{\alpha/\epsilon} Q(U^0(\xi), V^0(\xi))\, d\xi + o(\epsilon^{5/2}). \tag{6.36}$$

It remains to examine the integral I. Clearly by (6.35), $I = \mathcal{O}(\epsilon^{5/2+\beta})$. Since $II = \mathcal{O}(\epsilon^{5/2})$, it follows that $I = o(II)$, and returning to (6.36), we see that for both APB and IPB interfaces,

$$\frac{\partial}{\partial s}\mu^{1/2}(0+, t) = 0. \tag{6.37}$$

For IPB interfaces, this implies that

$$\mathcal{K}_s^{1/2}(0+, t) = 0, \tag{6.38}$$

and for APB interfaces, this yields

$$d_s(0+, t) = 0. \tag{6.39}$$

7 Summary.

In summary, it has been shown in the previous sections under the assumption that time scales like $\tau = \epsilon^{7/2} t$ and that the curvatures of the APBs and IPBs scale like $\epsilon^{3/2}$ and $\epsilon^{-1/2}$ respectively, that the limiting equations of motion are given by

$$W^0 = c_1 \mathcal{K}^{3/2} \text{ and } \frac{\partial^2}{\partial s^2}\mu^{1/2} = 0 \quad \text{along APBs,} \tag{7.40}$$

$$W^0 = -c_2 \frac{\partial^2 \mathcal{K}^{-1/2}}{\partial s^2} \text{ and } \mathcal{K}^{-1/2} = -\gamma_1 \mu^{1/2} \quad \text{along IPBs,} \tag{7.41}$$

where

$$c_1 = \frac{\int_{-\infty}^{\infty} \{(U_\rho^0)^2 + (V_\rho^0)^2\}\, d\rho}{\int_{-\infty}^{\infty} \frac{4(V_\rho^0)^2}{Q(U^0, V^0)}\, d\rho + \int_{-\infty}^{\infty} \frac{U^0(\rho) - U^0(-\infty)}{Q(U^0, V^0)}\, d\rho},$$

$$c_2 = \frac{4}{\{[U^0]_-^+\}^2} \int_{-\infty}^{\infty} Q(U^0, V^0)\, d\rho \cdot \int_{-\infty}^{\infty} \{(U_\rho^0)^2 + (V_\rho^0)^2\}\, d\rho,$$

and

$$\gamma_1 = [U^0]_-^+ \left[\int_{-\infty}^{\infty} \{(U_\rho^0)^2 + (V_\rho^0)^2\}\, d\rho \right]^{-1}.$$

At triple-junctions:

$$\text{Young's law:} \quad \tfrac{E_1}{\sin\theta_1} = \tfrac{E_2}{\sin\theta_2} = \tfrac{E_3}{\sin\theta_3} \quad E_i = \textstyle\int_{-\infty}^{\infty} F(U(\xi_i), V(\xi_i)) d\xi_i \tag{7.42}$$

$$\text{Balance of fluxes:} \quad \tfrac{\partial \mathcal{K}_1^{-1/2}}{\partial s_1}(0+, t) + \tfrac{\partial \mathcal{K}_2^{-1/2}}{\partial s_2}(0+, t) = \gamma_1 \tfrac{\partial \mu^{1/2}}{\partial s_3}(0+, t) \tag{7.43}$$

$$\text{Continuity of chemical potential:} \quad \mu_1^{1/2}(0+, t) = \mu_2^{1/2}(0+, t) = \mu_3^{1/2}(0+, t) \tag{7.44}$$

$$\text{A kinetic constraint:} \quad \text{Persistence of triple-junctions.} \tag{7.45}$$

At points of contact of interfaces with the external boundary $\partial\Omega$:

$$\text{APBs and IPBs intersect the external boundary at } \pi/2. \tag{7.46}$$

$$\frac{\partial \mu^{1/2}}{\partial s} = 0 \quad \text{along APBs} \quad \text{and} \quad \frac{\partial \mathcal{K}^{-1/2}}{\partial s} = 0 \quad \text{along IPBs.} \tag{7.47}$$

$$\text{APBs and IPBs do not detach from the external boundary.} \tag{7.48}$$

Certain properties of the limiting system are easy to ascertain. In particular,

Lemma 7.1 The area of the disordered phase is conserved.

Proof of Lemma 7.1

Recall [28] that if $r(t)$ is a closed curve, then

$$\dot{A} = \int_{r(t)} V\, ds, \tag{7.49}$$

where A is the area enclosed by the curve $r(t)$. From the information given in §2, disordered regions are considered to be bounded by a finite number of curves, connecting triple-junctions and points on the exterior boundary. These bounding curves must either be IPBs or segments of the exterior boundary. Let us denote by r^i_{IPB} for $i \in I_{IPB}$ the set of interphase boundary curves. Furthermore, let us denote by $A_{disordered}$ the total area of the disordered regions. For simplicity, the perturbational indices on $\mathcal{K}$ and μ will not be indicated.

Employing (7.49), and noting that the segments of the exterior boundary which surround disordered regions do not move, it follows by (7.41) that

$$\dot{A}_{disordered} = \sum_{i \in I_{IPB}} \int_{r^i_{IPB}} V\, ds = -c_2 \sum_{i \in I_{IPB}} \int_{r^i_{IPB}} \mathcal{K}_{ss}\, ds.$$

Hence, integrating

$$\dot{A}_{disordered} = -c_2 \sum_{i \in I_{IPB}} [\mathcal{K}_s(s^i_2) - \mathcal{K}_s(s^i_1)],$$

where s^i_2 and s^i_1 denote the upper and lower endpoints respectively of the curve $r^i(t)$. Let us now regroup the contributions to the above expression in terms of IPBs emerging from particular triple-junctions, noting in doing so that there is no contribution from the intersection of IPBs with the exterior boundary by (7.47). Thus,

$$\dot{A}_{disordered} = c_2 \sum_{j \in J_{triple}} [\mathcal{K}_s(s^j_1) + \mathcal{K}_s(s^j_2)],$$

where J_{triple} denotes an indexing of the set of triple-junctions and s^j_1 and s^j_2 denote the two IPBs at the point at which they emerge from the j^{th} triple-junction. Here, the convention has been employed that that locally at each triple-junction the parametrization along each IPB is taken to commence at the triple-junction. Employing the balance of fluxes condition (7.43), the above expression becomes

$$\dot{A}_{disordered} = -c_2 \gamma_1 \sum_{j \in J_{triple}} \mu_s(s^j_3).$$

Noting that each of the contributions lies on an APB, this last expression may be writtten as

$$\dot{A}_{disordered} = c_2 \gamma_1 \sum_{i \in I_{APB}} \int_{r^i_{APB}} \mu_{ss}\, ds,$$

which vanishes by virtue of (7.40). □

Lemma 7.2 The surface energy weighted interfacial length is a non-increasing function of time.

Proof of lemma 7.2

It is well known, see e.g. [28], that if $r(t)$ is a given curve in the plane, then

$$\frac{d}{dt}L_{r(t)} = -\int_{r(t)} \mathcal{K}V\, ds - (\dot{R}^+(t))_{tan} + (\dot{R}^-(t))_{tan}$$

where $L_{r(t)}$ is the length of the curve $r(t)$ and where $R^+(t)$, $R^-(t)$ denote the location of the endpoints of the curve $r(t)$, and $(\dot{R}^+(t))_{tan}$ and $(\dot{R}^-(t))_{tan}$ denote the tangential velocities of the endpoints; i.e.,

$$(\dot{R}^+(t))_{tan} = \dot{R}^+(t)\cdot T^+ \qquad (\dot{R}^-(t))_{tan} = \dot{R}^-(t)\cdot T^-$$

where $T^{\pm}$ denotes the unit tangent has been taken in the direction of the arc-length parametrization. Using the convention that $\tau^+ = T^+$ and $\tau^- = -T^-$ are unit tangent vectors emerging from the triple-junctions and external boundaries,

$$\frac{d}{dt}[\sigma_{IPB}L_{IPB} + \sigma_{APB}L_{APB}] = -\sigma_{APB}\sum_{i\in I_{APB}}\int_{r^i_{APB}} \mathcal{K}V\, ds - \sigma_{IPB}\sum_{i\in I_{IPB}}\int_{r^i_{IPB}} \mathcal{K}V\, ds$$

$$-\sigma_{APB}\sum_{i\in I_{APB}}\Big[\dot{R}^+_i(t)\cdot\tau^+ + \dot{R}^-_i(t)\cdot\tau^-\Big] - \sigma_{IPB}\sum_{i\in I_{IPB}}\Big[\dot{R}^+_i(t)\cdot\tau^+ + \dot{R}^-_i(t)\cdot\tau^-\Big]. \tag{7.50}$$

Note that all contributions in (7.50) are independent of the direction of the arc-length parametrization.

Claim: There is no net contribution from the motion of the endpoint of the curves $\{r^i_{APB}, r^i_{IPB}\}$ *to* (7.50).

Proof of the Claim.

It follows from (7.46)-(7.48) that there is no contribution from the points of intersection of the APB and IPB curves with the exterior boundary. Regrouping the remaining contributions by triple-junctions,

$$\text{Contributions from endpoints} \;=$$

$$\sum_{j\in J_{triple}}\Big[\sigma_{IPB}\{\dot{R}^j_1(t)\cdot\tau^j_1 + \dot{R}^j_2(t)\cdot\tau^j_2\} + \sigma_{APB}\{\dot{R}^j_3(t)\cdot\tau^j_3\}\Big]. \tag{7.51}$$

where $\dot{R}^j_i$ and τ^j_i denote respectively the velocity of the endpoint of Γ_i and the emergent tangent vector along the j^{th} triple-junction. The subscripts $i = 1, 2$ and $i = 3$ refer to properties of the two IPB's and of the APB respectively. It is easy to check that (7.42) implies that

$$\sigma_{APB} = 2\cos\theta\,\sigma_{IPB}, \tag{7.52}$$

where $\theta = \frac{1}{2}\theta_3$; i.e., half the angle at the triple-junction opposite the emerging APB. Persistence of triple-junctions implies the following kinetic condition

$$\dot{R}^j_1(t)\cdot\tau^j_1\cos\theta = \dot{R}^j_2(t)\cdot\tau^j_2\cos\theta = \dot{R}^j_3(t)\cdot\tau^j_3\cos\theta. \tag{7.53}$$

Substitution of (7.52) and (7.53) into (7.51) completes the proof of the *Claim*.

To complete the proof of the *lemma*, the second integral on the right hand side of (7.50) is integrated by part:

$$\sum_{i\in I_{IPB}} \int_{r^i_{IPB}} \mathcal{K}\mathcal{K}_{ss}\, ds = -\sum_{i\in I_{IPB}} \int_{r^i_{IPB}} \mathcal{K}^2\, ds + \sum_{i\in I_{IPB}} [\mathcal{K}(s^i_2)\mathcal{K}_s(s^i_2) - \mathcal{K}(s^i_1)\mathcal{K}_s(s^i_1)].$$

Taking arc-length parametrizations originating locally along each interface at every triple-junction and noting that by (7.47) it is possible to neglect contributions from intersections with exterior boundaries, we obtain

$$\sum_{i\in I_{IPB}} [\mathcal{K}(s^i_2)\mathcal{K}_s(s^i_2) - \mathcal{K}(s^i_1)\mathcal{K}_s(s^i_1)] = -\sum_{j\in J_{triple}} [\mathcal{K}(s^j_1)\mathcal{K}_s(s^j_2) + \mathcal{K}(s^j_1)\mathcal{K}_s(s^j_2)].$$

From continuity of the chemical potential across the interface, the above expression may be written as

$$= -\sum_{j\in J_{triple}} \mathcal{K}(s^j_1)[\mathcal{K}_s(s^j_1) + \mathcal{K}_s(s^j_2)],$$

or, employing the balance of fluxes and continuity of the chemical potential at the triple-junction,

$$= \sum_{j\in J_{triple}} \gamma_1^2 \mu(s^j_3)\mu_s(s^j_3).$$

Pairing the ends of APB curves

$$= \gamma_1^2 \sum_{i\in I_{APB}} [\mu(s^i_2)\mu_s(s^i_2) + \mu(s^i_1)\mu_s(s^i_1)].$$

Noting that by (7.40)

$$\mu_s(s^i_2) = -\mu_s(s^i_1),$$

and

$$\mu(s^i_2) = \mu(s^i_1) + \mu_s(s^i_1)(s^i_2 - s^i_1),$$

it follows that

$$I = -\sum_{i\in I_{APB}} \gamma_1^2 [\mu_s(s^i_1)]^2 (s^i_2 - s^i_1).$$

Returning to (7.50),

$$\frac{d}{dt}[\sigma_{APB}L_{APB} + \sigma_{IPB}L_{IPB}] =$$

$$-c_1 \sum_{i\in I_{APB}} \int_{r^i_{APB}} \mathcal{K}^2\, ds - c_2 \sum_{i\in I_{IPB}} \int_{r^i_{IPB}} \mathcal{K}_s^2\, ds - c_2\gamma_1^2 \sum_{i\in I_{APB}} \int_{r^i_{APB}} [\mu_s(s_1)]^2\, ds. \quad \square \qquad (7.54)$$

8 Discussion.

Under low temperature, long time, and scaling assumptions appropriate for modeling the Krzanowski instability, limiting equations of motion have been derived by formal asymptotics for an Allen-Cahn/Cahn-Hilliard system with a minor disordered phase. The resultant motion couples motion by mean curvature and motion by minus the surface Laplacian of the mean curvature, with quasi-static diffusion of the disordered phase along the APBs. Further numerical studies are necessary to test the applicability of the limiting equations to describe Krzanowski instabilities, sintering of small grains, and grain boundary grooving in polycrystalline films. A rough count of the number of equations derived indicates that the resultant system can be expected to be well posed, though questions of existence and uniqueness for the resulting system of equations can be resolved using the methods of [8] and [23].

Clearly though now that it has been shown to be feasible to couple differing types of geometric motions, it should be possible to implement our approach in the context of systems of Allen-Cahn/Cahn-Hilliard equations with degenerate mobilities and generalisations thereof, in order to capture via asymptotics an understanding of further modes of microstructural evolution.

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Figure Captions.

1.*i*. The limiting motion when the curvature of APBs is assumed to be $\mathcal{O}(\epsilon)$ and the curvature of IPBs is assumed to be $\mathcal{O}(1)$, see [13].

1.*ii*. The limiting equations of motion under the assumption that the curvature of APBs is $\mathcal{O}(\epsilon^{3/2})$ and the curvature of IPBs is $\mathcal{O}(\epsilon^{-1/2})$, see text.

5.*i*. The T_ϵ construction used at the triple-junction.

6.*i*. The R_ϵ construction used at points of intersection of APBs and IPBs with the external boundary.

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