GEOMETRIC MOTION FOR A DEGENERATE ALLEN-CAHN/CAHN-HILLIARD SYSTEM: THE PARTIAL WETTING CASE

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Abstract. Using formal asymptotics we demonstrate that in a low temperature coarsening limit, a degenerate Allen-Cahn/Cahn-Hilliard system yields a geometric problem in which small particles whose shape evolves according to surface diffusion move along a surface which itself moves by motion by mean curvature. The degenerate Allen-Cahn/Cahn-Hilliard system was developed in [7] to describe simultaneous ordering and phase separation, and within this context the particles which contain a minor disordered phase are embedded along grain boundaries which partition the system into two ordered phase variants. The limiting problem, though, can also be viewed as a diffuse interface approximation for various problems in materials science in which surface diffusion and motion by mean curvature are coupled, see, for example, [20, 28]. The present analysis extends a previous study [26] which focused on the complete wetting limit and on motions in the plane; here we treat the more generic partial wetting case and our analysis accommodates motion in three dimensions.

Keywords: Geometric free boundary problems, motion by mean curvature, surface diffusion, degenerate parabolic equations, higher order parabolic systems.

1. Introduction

In this paper we shall focus on the following Allen-Cahn/Cahn-Hilliard system of equations

$$(\mathbf{AC/CH})\quad \begin{cases} u_t &= 4\epsilon^2\nabla\cdot[Q(u,\,v)\nabla\mu], \\ \mu &= F_u(u,\,v)-\epsilon^2\triangle u, \\ v_t &= -\frac{1}{4}Q(u,\,v)[F_v(u,\,v)-\epsilon^2\triangle v], \end{cases}$$

for $(x,\,t)\in\Omega\times(0,\,T)$ where Ω is a smooth bounded domain in R^3 and $0<T<\infty$, in conjunction with the boundary conditions

$$\mathbf{n}\cdot Q(u,\,v)\nabla\mu=\mathbf{n}\cdot\nabla u=\mathbf{n}\cdot\nabla v=0, \tag{1.1}$$

for $(x,\,t)\in\partial\Omega\times(0,\,T)$, and its limiting motions. This system of equations was developed in [7] to model simultaneous phase separation and ordering in binary alloys. In AC/CH, u denotes an average concentration and v represents a nonconserved order variable. The mobility, $Q(u,v)$, is assumed to be nonnegative and to vanish at the "pure phases." This assumption, which reflects divergence of the time scale in a minimal entropy completely ordered system, implies degeneracy of the parabolic system AC/CH. The homogeneous free energy, F, will be assumed to contain two terms, one which reflects entropy contributions and another which accounts for the energy of mixing. The form which will be adopted for the entropy contribution will reflect the fact that in the original derivation both $u-v$ and $u+v$ acted as concentration variables.

Additional assumptions will be imposed on F in order to guarantee that the system will evolve in a partial wetting regime. Roughly speaking what is necessary in this context is to require that certain weighted geodesics connecting the ordered phases do not pass via an intermediary globally energy minimizing pure phase, see [27]. We remark that our analysis neglects effects which could lead to anisotropy or grain rotation; we do this for the sake of simplicity in order to focus on asymptotics which couple the two types of motions. We will amplify our assumptions further in the section which follows. For a discussion of models which are similar and related to AC/CH, we refer the reader to Eguchi & Ninomiya [12] and Chen et. al. [8, 30].

In the present paper we shall develop formal asymptotics to describe the long time limiting motion for the AC/CH system. Roughly speaking, the predicted limiting motion corresponds to a coarsening regime in which small grains or particles of disordered phase, whose surface evolves under motion by surface diffusion, are embedded within grain boundaries that are moving by mean curvature. Within this context the surface of the disordered grains are known as interphase boundaries (IPBs) and the grain boundaries are known as anti-phase boundaries (APBs). This description of coarsening corresponds qualitatively well with experiment, see e.g. Krzanowski & Allen [22]. Coupled surface diffusion and motion by mean curvature also occurs in materials science in contexts other than that of ordering and phase separation. For example in grain boundary motion where the grain boundary is connected to an external surface via a thermal groove [20] and in sintering [28], such a description is appropriate under suitable assumptions. However, while motion by mean curvature and motion by surface diffusion have been discussed in numerous contexts in the past, their coupled motion has only recently been obtained as a limiting motion from a diffuse interface model; i.e., from a system of equations such as AC/CH which are prescribed in terms of variables which are defined at all points in Ω, [26]. There, however, the assumptions were such that the dihedral angle between two IPBs which connected up to an APB was zero to leading order. This feature, which can be associated with proximity to a complete wetting limit, is non-generic and causes the limiting equations to be in some sense singular.

The asymptotic analysis leading to the coupling of motion by mean curvature and surface diffusion is somewhat delicate even in the partial wetting case, since rough time scale arguments would lead one to expect motion by mean curvature to evolve on a much faster scale than motion by surface diffusion, hence their coupling on the same time scale would be seemingly inconsistent. However, the coupling becomes possible when the "aspect ratio" (given by the ratio of a typical length scale for the volumes which evolve by surface diffusion to a typical length scale for the volumes which evolve by motion by mean curvature) is sufficiently small. Ideally, one should like to obtain predictions for the manner in which the length scales of the system increase with time during the long time coarsening regime, such as those obtained for example, by Kohn & Otto [21] in the context of the Cahn-Hilliard equation in the deep quench limit. Though this has so far not been accomplished in the present context, this may be possible to undertake within the framework of the limiting equations which we obtain here. We remark that some degree of "self-similarity" in length scale growth must be assumed in order to guarantee the validity of the "aspect ratio" assumption described above during coarsening.

Ideally we should like to be able to rigorously prove a connection between the dynamics of AC/CH and the limiting asymptotic motions which we derive. We note that the connection between the dynamics of diffuse interface equations and limiting asymptotics motions has been rigorously established in a number of contexts, see for example Caginalp & Chen [4] and references therein. We point out that in order to accomplish such a program in the present context, a number of nontrivial steps are required. In particular, existence and regularity must be established both for the AC/CH system and for the limiting equations of motion which we obtain.

With regard to proving existence and regularity for the AC/CH system, so far this has only been accomplished for one-dimensional domains, [10]. Progress in this direction is hindered by the degeneracy of the problem and by the paucity of symmetry in the structure of the equations. We note that existence and regularity has been established for the Cahn-Hilliard equation with degenerate mobility in three dimensions in [13], even though the degeneracy there is of the same level as in the present context. However the proof there is facilitated by the additional structure which occurs in that context. Notably degenerate fourth order parabolic equations and systems are also encountered in the context of the thin film equation and related systems. Similar issues occur there with regard to existence and regularity, and have been a topic of much recent interest and development, see e.g. [11]. With regard to establishing existence and regularity for the limiting equations, this appears to be not too difficult to undertake, and results in this direction should be forthcoming soon. This has been accomplished for example in [16] for the limiting motion which arises from a system of degenerate Cahn-Hilliard equations. In particular, it should be easier to prove existence for the limiting dynamics which are obtained here, as compared with establishing existence for limiting equations of motion coupling surface diffusion with motion by mean curvature when complete wetting is predicted to leading order since additional degeneracy is implied in that context. We remark that even when the two steps above have been established, it cannot be expected that establishing a rigorous connection will be straightforward. Note that although limiting motions were derived formally for the degenerate Cahn-Hilliard equation in [6], and existence and regularity for both the degenerate Cahn-Hilliard equation and for its limiting motions have been established in [13] and [14] respectively, a rigorous connection between the two has yet to be proven. Thus results in this direction in the present context cannot be expected to be forthcoming too rapidly. However, it is our hope that by presenting the formal asymptotics in a careful and consistent manner, confidence and interest in our methodology will be enhanced and the goals which we have outlined shall eventually be achieved.

We remark that once a clear connection has been established between the AC/CH diffuse interface model and the limiting motions which we outline here, even before the connection has become rigorously established, the AC/CH system can be looked upon as an approximation of the geometric problem. As such, the system can be implemented as a numerical tool for studying the limiting geometric problem. Notably, fully practical numerical schemes have been developed for the AC/CH system both for the degenerate and the non-degenerate cases [1, 2].

The present paper backs away from the more technically involved analysis in [26] and puts things in an easier and more generic setting. Considerable effort is devoted here to making the formal steps in the asymptotic analysis more transparent than in [6] and [26]. Some of the technical discussions which we present here are reminiscent of discussions which appear in [6, 26], but they have been included here and in some cases modified for the sake of completeness, clarity, and accessability. Hopefully the technical transparency of our presentation will promote more rapid validification of the predicted limiting motions for degenerate CH equations and systems as well as for the AC/CH system.

The outline of this paper is as follows. In §2, the basic assumptions and notation for our analysis are given, and the strategy for the asymptotic analysis is presented. In §3, and specific ansatzes are introduced for the asymptotic expansions in the outer solution and are demonstrated to be self-consistent. §4 contains the derivation of the limiting motions for APBs and IPBs. The laws governing triple junctions are derived in §5, and the laws governing the intersections of APBs and IPBs with the external boundary $\partial\Omega$ are obtained in §6. In §7, our results are summarized for the limiting geometric problem. We invite the interested reader to turn now to Figure 6 for a rapid overview of these results.

FIGURE 1. The region, $B := \{(u,\, v) \in R^2 |\, 0 < u + v < 1,\, 0 < u - v < 1\}$

2. Preliminaries

In this paper, we shall consider the degenerate Allen-Cahn/Cahn-Hilliard system (AC/CH) for $(x,\, t) \in \Omega \times (0,\, T)$, where Ω is a smooth bounded domain in R^3 and $0 < T < \infty$, together with the boundary conditions (1.1) for $(x,\, t) \in \partial\Omega \times (0,\, T)$. The first boundary condition represents a no flux boundary condition; the second and third reflect "free" or energy minimizing boundary conditions. Here u, v, and μ are scalar functions representing respectively the concentration, the order parameter, and the chemical potential. It is constructive to note that

$$\vec{j} := -Q(u,\, v)\nabla\mu \tag{2.1}$$

expresses the mass flux.

In AC/CH, $F(u,\, v)$ is the homogeneous free energy which will be assumed to be of the form:

$$F(u,\, v) = \frac{\Theta}{2}\Big[G(u+v) + G(u-v)\Big] + E(u,\, v), \tag{2.2}$$

where Θ represents a dimensionless temperature,

$$G(s) = s \ln s + (1-s)\ln(1-s)$$

expresses the entropy density of the system, and E reflects the interaction energy density of the system which we assume to be a polynomial of degree k,

$$E = \sum_{i,\, j=0}^{k} a_{ij}\, u^i v^j. \tag{2.3}$$

We remark that in the existence proof in [10], E was taken as a specific quadratic polynomial. Restrictions on the coefficients a_{ij} will be implied by our assumptions with regard to certain properties of $F(u,\, v)$, as we shall explain shortly.

In order that $F(u,\, v)$ be well defined, $(u,\, v)$ must lie in the closure of the diamond shaped region

$$B := \{\, (u,\, v) \;|\; 0 < u - v < 1, \quad 0 < u + v < 1\,\}.$$

See Figure 1. Off-hand, it is not obvious that by restricting the initial data to lie in $\overline{B}$, that solutions will continue to lie in $\overline{B}$ and that the initial value problem for AC/CH will be well-posed. However, it was proven in [10] in one-dimension that this restriction, in conjunction with the constraint that the average concentration $\overline{u} := \frac{1}{|\Omega|}\int_\Omega u\, dx$ satisfies $\overline{u} \in (0,\, 1)$ and with appropriate degeneracy assumptions on $Q(u,\, v)$, was in fact sufficient to guarantee existence, though not uniqueness of solutions lying within $B \cup \{0,\, 0\} \cup \{1,\, 0\}$. In higher dimensions such as $N = 3$ as we shall be considering here, in the absence of appropriate analytical results, *we shall assume the existence of smooth solution* $(u,\, v)$ *which lie entirely within* B. While analytically it is of interest to consider solutions with nontrivial support of the set $\{0,\, 0\} \cup \{1,\, 0\}$, energetic considerations based on the assumptions to be made on $F(u,\, v)$ lead one not to expect persistence over time of nontrivial support for this set to occur generically.

In AC/CH, the function $Q(u, v)$ represents the mobility. *We shall assume $Q(u, v)$ to be degenerate at the corners of $\overline{B}$* . More specifically, we will assume as in [10] that

$$Q(u, v) = P(u, v)\widetilde{Q}(u, v), \tag{2.4}$$

where $P(u, v) = u(1-u)(\frac{1}{4} - v^2)$ and $\widetilde{Q}(u, v)$ is a smoothly defined function which is non-vanishing throughout $\overline{B}$. Note that $P(u, v)$ has simple roots at the corners of $\overline{B}$,

$$\{(0, 0), (1/2, 1/2), (1/2, -1/2), (1, 0)\} \tag{2.5}$$

This assumption can be seen as a generalization of the classical notion [5, 15] that mobilities should vanish in pure phases since the exchange probabilities which determine the mobilities vanish in a perfectly ordered environment.

In accordance with the assumption that v represents an ordering variable and that $v \to -v$ represents the exchange of one phase variant by another energetically and kinetically equivalent one, *we shall assume that $F(u, v)$ and $Q(u, v)$ are even functions of the variable v,*

$$F(u, v) = F(u, -v), \quad Q(u, v) = Q(u, -v). \tag{2.6}$$

We shall assume that the interaction energy $E(u, v)$ is concave, its coefficients a_{ij} (see (2.3)) are $\mathcal{O}(1)$, and that it has two global minimizers located at $(\frac{1}{2}, \pm\frac{1}{2})$ and two minimizers located at $(0, 0)$ and $(1, 0)$ which are local but not global minimizers. This implies that when Θ is positive and sufficiently small (see (2.2)), the homogeneous free energy $F(u, v)$ possesses 4 minimizers within B which are located transcendentally close to the extreme points, (2.5). Moreover, for small positive values of Θ; e.g. when Θ is positive and $\mathcal{O}(\epsilon^{1/2})$, it is readily seen that there exists a Lagrange multiplier, λ, such that the "tilted" free energy $F(u, v) + \lambda u$ possesses precisely three equal depth global minimizers within B which are located transcendentally close ($\mathcal{O}(e^{-c/\Theta})$) to the extreme points of B for sufficiently small positive values of Θ. The information with regard to the location of the equilibria will be critical in evaluating the behavior of the inner solutions near $\pm\infty$. *Henceforth, we shall incorporate the effect of the Lagrange multiplier into the free energy density, setting $F + \lambda u \to F$ which shall be referred to simply as "the free energy".* This implies in particular that

$$F_{uu}, F_{vv} > 0, \quad F_{uu}F_{vv} - (F_{uv})^2 > 0 \tag{2.7}$$

at the global minima. Finally, *without loss of generality, we may assume that $F = 0$ at the global minimizers.*

So that our analysis will reflect the partial wetting case, we shall rely on the properties of certain energy minimizing paths. *We let $\alpha_\pm$ denote the global minimizers of F located near $(1/2, -1/2)$ and $(1/2, 1/2)$, respectively, which we shall refer to as the ordered phase variants, and let α_0 denote to the global minimizer of F which is located near $(0, 0)$ which we shall refer to as the disordered phase. We shall assume that the coefficients in (2.3) are such that there exists a unique minimizing path connecting $\alpha_\pm$* where

$$\liminf_{(u, v) \in A_\pm} \int_0^1 \sqrt{F(u, v)\{\dot{u}^2 + \dot{v}^2\}}\, dt, \tag{2.8}$$

is attained, where

$$A_-^+ := \{ (u, v) \in C^1[0, 1], (u(0), v(0)) = \alpha_-, (u(1), v(1)) = \alpha_+, (u(t), v(t)) \in B \quad \forall t \in [0, 1]\},$$

which does not pass via the global minimizer, α_0. Were the geodesic to pass via α_0, then it would be implied (see [27]) that the surface energy of the transition from one phase variant to the other was precisely equally to twice the surface energy of a transition from one of the phase variants to to the disordered phase, and this would correspond to the complete wetting case which is not being treated here. *In fact we shall make the slightly stronger assumption that the geodesic path stays boundedly away from* α_0. This assumption can be interpreted as saying that our system will be assumed to be in the generic partially wetting regime and not asymptotically close to complete wetting.

We call to the reader's attention that in the partial wetting case, the geodesic may or may not pass via a local minimizers. If the geodesic passes via a local minimizer, then the system is said to be prewetting. Otherwise, there is said to be absorption unless there is no variation at all in concentration along the transition from one phase variant to the other. *For simplicity we shall also assume that the geodesic path stays boundedly away from* $(1, 0)$. We remark that such an assumption is not unreasonable, since even in the prewetting case, under quite minimal assumptions on $F(u, u)$, the geodesic path can be shown not to cross a local minimizer located near $(1, 0)$, if such a local minimizer exists. Suppose, for example, that we were to assume that in addition to the $v \to -v$ symmetry, prior to "tilting" by the Lagrange multiplier λ, the free energy $F(u, v)$ also exhibits $u \to 1/2 - u$ symmetry. Then it is readily seen that if $0 < \bar{u} < 1/2$ as we have assumed, an energy minimizing geodesic cannot come too close to $(1, 0)$, since this would imply that one could readily construct a path lying to the left of $u = 1/2$ with lower energy, which would contradict the assumption that the original path described was itself energy minimizing.

For the analysis which follows, *we shall also make use of the minimizing paths connecting* $\alpha_\pm$ *with* α_0. Analytically, these are the paths where

$$\liminf_{(u,\, v)\in A_0^\pm} \int_0^1 \sqrt{F(u,\, v)\{\dot{u}^2+\dot{v}^2\}}\, dt$$

is attained, where

$$A_0^\pm := \{\, (u,\, v) \in C^1[0,\, 1],\, (u(0),\, v(0)) = \alpha_0,\, (u(1),\, v(1)) = \alpha_\pm, \quad (u(t),\, v(t)) \in B \quad \forall t \in [0,\, 1]\}.$$

We shall assume this minimizing path to be uniformly bounded an $\mathcal{O}(e^{-c/\Theta})$ *distance away from* ∂B. We remark that the limit $\Theta \to 0$ is a singular limit, known in the literature [29] as the deep-quench limit. In this limit, the minimizers of F go to the corners of $\overline{B}$, and the geodesics may be totally or partially contained in ∂B.

We point out to the reader that inherently the partial wetting case is far more generic than the complete wetting case. In [27], it is demonstrated analytically that interaction energy $E(u, v) = \alpha u(1-u) - \beta v^2$ with $0 < \alpha < \beta$ which was employed in [26] indeed implies complete wetting when $\bar{u} \in (0, 1/2)\cup(1/2, 1)$ at $\Theta = 0$, and some simple examples are given of interaction energies which imply partial wetting.

In accordance with the discussion in [26], *we shall introduce a slow time scale,* $\tau = \epsilon^{7/2}t$, *into the AC/CH equations and set* $\tau = t$ *for notational convenience.* In this manner, we obtain

$$\begin{aligned} \epsilon^{5/2}u_t &= 4\epsilon\nabla\cdot[Q(u,\, v)\nabla\mu_u], \\ \mu &= F_u(u,\, v) - \epsilon^2\triangle u, \\ \epsilon^{7/2}v_t &= -\tfrac{1}{4}Q(u,\, v)[F_v(u,\, v) - \epsilon^2\triangle v]. \end{aligned} \tag{2.9}$$

Having thus rescaled time, *all dynamic phenomena of interest will be assumed to occur on a* $\mathcal{O}(1)$ *time scale.*

To accommodate with our assumption that we shall be considering a low temperature limit, *we shall assume that* $\Theta = \mathcal{O}(\epsilon^{1/2})$, or more specifically, that

$$\Theta = \epsilon^{1/2}. \tag{2.10}$$

Note that by (2.2) in fact $F = F(u, v; \Theta)$ and hence $F_u = F_u(u, v; \Theta)$ and $F_v = F_v(u, v; \Theta)$. However, as we have noted above, the deep quench limit is singular. Therefore, whenever expanding F or any of its u, v derivatives about a given states, *we shall maintain the Θ dependence even though by assumption $\Theta = \mathcal{O}(\epsilon^{1/2})$ in order to avoid this singular limit. For simplicity, however, we shall not make the dependence of F on Θ explicit in our notation.* We remark that limiting equations of motion for the degenerate Cahn-Hilliard equation were obtained in [6] both in the deep quench limit and when $0 < \Theta << 1$. In the deep quench limit, though, the asymptotics were obtained there directly at $\Theta = 0$ and not by taking a $\Theta \to 0$ limit in the low temperature asymptotics.

As mentioned in the Introduction, *we shall assume that the disordered phase constitutes a minor phase*; i.e., that the volume fraction of Ω which is occupied by the disordered phase is small. This shall be further reflected in *an assumption that the curvature of particles which contain the disordered phase is very large,* or more specifically that

$$H_{IPB} = \mathcal{O}(\epsilon^{-1/2}), \tag{2.11}$$

where H_{IPB} denotes the mean curvature at points along IPBs. Note that the structure of (2.9) is mass conservative. These assumptions imply that the mean concentration of the system as a whole must be close to 1/2, the concentration of the ordered phase variants. We may quantify this requirement by setting

$$1/2 - \bar{u} = \mathcal{O}(\epsilon^{3/2}),$$

where

$$\bar{u} := \frac{1}{|\Omega|} \int_\Omega u \, dx.$$

In parallel with (2.11) and in analogy with the assumptions made in [26], *we shall assume that the curvature of the APBs in very small,* or more specifically that

$$H_{APB} = \mathcal{O}(\epsilon^{3/2}), \tag{2.12}$$

where H_{APB} denotes the mean curvature at points along APBs. Note that the analogous requirement in [26] was that $1/2 - \bar{u} = \mathcal{O}(\epsilon)$. This alteration in the assumptions is in order to attain scaling consistency with the scaling requirement (2.11) when three rather than two dimensions are being considered. By reverting to the assumption that $1/2 - \bar{u} = \mathcal{O}(\epsilon)$, the analysis in this paper could readily be adapted for the case $N = 2$.

If $F(u, v; 0)$ is sufficiently convex, then it is reasonable to expect that if $1/2 - \overline{u} = \mathcal{O}(\epsilon^{3/2})$, but $\overline{u} \neq 1/2$, and if $(u(t), v(t))$ denotes the geodesics connecting α_- and α_+, then

$$\int_0^1 \frac{u(s) - u(0)}{Q(u(s), v(s))} \, ds \neq 0. \tag{2.13}$$

We shall assume here that (2.13) holds.

Some words on "strategy" follow at this point.

3. The outer solution

As in [26], we shall not actually solve explicitly for the outer solution. Rather we shall make a number of ansatzes with regard to the form of the perturbations expansions which are then shown to be self-consistent and which allow the inner and outer solutions to be determined by the asymptotics to leading order. More specifically, let $\alpha_i := (u^{0,i}, v^{0,i})$, $i = 1, 2, 3$ denote the global minimizers of the free energy, and let the distance of these minimizers to the nearest extreme point of B be given as $\mathcal{O}(e^{-c/\sqrt{\epsilon}})$, where c is a fixed constant. In accordance with the discussion in §2, the minimizers $(u^{0,\,i},\, v^{0,\,i})$, $i = 1,\, 2,\, 3$ are bounded an $\mathcal{O}(e^{-c/\sqrt{\epsilon}})$ distance away from the boundary of B, ∂B. *Throughout the outer region, we shall assume perturbation expansion of the form*

$$u(x,\, t) = u^{0,\,i} + (u^0 + \epsilon^{1/2} u^{1/2} + \epsilon u^1 + \epsilon^{3/2} u^{3/2} + \mathcal{O}(\epsilon^2)) e^{-c/\sqrt{\epsilon}}, \tag{3.1}$$

$$v(x,\, t) = v^{0,\,i} + (v^0 + \epsilon^{1/2} v^{1/2} + \epsilon v^1 + \epsilon^{3/2} v^{3/2} + \mathcal{O}(\epsilon^2)) e^{-c/\sqrt{\epsilon}}, \tag{3.2}$$

to be valid, where c is the same constant as before. In (3.1)-(3.2) the superscripts refer to the order of the various terms in the perturbation expansion in which they appear. We shall employ this notational convention throughout the text, clarifying further only where necessary. *Similarly with regard to the mass flux, $\vec{j}$, we shall assume that*

$$\vec{j}(x,\, t) = (\vec{j}^{\,0} + \epsilon^{1/2} \vec{j}^{\,1/2} + \epsilon \vec{j}^{\,1} + \epsilon^{3/2} \vec{j}^{\,3/2} + \mathcal{O}(\epsilon^2)) e^{-c/\sqrt{\epsilon}}, \tag{3.3}$$

where again c is the same as above. *And finally with regard to μ we shall make the scaling ansatz that*

$$\mu(x,\, t) = \mu^0 + \epsilon^{1/2} \mu^{1/2} + \epsilon \mu^1 + \epsilon^{3/2} \mu^{3/2} + \mathcal{O}(\epsilon^2). \tag{3.4}$$

We remark that the terms u^0 and v^0 are necessary in order to guarantee the overall self-consistency of our asymptotic framework. By including these terms, our assumptions on the form of the perturbation expansions for u and v are seen to parallel the form which is assumed for $\vec{j}$.

Let us now ascertain the implications of our scaling assumptions. For ease of presentation we shall employ in this section only, the following notation

$$\mu_u := \mu = F_u(u,\, v) + \epsilon^2 \triangle u,$$

and

$$\mu_v := F_v(u,\, v) + \epsilon^2 \triangle v.$$

Taylor expanding $F_u(u,\, v)$ about one of the global minimizers $(u^{0,i},\, v^{0,i})$, $i = 1, 2,$ or 3, we obtain that

$$F_u(u,\, v) = \epsilon^{1/2} F_u^{1/2} + \epsilon F_u^1 + \mathcal{O}(\epsilon^{3/2},$$

where $F_u^{1/2} = (F_{uu}^0 u^0 + F_{uv}^0 v^0) \epsilon^{-1/2} e^{-c/\sqrt{\epsilon}}$ and $F_u^1 = (F_{uu}^0 u^{1/2} + F_{vv}^0 v^{1/2}) e^{-c/\sqrt{\epsilon}}$, where F_{uu}^0 denotes F_{uu} evaluated at the global minimizer about which we are expanding. We point out here, that in accordance with our remarks in §2, the dependence of F and its derivatives on Θ is maintained at all levels of the expansions. Similarly, we obtain that

$$F_v(u,\, v) = \epsilon^{1/2} F_v^{1/2} + \epsilon F_v^1 + \mathcal{O}(\epsilon^{3/2}),$$

where the definitions of $F_v^{1/2}$, F_v^1 are analogous to those of $F_u^{1/2}$, F_u^1. By considering the assumed form for F given in (2.2) and recalling (2.10) and our assumptions on the location of the minimizers $(u^{0,i},\, v^{0,i})$, we see that F_{uu}^0, F_{uv}^0, F_{vv}^0 are $\mathcal{O}(\epsilon^{1/2} e^{c/\sqrt{\epsilon}})$. From the Taylor expansions given above for $F_u(u,\, v)$ and $F_v(u,\, v)$, we obtain that $F_u(u,\, v)$ and $F_v(u,\, v)$ are $\mathcal{O}(\epsilon^{1/2})$ and have regular perturbation expansions in $\epsilon^{1/2}$. Thus, the ansatz given in (3.4) is, in fact, appropriate for μ_v as well as for μ_u and the assumed scalings are self-consistent within the framework of the second and third equations in (2.9) in that all terms have regular perturbation expansions in $\epsilon^{1/2}$. In particular, it follows that

$$\mu_u^0 = 0, \quad \mu_v^0 = 0. \tag{3.5}$$

Note that from the assumptions above it follows that

$$\begin{aligned}\mu_u^{1/2} &= (F_{uu}^0 u^0 + F_{uv}^0 v^0)\epsilon^{-1/2} e^{-c/\sqrt{\epsilon}} \\ \mu_v^{1/2} &= (F_{uv}^0 u^0 + F_{vv}^0 v^0)\epsilon^{-1/2} e^{-c/\sqrt{\epsilon}},\end{aligned}$$

from which we may conclude, in conjunction with the inequality from $F_{uu}^0 F_{vv}^0 - (F_{uv}^0)^2 > 0$ from §2, that u^0 and v^0 are determined in the outer solution by $\mu_u^{1/2}$ and $\mu_v^{1/2}$.

With regard to the mobility, Taylor expanding $Q(u, v)$ about the nearest corner in B to $(u^{0,i}, v^{0,i})$ which we shall denote as $(\bar{u}^{0,i}, \bar{v}^{0,i})$, we obtain

$$Q(u, v) = [\bar{Q}^0 + \epsilon^{1/2}\bar{Q}^{1/2} + \epsilon\bar{Q}^1 + \mathcal{O}(\epsilon^{3/2})]e^{-c/\sqrt{\epsilon}},$$

where

$$\begin{aligned}\bar{Q}^0 &:= Q_u^0((u^{0,i} - \bar{u}^{0,i})e^{c/\sqrt{\epsilon}} + u^0) + Q_v^0((v^{0,i} - \bar{v}^{0,i})e^{c/\sqrt{\epsilon}} + v^0), \\ \bar{Q}^{1/2} &:= Q_u^0 u^{1/2} + Q_v^0 v^{1/2}, \quad \bar{Q}^1 := Q_u^0 u^1 + Q_v^0 v^1,\end{aligned}$$

and where Q_u^0 and Q_v^0 denote respectively Q_u and Q_v evaluated at $(\bar{u}^{0,i}, \bar{v}^{0,i})$. Note that the assumptions on Q, u, and v imply that $Q(u, v)$ is $\mathcal{O}(e^{-c/\sqrt{\epsilon}})$ with the same constant c as above. Hence referring to (3.1), (3.2), (3.4), we see that the scaling in the first equation in (2.9) is self-consistent in that all terms are of the form $e^{-c/\sqrt{\epsilon}}$ times a regular perturbation expansion in $\epsilon^{1/2}$. Finally, consideration of (3.3) and (2.1) yields that

$$\vec{j}^0 = 0. \tag{3.6}$$

Geodesics We recall that $(U^0(\rho), V^0(\rho))$ as it was defined in §2 corresponds to a reparameterization of the geodesic path connecting the two ordered variants. Because the geodesic is an energy minimizing path and because of the $v \to -v$ symmetry which has been assumed for $F(u, v)$, it is easy to show that

$$V^0(\rho) \geq 0 \;\text{ for }\; \rho \geq 0, \tag{3.7}$$

since the energy as defined in (2.8) may be lowered if (3.7) does not hold. Note that (3.7) implies in particular that $V^0(\rho)$ will stay $\mathcal{O}(1)$ away from $-V^\infty$ for $\rho \in (0, \infty)$. Moreover, because the geodesic is an energy minimizing path, it is not difficult to argue that for $\rho \in (-\rho_0, \rho_0)$, for $\rho_0 = \mathcal{O}(1)$, $(U^0(\rho), V^0(\rho))$ will stay $\mathcal{O}(1)$ away from $(U^\infty, \pm V^\infty)$ which constitute global minimizers of $F(u, v)$. As noted in §2, the geodesic path traced out by $(U^0(\rho), V^0(\rho))$ can also be assumed to stay $\mathcal{O}(1)$ away from (0, 0) and (1, 0).

4. The inner solutions

As discussed in the Introduction, we shall assume that throughout the coarsening regime, there exist thin domains of rapid spatial variation which partition $\Omega \subset R^3$ into various regions in which the outer solutions is valid. These thin domains or inner regions are assumed to have an $\mathcal{O}(\epsilon)$ width and we shall parameterize these inner regions via a locally defined orthonormal system, (r, s) where $r = r(x, t)$ measures normal distance from the mid-surface of the inner region, and $s(x, t) = (s_1(x, t), s_2(x, t))$ constitutes an orthonormal frame relative to the mid-surface of the inner region, so that $|\nabla r| = |\nabla s_1| = |\nabla s_2| = 1$ and $\nabla r \cdot \nabla s_1 = \nabla r \cdot \nabla s_2 = \nabla s_1 \cdot \nabla s_2 = 0$. Clearly, there is some variability in how the mid-surface of the inner region is to be chosen. This difficulty can be treated by implementing a suitable normalization condition, as we shall explain in the sequel.

It is readily verified that

$$\triangle r = -2H, \quad \text{and} \quad r_t = -W, \tag{4.1}$$

where $H = \frac{1}{2}(\kappa_1 + \kappa_2)$ denotes the mean curvature and $W(x,\, t)$ denotes the normal velocity of the interface in the direction in which normal distance is measured. From (4.1), the orientation of the curvature can be inferred. Recalling that time has been assumed to be scaled so that all temporal variation will occur on an $\mathcal{O}(1)$ scale, *we shall assume that*

$$W = W^0 + \mathcal{O}(\epsilon^{1/2}), \tag{4.2}$$

and our assumptions for H will be in accordance with (2.11),(2.12).

Since the thickness of the inner region is being taken to be $\mathcal{O}(\epsilon)$, *we introduce the stretched inner variable* $\rho = r/\epsilon$. In terms of the variables $(\rho,\, s)$ where $s = (s_1,\, s_2)$, the functions u, v, μ, *and* $\vec{j}$ *will be assumed to be expressible via the following regular perturbation expansions*

$$\begin{aligned}
u(x,\, t) &= U(s,\, \rho,\, t) = U^0 + \epsilon^{1/2} U^{1/2} + \epsilon U^1 + \mathcal{O}(\epsilon^{3/2}),\\
v(x,\, t) &= V(s,\, \rho,\, t) = V^0 + \epsilon^{1/2} V^{1/2} + \epsilon V^1 + \mathcal{O}(\epsilon^{3/2}),\\
\mu(x,\, t) &= \mu(s,\, \rho,\, t) = \mu^0 + \epsilon^{1/2}\mu^{1/2} + \epsilon\mu^1 + \mathcal{O}(\epsilon),\\
\vec{j}(x,\, t) &= \vec{J}(s,\, \rho,\, t) = \vec{J}^{-1}\epsilon^{-1} + \vec{J}^{-1/2}\epsilon^{-1/2} + \vec{J}^0 + \epsilon^{1/2}\vec{J}^{1/2} + \epsilon\vec{J}^1 + \mathcal{O}(\epsilon^{3/2}).
\end{aligned}$$

Since the geodesics connecting between the minimizers of the free energy have been assumed to bounded away from the boundary of B, based on the notion that the solution in the inner region should also take in some approximate minimal path between approximate minimizers, *we shall assume* (U, V) *to be bounded away from the minimizers* $(u^{0,i},\, v^{0,i})$ *and from the boundary of* B *within the inner region*, and hence $F(U,\, V)$ and its derivatives to be Taylor expandable about $(U^0,\, V^0)$ with $\mathcal{O}(1)$ coefficients.

4.1. **The inner solution along IPBs.** Proceeding within the framework outlined at the beginning of the section, let us consider an inner region with an ordered variant lying "ahead" in the positive r direction and with a disordered region lying "behind" in the negative r direction. *Referring to the ordered minimizer which is approximately reached in the outer region lying ahead as* $(u^{0,+},\, v^{0,+})$ *and the disordered minimizer which is approximately reached behind as* $(u^{0,-},\, v^{0,-})$, *we may normalize our coordinates by setting*

$$U(s,\, 0,\, t) = \frac{1}{2}(u^{0,+} + u^{0,-}). \tag{4.1.1}$$

Note that (4.1) implies in the context of the scaling assumption (2.11) that

$$\triangle r = -2\epsilon^{-1/2} H^{-1/2} - 2H^0 - 2\epsilon^{1/2} H^{1/2} + \mathcal{O}(\epsilon). \tag{4.1.2}$$

To obtain an evolution equation for the IPB interface, we employ the expansions outlined at the beginning of the section and solve the relevant equations at orders $\mathcal{O}(\epsilon^{-1})$ though $\mathcal{O}(\epsilon)$. The analysis here is similar and in fact somewhat easier than in the APB case which follows in §4.2.

At $\mathcal{O}(\epsilon^{-1})$, it follows from the first equation in (2.9) and (2.1) that

$$4(Q^0 \mu^0_\rho)_\rho = 0, \tag{4.1.3}$$

$$\vec{J}^{-1} \cdot \vec{n} = -4Q^0 \mu^0_\rho, \tag{4.1.4}$$

where $Q^0 = Q(U^0,\, V^0)$. Integrating (4.1.3) and employing (4.1.4), we obtain that

$$Q^0 \mu^0_\rho = f^{-1}(s,\, t) = -\vec{J}^{-1} \cdot \vec{n}.$$

Now matching with the outer region, it follows that $Q^0 \mu^0_\rho = 0$. Recalling that $Q(U,\, V)$ vanishes only at the corners of B, $(\bar{u}^{0,i},\, \bar{v}^{0,i})$, and taking $(U^0,\, V^0)$ to lie strictly within the interior of B

throughout the inner region, we may conclude that Q^0 should be non-vanishing throughout the inner region, and hence that

$$\mu_\rho^0 = 0.$$

Integrating this last equation and matching with the outer region we find that

$$\mu^0 = 0. \tag{4.1.5}$$

At $\mathcal{O}(\epsilon^{-1/2})$, we obtain from the first equation in (2.9) and from (2.1) that

$$4(Q^0\mu_\rho^{1/2})_\rho = 0, \tag{4.1.6}$$

$$\vec{J}^{-1/2}\cdot\vec{n} = -4Q^0\mu_\rho^{1/2}. \tag{4.1.7}$$

As in the analysis at $\mathcal{O}(\epsilon^{-1})$, we obtain that

$$\mu_\rho^{1/2} = 0, \tag{4.1.8}$$

though we cannot now conclude that $\mu^{1/2} = 0$.

At $\mathcal{O}(1)$, noting (4.1.5) and(4.1.8), it follows from (2.9) and (2.1) that

$$0 = 4(Q^0\mu_\rho^1)_\rho, \tag{4.1.9}$$

$$0 = F_U^0 - U_{\rho\rho}^0, \tag{4.1.10}$$

$$0 = -\frac{1}{4}Q^0[F_V^0 - V_{\rho\rho}^0], \tag{4.1.11}$$

$$\vec{J}^0\cdot\vec{n} = -4Q^0\mu_\rho^1, \tag{4.1.12}$$

where $F_U^0 = F_U(U^0, V^0)$ and $F_V^0 = F_V(U^0, V^0)$. From (4.1.9) and (4.1.12), we obtain by integrating, matching, and recalling (3.6) that

$$\mu_\rho^1 = 0. \tag{4.1.13}$$

Since Q^0 is being taken to be non-vanishing within the inner region, it follows from (4.1.11)-(4.1.10) and (4.1.5) that

$$\begin{cases} F_U^0 - U_{\rho\rho}^0 = 0, \\ F_V^0 - V_{\rho\rho}^0 = 0. \end{cases} \tag{4.1.14}$$

Equations (4.1.14) and the boundary conditions obtained by matching with the outer solutions determine $(U^0(\rho), V^0(\rho))$ uniquely up to a $\rho \to \rho + \bar{\rho}$ transition, as the heteroclinic orbit connecting the energy minimizing disordered phase with one of the two ordered variants. This degree of freedom is eliminated by the normalization condition (4.1.1) which implies here that $U^0(0) = \frac{1}{2}(u^{0,+} + u^{0,-})$. Equation (4.1.14) can be viewed as a re-parameterization of the geodesic connecting one of the two ordered variants with the energy minimizing disordered phase which was described in §2; see the discussion in [27]. Note that to leading order the inner solution indeed approximates the geodesic and stays strictly within the interior of B, which is self-consistence with the assumptions given at the beginning of this section.

At $\mathcal{O}(\epsilon^{1/2})$, taking (4.1.5), (4.1.8), (4.1.13), and (4.1.14) into account, we obtain from (2.9) and (2.1) that

$$0 = 4(Q^0\mu_\rho^{3/2})_\rho, \tag{4.1.15}$$

$$\mu^{1/2} = F_U^{1/2} - U_{\rho\rho}^{1/2} + 2U_\rho^0 H^{-1/2}, \tag{4.1.16}$$

$$0 = -\frac{1}{4}Q^0[F_V^{1/2} - V_{\rho\rho}^{1/2} + 2V_\rho^0 H^{-1/2}], \tag{4.1.17}$$

$$\vec{J}^{1/2} \cdot \vec{n} = -4Q^0 \mu_\rho^{3/2}, \tag{4.1.18}$$

where $F_U^{1/2}$ and $F_V^{1/2}$ are the respective coefficients of $\epsilon^{1/2}$ in the Taylor expansion of $F_U(U, V)$ and $F_V(U, V)$ about (U^0, V^0), namely

$$\begin{aligned} F_U^{1/2} &:= F_{UU}(U^0, V^0)U^{1/2} + F_{UV}(U^0, V^0)V^{1/2}, \\ F_V^{1/2} &:= F_{VU}(U^0, V^0)U^{1/2} + F_{VV}(U^0, V^0)V^{1/2}. \end{aligned}$$

From (4.1.15) and (4.1.18), we may conclude by integrating and matching that

$$Q^0 \mu_\rho^{3/2} = f^{3/2}(s, t) = \vec{J}^{1/2} \cdot \vec{n}, \tag{4.1.19}$$

where $f^{3/2}(s, t)$ is transcendentally small. Since Q^0 does not vanish throughout the inner region, it follows from (4.1.17) and (4.1.16) that

$$\begin{cases} F_U^{1/2} - U_{\rho\rho}^{1/2} &= -2U_\rho^0 H^{-1/2} + \mu^{1/2}, \\ F_V^{1/2} - V_{\rho\rho}^{1/2} &= -2V_\rho^0 H^{-1/2}, \end{cases}$$

Multiplying this system by (U_ρ^0, V_ρ^0), integrating over the interval $(-\infty, \infty)$, using (4.1.8) and (4.1.14), then matching with the outer region,

$$\mu^{1/2} = \frac{2H^{-1/2}}{[U^0]_{-\infty}^{\infty}} \int_{-\infty}^{\infty} [(U_\rho^0)^2 + (V_\rho^0)^2]\, d\rho. \tag{4.1.20}$$

At $\mathcal{O}(\epsilon)$, taking into account (4.1.5), (4.1.8), and (4.1.13), the first equation in (2.9) and (2.1) yield

$$0 = 4(Q^0 \mu_\rho^2 + Q^{1/2} \mu_\rho^{3/2})_\rho, \tag{4.1.21}$$

$$\vec{J}^1 \cdot \vec{n} = -4Q^0 \mu_\rho^2 - 4Q^{1/2} \mu_\rho^{3/2}, \tag{4.1.22}$$

where $Q^{1/2}$ is the coefficient of $\epsilon^{1/2}$ in the Taylor expansion of $Q(U, V)$ about (U^0, V^0), namely, $Q^{1/2} := Q_U(U^0, V^0)U^{1/2} + Q_V(U^0, V^0)V^{1/2}$. From (4.1.21) and (4.1.22), integrating and matching,

$$Q^0 \mu_\rho^2 + Q^{1/2} \mu_\rho^{3/2} = f^1(s, t) = \vec{J}^1 \cdot \vec{n}, \tag{4.1.23}$$

where $f^1(s, t)$ is T.S.T., where the notation T.S.T. is being used to denote *transcendentally small terms*. In order to obtain an evolution for the IPB interface, it is not necessary to consider the second and third equations in (2.9).

At $\mathcal{O}(\epsilon^{3/2})$, taking into account (4.1.5), (4.1.8), and (4.1.13), the first equation in (2.9) and (2.1) may be written as

$$-U_\rho^0 W^0 = 4(Q^0 \mu_\rho^{5/2} + Q^{1/2} \mu_\rho^2 + Q^1 \mu_\rho^{3/2})_\rho + Q^0 \triangle_s \mu^{1/2}, \tag{4.1.24}$$

$$\vec{J}^{3/2} \cdot \vec{n} = -4Q^0 \mu_\rho^{5/2} - 4Q^{1/2} \mu_\rho^2 - 4Q^1 \mu_\rho^{3/2}, \tag{4.1.25}$$

where $\triangle_s$ denotes the Laplace-Beltrami operator on the mid-surface of the inner region defined by $r = 0$, and Q^1 is the coefficient of ϵ in the Taylor expansion of $Q(U, V)$ about (U^0, V^0). Noting that (4.1.24) may be written as

$$-U_\rho^0 W^0 = 4(\vec{J}^{3/2} \cdot \vec{n})_\rho + Q^0 \triangle_s \mu^{1/2},$$

then integrating this equation over the interval $(-\epsilon^{-1/4},\, \epsilon^{-1/4})$ and matching with the outer solution, we obtain

$$W^0 = -\frac{2\triangle_s H^{-1/2}}{([U^0]_{-\infty}^{\infty})^2}\int_{-\infty}^{\infty}[(U_\rho^0)^2 + (V_\rho^0)^2]\, d\rho \int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} Q^0\, d\rho + TST, \tag{4.1.26}$$

which implies that in the limit $\epsilon \to 0$

$$W^0 = -c_{IPB}\triangle_s H^{-1/2}, \tag{4.1.27}$$

where

$$c^{IPB} = \lim_{\epsilon\to 0}\left[\frac{2}{([U^0]_{-\infty}^{\infty})^2}\int_{-\infty}^{\infty}[(U_\rho^0)^2 + (V_\rho^0)^2]\, d\rho \int_{-\infty}^{\infty} Q^0\, d\rho\right].$$

It would be seemingly preferable and simpler to integrate Q^0 over the interval $(-\infty,\, \infty)$ in the discussion above, however the integral $\int_{-\infty}^{\infty} Q^0\, d\rho$ is divergent since $Q(U^0,\, V^0) \to Q(u^{0,i},\, v^{0,i})$ as $\rho \to \pm\infty$ where $Q(u^{0,i},\, v^{0,i})$ is TST though non-vanishing. Therefore it is reasonable to inquire in what sense the integral over Q^0 in (4.1.27) is robustly defined. Note that by relying on [9, Section 13], one may show that for $\rho > \rho_0$ where ρ_0 is $\mathcal{O}(1)$

$$U^0 - U^\infty = C_U e^{-f(\epsilon)\rho} + o(e^{-f(\epsilon)\rho}), \quad V^0 - V^\infty = C_V e^{-f(\epsilon)\rho} + o(e^{-f(\epsilon)\rho}), \tag{4.1.28}$$

where $(U^\infty,\, V^\infty) = \lim_{\rho\to\infty}(U(\rho),\, V(\rho)$, C_U and C_V are $\mathcal{O}(1)$, and $f(\epsilon) = \Theta^{1/2}e^{c/2\Theta}$ where c is the same constant which was used in §2 to describe the location of the minimizers of $F(u,\, v)$, with similar predictions at $-\infty$. Using (4.1.28), it is not difficult to demonstrate that the integral over Q^0 in (4.1.26) is $\mathcal{O}(1)$ and that the limits of integration may be taken as $\pm l(\epsilon)$ where $l(\epsilon)$ is any algebraically large function of ϵ, and the resultant variation (4.1.26) will only be TST small. We remark that it is reasonable to require that $l(\epsilon) = o(\epsilon^{-1})$, since the width of the inner region given in terms of the original variables is ϵ.

4.2. **The inner solution along APBs.** We proceed again according to the framework outlined at the beginning of this section, and it we consider an inner region which has one of the two ordered variants lying "ahead" of it, in the positive r direction, and the other of the two ordered variants lying at its rear. We adopt the normalization that $V(s,\, 0,\, t) = 0$. Equation (4.1) implies in the context of the scaling assumption (2.12) that

$$\triangle r = -2\epsilon^{3/2}H^{3/2} + \mathcal{O}(\epsilon^2). \tag{4.2.1}$$

To obtain an evolution equation for the APB interface, we employ the expansions outlined earlier, as in the IPB case. This time, however, the relevant equations will be solved at orders $\mathcal{O}(\epsilon^{-1})$ though $\mathcal{O}(\epsilon^{5/2})$. The analysis at orders $\mathcal{O}(\epsilon^{-1})$ through $\mathcal{O}(1)$ is identical to the APB analysis. At higher orders we ,ale use of certain symmetry properties which will be demonstrated to hold for the heteroclinic orbit connecting the two ordered variants.

At $\mathcal{O}(\epsilon^{-1})$, as in the IPB case

$$4(Q^0\mu_\rho^0)_\rho = 0,$$
$$\vec{J}^{-1}\cdot\vec{n} = -4Q^0\mu_\rho^0,$$

where $Q^0 = Q(U^0,\, V^0)$, which implies

$$\mu^0 = 0.$$

At $\mathcal{O}(\epsilon^{-1/2})$, we obtain that

$$4(Q^0\mu_\rho^{1/2})_\rho = 0,$$

$$\vec{J}^{-1/2} \cdot \vec{n} = -4Q^0 \mu_\rho^{1/2},$$

which imply that

$$\mu_\rho^{1/2} = 0.$$

At $\mathcal{O}(1)$, one gets

$$0 = 4(Q^0 \mu_\rho^1)_\rho,$$
$$0 = F_U^0 - U_{\rho\rho}^0,$$
$$0 = -\frac{1}{4} Q^0 [F_V^0 - V_{\rho\rho}^0],$$
$$\vec{J}^0 \cdot \vec{n} = -4Q^0 \mu_\rho^1,$$

where $F_U^0 = F_U(U^0, V^0)$ and $F_V^0 = F_V(U^0, V^0)$, which yields that

$$\mu_\rho^1 = 0, \tag{4.2.2}$$

and that

$$F_V^0 - V_{\rho\rho}^0 = 0, \tag{4.2.3}$$
$$F_U^0 - U_{\rho\rho}^0 = 0. \tag{4.2.4}$$

In the present context, equations (4.2.3)-(4.2.4) and the boundary conditions obtained by matching with the outer solutions now determine $(U^0(\rho), V^0(\rho))$ uniquely, up to $\rho \to \rho + \bar{\rho}$ translations, as the heteroclinic orbit connecting the two ordered variants, which can be viewed as a re-parameterization of the geodesic connecting the two ordered variants. It is important to note that the assumption (2.6) with regard to the $v \to -v$ symmetry of $F(u, v)$ implies that the unique globally energy minimizing geodesic which connects the two ordered variants, which are symmetrically located within B, must itself be symmetric with respect to $v \to -v$ reflection. (If it were not symmetric, a symmetric path with lower energy could be constructed which would yield a contradiction, see e.g. [23, Lemma 1].) The normalization $V(s, 0, t) = 0$ implies now that $V^0(0) = 0$, and hence that

$$(U^0(\rho), V^0(\rho)) = (U^0(-\rho), -V^0(-\rho)), \text{ for all } \rho \in (-\infty, \infty).$$

In other words, $U^0(\rho)$ is an even function, and $V^0(\rho)$ is an odd function. Since the relevant geodesics have been taken to lie strictly within the interior of B, we obtain that Q^0 is non-vanishing throughout the inner region.

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

$$0 = 4(Q^0 \mu_\rho^{3/2})_\rho,$$
$$\mu^{1/2} = F_U^{1/2} - U_{\rho\rho}^{1/2},$$
$$0 = -\frac{1}{4} Q^0 [F_V^{1/2} - V_{\rho\rho}^{1/2}],$$
$$\vec{J}^{1/2} \cdot \vec{n} = -4Q^0 \mu_\rho^{3/2},$$

where $F_U^{1/2}$ and $F_V^{1/2}$ are the coefficients of $\epsilon^{1/2}$ in the Taylor expansion of $F_U(U, V)$ and $F_V(U, V)$ about (U^0, V^0), as in the IPB analysis. From these equations, it follows that, in analogy with the IPB analysis,

$$Q^0 \mu_\rho^{3/2} = g^{3/2}(s, t) = \vec{J}^{1/2} \cdot \vec{n}, \tag{4.2.5}$$

where $g^{3/2}(s,\, t)$ is transcendentally small, and that

$$\left\{ \begin{array}{rcl} F_U^{1/2} - U_{\rho\rho}^{1/2} &=& \mu^{1/2}, \\ F_V^{1/2} - V_{\rho\rho}^{1/2} &=& 0, \end{array} \right. \tag{4.2.6}$$

where $F_U^{1/2} := F_{UU}^0 U^{1/2} + F_{UV}^0 V^{1/2}$ and $F_V^{1/2} := F_{UV}^0 U^{1/2} + F_{VV}^0 V^{1/2}$ are the coefficients of $\epsilon^{1/2}$ in the respective Taylor expansions of $F_U(U,\, V)$ and $F_V(U,\, V)$ about $(U^0,\, V^0)$. Multiplying this system by $(U_\rho^0,\, V_\rho^0)$, integrating over the interval $(-\infty,\, \infty)$, and matching with the outer region, we get now that

$$0 = \int_{-\infty}^{\infty} U_\rho^0\, \mu^{1/2}\, d\rho. \tag{4.2.7}$$

Since U_ρ^0 is odd and $\mu^{1/2}$ is independent of ρ, no new information is gained from (4.2.7). However, since $\mu^{1/2}$ is independent of ρ, the right hand side of the first equation in (4.2.6) is an even function of ρ and the right hand side of the second equation in (4.2.6) can be considered an odd function of ρ. Note that $(U_\rho^0,\, V_\rho^0)$ constitutes a homogeneous solution to (4.2.5) such that $(U_\rho^0(\pm\infty),\, V_\rho^0(\pm\infty)) = 0$. Hence given any solution to (4.2.5) which satisfies prescribed Dirichlet boundary matching conditions at $\pm\infty$, may be written as $(U^{1/2},\, V^{1/2}) + k(U_\rho^0,\, V_\rho^0)$, where $k = k(s,t)$ is an arbitrary function and

$$(U^{1/2},\, V^{1/2}) \perp (U_\rho^0,\, V_\rho^0). \tag{4.2.8}$$

The condition (4.2.8) This normalization condition can be seen to imply that $U^{1/2}$ is an even function of ρ and $V^{1/2}$ is an odd function of ρ. See Appendix I for a detailed proof. In particular, it yields that $V^{1/2}(0,s) = 0$. Since the boundary conditions at $\pm\infty$ and the fact that $V^0(0) = 0$ imply that $V_\rho^0(0) \neq 0$, it follows from the normalization condition that $k(s,\, t) = 0$.

At $\mathcal{O}(\epsilon)$, taking into account our results in this section up to now, we get that

$$0 = 4(Q^0\mu_\rho^2 + Q^{1/2}\mu_\rho^{3/2})_\rho, \tag{4.2.9}$$

$$\vec{J}^1 \cdot \vec{n} = -4Q^0\mu_\rho^2 - 4Q^{1/2}\mu_\rho^{3/2}, \tag{4.2.10}$$

$$0 = -\frac{1}{4}Q^0[F_V^1 - V_{\rho\rho}^1], \tag{4.2.11}$$

$$\mu^1 = F_U^1 - U_{\rho\rho}^1, \tag{4.2.12}$$

where $Q^{1/2}$ is the coefficient of $\epsilon^{1/2}$ in the Taylor expansion of $Q(U,\, V)$ about $(U^0,\, V^0)$, and F_U^1 and F_V^1 are the coefficients of ϵ in the respective Taylor expansions of $F_U(U,\, V)$ and $F_V(U,\, V)$ about $(U^0,\, V^0)$. From (4.2.9) and (4.2.10), we may conclude as in the IPB analysis that

$$-4Q^0\mu_\rho^2 - 4Q^{1/2}\mu_\rho^{3/2} = g^1(s,\, t) = \vec{J}^1 \cdot \vec{n}, \tag{4.2.13}$$

where $g^1(s,\, t)$ is T.S.T.. From (4.2.11) and (4.2.12), we obtain a system which we may write as

$$\left\{ \begin{array}{rcl} F_{UU}^0 U^1 + F_{UV}^0 V^1 - U_{\rho\rho}^1 &=& \mu^1 - \frac{1}{2}[F_{UUU}^0 (U^{1/2})^2 + 2F_{UUV}^0 U^{1/2}V^{1/2} + F_{UVV}^0 (V^{1/2})^2], \\ F_{UV}^0 U^1 + F_{VV}^0 V^1 - V_{\rho\rho}^1 &=& -\frac{1}{2}[F_{VUU}^0 (U^{1/2})^2 + 2F_{UVV}^0 U^{1/2}V^{1/2} + F_{VVV}^0 (V^{1/2})^2]. \end{array} \right. \tag{4.2.14}$$

We proceed as in the $\mathcal{O}(\epsilon^{1/2})$ analysis and write the solution to (4.2.14) as $(U^1,\, V^1) + k(U_\rho^0,\, V_\rho^0)$ where $(U^1,\, V^1) \perp (U_\rho^0,\, V_\rho^0)$. We now wish to show that the constraint $(U^1,\, V^1) \perp (U_\rho^0,\, V_\rho^0)$ implies that U^1 is even and V^1 is odd, as functions of ρ. To accomplish this, we make use of the following considerations. By induction it is easy to see that (2.6) implies that for any integers j and k

$$\frac{\partial^{j+k}}{\partial U^j \partial V^k} F(U,\, V) = (-1)^k \frac{\partial^{j+k}}{\partial U^j \partial V^k} F(U,\, -V). \tag{4.2.15}$$

Since $U^0(\rho)$ is an even function of ρ and $V^0(\rho)$ is an odd function of ρ, it follows from (4.2.15) that $\frac{\partial^{j+k}}{\partial U^j \partial V^k} F(U^0(\rho),\, V^0(\rho))$ is an even function of ρ if k is even and it is an odd function of ρ if k is odd. From this remark and since μ^1 is independent of ρ, we may readily verify that the right hand side of the first equation in (4.2.14) is even and the right hand side of the second equation in (4.2.14) is odd, with respect to ρ. Hence, we may use Appendix I to conclude that indeed U^1 is even and V^1 is odd, with respect to ρ, and therefore we may sat $k(s,\, t) = 0$ as earlier. We note that if we now take the inner product of (4.2.14) with $(U^0_\rho,\, V^0_\rho)$, as in the analysis at $\mathcal{O}(\epsilon^{1/2})$ no additional information is gained.

At $\mathcal{O}(\epsilon^{3/2})$, taking into account our results so far, we find that

$$-W^0 U^0_\rho = 4(Q^0 \mu^{5/2}_\rho + Q^{1/2}\mu^2_\rho + Q^1 \mu^{3/2}_\rho)_\rho + 4Q^0 \triangle_s \mu^{1/2}, \tag{4.2.16}$$

$$\vec{J}^{3/2} \cdot \vec{n} = -4Q^0 \mu^{5/2}_\rho - 4Q^{1/2}\mu^2_\rho - 4Q^1 \mu^{3/2}_\rho, \tag{4.2.17}$$

$$0 = -\frac{1}{4} Q^0 [F^{3/2}_V - V^{3/2}_{\rho\rho}], \tag{4.2.18}$$

$$\mu^{3/2} = F^{3/2}_U - U^{3/2}_{\rho\rho}, \tag{4.2.19}$$

where Q^1 is the coefficient of ϵ in the Taylor expansion of $Q(U,\, V)$ about $(U^0,\, V^0)$ and $F^{3/2}_U$ and $F^{3/2}_V$ are the coefficients of $\epsilon^{3/2}$ in the Taylor expansion of $F_U(U,\, V)$ and $F_V(U,\, V)$ about $(U^0,\, V^0)$, and where $\triangle_s$ is the Laplace-Beltrami.

Note now that we may write (4.2.16) as

$$-W^0 U^0_\rho = -(\vec{J}^{3/2} \cdot \vec{n})_\rho + 4Q^0 \triangle_s \mu^{1/2}. \tag{4.2.20}$$

We now integrate this equation with respect to ρ over the interval $(-\epsilon^{-\frac{1}{4}},\, \epsilon^{-\frac{1}{4}})$. Since U^0 is even and goes exponentially to U^∞, where $U^\infty := \lim_{\rho\to\pm\infty} U^0(\rho)$ and since $\mu^{1/2}$ is independent of ρ, we obtain that

$$4\triangle_s\, \mu^{1/2} \int_{-\epsilon^{-\frac{1}{4}}}^{\epsilon^{-\frac{1}{4}}} Q(U^0,\, V^0)\, d\rho = T.S.T..$$

As in the IPB analysis, it is readily seen that the integral on the left hand side is $\mathcal{O}(1)$ and robustly defined. Hence

$$\triangle_s\, \mu^{1/2} = T.S.T.. \tag{4.2.21}$$

With regard to equations (4.2.18) and (4.2.19), proceeding as we did with equations (4.2.11) and (4.2.12) at $\mathcal{O}(\epsilon)$, we find that

$$\int_{-\infty}^{\infty} \mu^{3/2} U^0_\rho\, d\rho = 0.$$

Integrating the above equation by parts yields

$$\{\mu^{3/2}(U^0(\rho) - U^\infty)\}|^{\infty}_{-\infty} - \int_{-\infty}^{\infty} \mu^{3/2}_\rho (U^0 - U^\infty)\, d\rho = 0.$$

Since matching implies that $\lim_{\rho\to\pm\infty}\mu^{3/2}$ is bounded or has at most linear behavior, and since we may conclude as in (4.1.28) that $\lim_{\rho\to\pm\infty}(U^0-U^\infty)$ is exponentially decaying, the first term vanishes and hence

$$\int_{-\infty}^{\infty}\mu_\rho^{3/2}(U^0-U^\infty)\,d\rho=0.$$

Recalling (4.2.5), this implies that

$$g^{3/2}\int_{-\infty}^{\infty}\frac{(U^0-U^\infty)}{Q(U^0,\,V^0)}\,d\rho=0.$$

In accordance with (2.13), we assume the integral in the expression to be non-vanishing. Therefore, $g^{3/2}=0$, and hence

$$\mu_\rho^{3/2}=0.$$

Returning to (4.2.13), we find that

$$-4Q^0\mu_\rho^2=g^1=TST.$$

Finally, from (4.2.18),(4.2.19), the normalization condition, and Appendix I, we find that $(U^{3/2},\,V^{3/2})\perp(U_\rho^0,\,V_\rho^0)$ and hence that $U^{3/2}$ is even and $V^{3/2}$ is odd, with respect to ρ.

At $\mathcal{O}(\epsilon^2)$, proceeding as above, we now obtain

$$-W^{1/2}U_\rho^0-W^0U_\rho^{1/2}=4(Q^0\mu_\rho^3+Q^{1/2}\mu_\rho^{5/2}+Q^1\mu_\rho^2)_\rho+4Q^0\triangle_s\mu^1+4Q^{1/2}\triangle_s\mu^{1/2},\qquad(4.2.22)$$

$$\vec{J}^2\cdot\vec{n}=-4Q^0\mu_\rho^3-4Q^{1/2}\mu_\rho^{5/2}-4Q^1\mu_\rho^2,\qquad(4.2.23)$$

$$0=-\frac{1}{4}Q^0[F_V^2-V_{\rho\rho}^2],\qquad(4.2.24)$$

$$\mu^2=F_U^2-U_{\rho\rho}^2,\qquad(4.2.25)$$

where F_U^2 and F_V^2 are the coefficients of ϵ^2 in the Taylor expansion of $F_U(U,\,V)$ and $F_V(U,\,V)$ about $(U^0,\,V^0)$.

Treating equations (4.2.22) and (4.2.23) as we treated equations (4.2.16) and (4.2.17) earlier and using (4.2.21), we obtain

$$\triangle_s\,\mu^1=T.S.T..\qquad(4.2.26)$$

With regard to equations (4.2.24) and (4.2.25), we may proceed as with equations (4.2.18) and (4.2.19) and conclude that

$$\mu_\rho^2=0,$$

which implies in conjunction with (4.2.20) and the results above that

$$-W^0(U^0-U^\infty)=4Q^0\mu_\rho^{5/2}+T.S.T.,\qquad(4.2.27)$$

or, to be more precise,

$$-W^0(U^0-U^\infty)=4Q^0\mu_\rho^{5/2}-W^0(U^0(-\epsilon^{-1/4})-U^\infty)-\vec{J}^{3/2}\cdot\vec{n}|_{\rho=-\epsilon^{-1/4}}+4\triangle_s\,\mu^{1/2}\int_{-\epsilon^{-1/4}}^{\rho}Q^0\,d\rho.\qquad(4.2.28)$$

Moreover, proceeding as earlier, we find that $U^2(\rho)$ is an even function of ρ and $V^2(\rho)$ is an odd function of ρ.

At $\mathcal{O}(\epsilon^{5/2})$, it suffices to consider two of the four equations which govern at this level. Using our results so far, these equations may be written as

$$\mu^{5/2}=F_U^{5/2}-U_{\rho\rho}^{5/2}+2U_\rho^0\,H^{3/2},\qquad(4.2.29)$$

$$-V^0_\rho W^0 = -\frac{1}{4} Q^0 [F^{5/2}_V - V^{5/2}_{\rho\rho} + 2V^0_\rho\, H^{3/2}], \tag{4.2.30}$$

where now $F^{5/2}_U$ and $F^{5/2}_V$ are the coefficients of $\epsilon^{5/2}$ in the Taylor expansions of $F_U(U,\, V)$ and $F_V(U,\, V)$ about $(U^0,\, V^0)$. Dividing (4.2.30) by $-\frac{1}{4}Q^0$ and taking the inner product of the resultant system with $(U^0_\rho,\, V^0_\rho)$ over the interval $(-\epsilon^{-1/4},\, \epsilon^{-1/4})$ yields

$$\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \mu^{5/2} U^0_\rho \, d\rho + W^0 \int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \frac{4(V^0_\rho)^2}{Q(U^0,\, V^0)} \, d\rho = 2H^{3/2} \int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \{(U^0_\rho)^2 + (V^0_\rho)^2\} \, d\rho. \tag{4.2.31}$$

Integrating the first integral on the left hand side of the above expression by parts

$$\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \mu^{5/2} U^0_\rho \, d\rho = \{\mu^{5/2}(U^0 - U^\infty)\}|^{\epsilon^{-1/4}}_{-\epsilon^{-1/4}} - \int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \mu^{5/2}_\rho (U^0 - U^\infty) \, d\rho. \tag{4.2.32}$$

We now demonstrate that

$$\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \mu^{5/2} U^0_\rho \, d\rho = W^0 \int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \frac{(U^0 - U^\infty)^2}{4Q(U^0,\, V^0)} \, d\rho + TST., \tag{4.2.33}$$

To verify (4.2.33), we first examine somewhat carefully the qualitative behavior of $(U^0(\rho),\, V^0(\rho))$. As in §4.1, we may rely on the approach of [9, Chapter 13] to show that for $|\rho| > |\rho_0|$, where $\rho_0 = \mathcal{O}(1)$

$$U^0 - U^\infty = C_U e^{-f(\epsilon)|\rho|} + o(e^{-f(\epsilon)|\rho|}), \quad V^0 - V^\infty = C_V e^{-f(\epsilon)|\rho|} + o(e^{-f(\epsilon)|\rho|}), \tag{4.2.34}$$

where C_U and C_V are $\mathcal{O}(1)$, $f(\epsilon) = \Theta^{1/2} e^{c/2\Theta}$, and c is the same constant that appeared in §2 to describe the location of the minimizers of $F(u,\, v)$. In particular (4.2.34) implies that the first term on the right hand side of (4.2.32) is T.S.T.. Note now that (4.2.28) implies that

$$\mu^{5/2}_\rho = -\frac{W^0}{4Q^0}(U^0 - U^\infty) + \frac{W^0}{4Q^0}(U^0(-\epsilon^{-1/4}) - U^\infty) + \frac{1}{4Q^0}\vec{J}^{3/2} \cdot n|_{\rho=-\epsilon^{-1/4}} - \triangle_s \mu^{1/2} \frac{1}{Q^0} \int_{-\epsilon^{-1/4}}^{\rho} Q^0.$$

Thus

$$\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \mu^{5/2} U^0_\rho \, d\rho = W^0 \int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \left\{ \frac{(U^0 - U^\infty)^2}{4Q(U^0,\, V^0)} \right\} d\rho + A + B + C + T.S.T., \tag{4.2.35}$$

where

$$(A) := \tfrac{W^0}{4}(U^0(-\epsilon^{-1/4}) - U^\infty) \textstyle\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \frac{U^0 - U^\infty}{Q^0} \, d\rho,$$

$$(B) := \tfrac{1}{4}\vec{J}^{3/2} \cdot n|_{\rho=-\epsilon^{-1/4}} \textstyle\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \frac{U^0 - U^\infty}{Q^0} \, d\rho,$$

$$(C) := -\triangle_s \mu^{1/2} \textstyle\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \left\{ \int_{-\epsilon^{-1/4}}^{\rho} Q^0 \right\} \frac{U^0 - U^\infty}{Q^0} \, d\rho.$$

By (4.2.34), $(U^0(-\epsilon^{-1/4}) - U^\infty) = T.S.T.$ and by matching with the outer solution it follows that $\vec{J}^{3/2} \cdot n|_{\rho=-\epsilon^{-1/4}} = T.S.T.$. Moreover by (4.2.21), $\triangle_s \mu^{1/2} = T.S.T.$. Also, by the assumptions in §2 on $Q(u,\, v)$, it follows that $\max_{(u,\, v) \in \bar{B}} |Q(u,\, v)| = \mathcal{O}(1)$. Therefore $\sup_{\rho \in (-l(\epsilon),\, l(\epsilon))} | \int_{-\epsilon^{-1/4}}^{\rho} Q^0 \, d\rho| = \mathcal{O}(l(\epsilon))$, where $l(\epsilon)$ is algebraically large. Hence,

$$A + B + C = T.S.T., \tag{4.2.36}$$

if we can demonstrate that

$$\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \left| \frac{(U^0 - U^\infty)}{Q(U^0,\, V^0)} \right| d\rho \le C_2(\epsilon), \tag{4.2.37}$$

where $C_2(\epsilon)$ has at most algebraic growth. This may be accomplished by showing that

$$\Phi(\rho) := \left|\frac{U^0 - U^\infty}{Q(U^0, V^0)}\right| \le C_3, \quad \rho \in (-\infty, \infty), \tag{4.2.38}$$

where $C_3 = \mathcal{O}(1)$, and clearly by symmetry it suffices to demonstrate (4.2.38) for $\rho \in (0, \infty)$. By the assumptions on $Q(u, v)$ given in (2.4) (optimal-where..), we have that

$$\Phi(\rho) \le C_4 \left|\frac{U^0 - U^\infty}{U^0(1 - U^0)(1/2 - V^0)(1/2 + V^0)}\right|, \quad \rho \in (0, \infty),$$

where $C_4 = \mathcal{O}(1)$. And from the assumptions on the geodesics and the discussion in §2, we have that for $\rho \in (0, \infty)$, the function $U^0(\rho)$ stays uniformly bounded away from 0 and 1, $V^0(\rho)$ is uniformly bounded away from $-1/2$, and $|1/2 - V^0(\rho)| \ge |V^\infty - V^0(\rho)|$. Therefore,

$$\Phi(\rho) \le C_5 \left|\frac{U^0 - U^\infty}{1/2 - V^0}\right| \le C_5 \left|\frac{U^0 - U^\infty}{V^0 - V^\infty}\right|, \quad \rho \in (0, \infty),$$

where $C_5 = \mathcal{O}(1)$. Recalling the limiting behavior of $(U^0(\rho), V^0(\rho))$ given in (4.2.34), a bound of the form (4.2.38) now readily follows and (4.2.36) is obtained.

Thus

$$\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \mu^{5/2} U^0_\rho \, d\rho = W^0 \int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \left\{\frac{(U^0 - U^\infty)^2}{4Q(U^0, V^0)}\right\} d\rho + T.S.T.. \tag{4.2.39}$$

Note that the bound on $\Phi(\rho)$ obtained above in conjunction with the estimate (4.2.34) also implies that

$$\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \left\{\frac{(U^0 - U^\infty)^2}{4Q(U^0, V^0)}\right\} d\rho = \int_{-\infty}^{\epsilon^\infty} \left\{\frac{(U^0 - U^\infty)^2}{4Q(U^0, V^0)}\right\} d\rho + T.S.T..$$

Moreover, it is not difficult to use similar bounds as well as estimates for V^0_ρ of the form (4.1.28) to obtain that

$$\int_{-\epsilon^{-1/4}}^{\epsilon^{-1/4}} \left\{\frac{(V^0_\rho)^2}{4Q(U^0, V^0)}\right\} d\rho = \int_{-\infty}^{\epsilon^\infty} \left\{\frac{(V^0_\rho)^2}{4Q(U^0, V^0)}\right\} d\rho + T.S.T..$$

Therefore, it follows from (4.2.31) and (4.2.33) that to within transcendentally small terms

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

In other words, to leading order

$$W^0 = c_{APB} H^{3/2}, \tag{4.2.40}$$

where

$$c_{APB} = \frac{2\int_{-\infty}^{\infty} \{(U^0_\rho)^2 + (V^0_\rho)^2\} \, d\rho}{\int_{-\infty}^{\infty} \left\{\frac{(U^0 - U^\infty)^2}{4Q(U^0, V^0)} + \frac{4(V^0_\rho)^2}{Q(U^0, V^0)}\right\} d\rho.} \tag{4.2.41}$$

We conclude this section by noting that (4.2.21) and (4.2.26) together imply that

$$\triangle_s \mu = \mathcal{O}(\epsilon^{3/2}). \tag{4.2.42}$$

FIGURE 2. A line of triple junctions where two IPBs and one APB meet.

FIGURE 3. An isosceles triangle in the plane normal to the line of triple junctions.

Remark 4.1. *We shall again see that the limits of integrations in the above integrals may be equally well taken to be* $\pm l(\epsilon)$, *where* $l(\epsilon)$ *is any algebraically large function of* ϵ *which is* $o(\epsilon^{-1})$, *and the resultant variation in the final results will be only T.S.T..*

5. TRIPLE JUNCTION CONDITIONS

In this section we show how the conditions at the triple junction line are obtained, primarily outlining out how the analysis may be reduced to that which appears in [26].

5.1. **Young's law.** To derive Young's law to leading order, we introduce the stretched variable $\eta = \frac{x-m(t)}{\epsilon}$ where $m(t)$ denotes the location of the triple junction. A prism, P, is constructed whose cross section is taken to be given by an isosceles triangle with base length proportional to ϵ^β and whose height is taken to be ϵ^α. See Figure 2. We shall assume that $\alpha = 2\beta$, and that $7/8 < \beta < 1$. The triple junction line is assumed to pass normally through the median plane of the prism, and the base of the isosceles triangle which lies in the median plane is taken to be orthogonal to one of the three interfaces which meet along the triple junction line. An orthonormal co-ordinate system $\eta = (\zeta, \xi, z)$ is constructed so that ζ is tangent at the triple junction to the interface which intersects the base of the triangle and points outward and z is tangent to the triple junction line at $\eta = 0$. See Figure 3.

We now reduce the analysis here to the analysis presented in [26, 3]. To do so, we write the first two equations in (2.9) in terms of $\eta = (\zeta, \xi, z)$ and $U = U(\eta)$, $V = V(\eta)$,

$$\epsilon^{7/2}(W_t - \epsilon^{-1} m_t \cdot \nabla_\eta V) = -\frac{1}{4} Q(U, V)[F_v - \triangle_\eta V], \tag{5.1.1}$$

$$\mu = F_u - \triangle_\eta U. \tag{5.1.2}$$

If time has been appropriately scaled in our problem, we may assume that $V_t = \mathcal{O}(1)$ and $m_t = \mathcal{O}(1)$. Moreover, assuming the spatial variation in U and V to be no more rapid in the vicinity of the triple junction line than it is within the inner region, then $\nabla_\eta V = \mathcal{O}(1)$. These estimates allow us to conclude from (5.1.1) that

$$-\frac{1}{4} Q(U, V)[F_v - \triangle_\eta V] = \mathcal{O}(\epsilon^{5/2}). \tag{5.1.3}$$

We consider now the implications of (5.1.3) on the size of the term in square brackets. Note that according to §3, within the outer region $Q = \mathcal{O}(e^{-c/\sqrt{\epsilon}})$ and $F_v - \triangle_\eta V = \mathcal{O}(\epsilon^{1/2})$. And within the inner regions, we have seen in §4.1−§4.2 that $Q = \mathcal{O}(1)$ and that $F_v - \triangle_\eta V$ is $\mathcal{O}(\epsilon)$ along IPBs and $\mathcal{O}(\epsilon^{5/2})$ along APBs. If the behavior at the triple junction is not more singular than elsewhere, the mildest assumption which is consistent with (5.1.3) and the above estimates is that

$$F_v - \triangle_\eta V = \mathcal{O}(\epsilon^{1/2}). \tag{5.1.4}$$

Note that stronger assumptions were made in [26], but (5.1.4) is more modest and suffices for the analysis which follows.

Multiplying (5.1.2) by U_ξ and (5.1.4) by V_ξ, then adding, integrating over $\widetilde{P}$ where $\widetilde{P}$ corresponds to the prism P after its dimensions have been stretched by ϵ^{-1}, and using Gauss' theorem, we obtain

$$\int_{\partial \widetilde{P}_{sides}} \Big\{[F - \mu U + \frac{1}{2}(U_\zeta^2 + V_\zeta^2) - \frac{1}{2}(U_\xi^2 + V_\xi^2)]\hat{e}_\xi - (U_\zeta U_\xi + V_\zeta V_\xi)\hat{e}_\zeta\Big\} \cdot \hat{n}\, dS$$
$$= A + B + C + D, \tag{5.1.5}$$

where $\hat{e}_\zeta$ and $\hat{e}_\xi$ denote unit vectors in the positive ζ and ξ directions respectively, $\hat{n}$ denotes a unit exterior normal to $\partial \widetilde{P}_{sides}$, and

$$A := \Big[\int_{\partial \widetilde{P}_{top}} - \int_{\partial \widetilde{P}_{bottom}}\Big](U_z U_\xi + V_z V_\xi)\, dS,$$
$$B := \mathcal{O}(\epsilon^{1/2}) \int_{\widetilde{P}} V_\xi\, dV,$$
$$C := \int_{\widetilde{P}} \mu_\xi\, U\, dV,$$
$$D := -\frac{1}{2}\int_{\partial \widetilde{P}_{sides}} (U_z^2 + V_z^2)\, \hat{e}_\xi \cdot \hat{n}\, dS$$

We now estimate the terms A, B, C, and D. One readily estimates that $A \le \sup_{\widetilde{P}} |(U_\xi U_z + V_\xi V_z)_z| C\epsilon^{\alpha+\beta-2}$, where $C\epsilon^{\beta-1}$ represents the area of $\partial \widetilde{P}_{top}$. Assuming, as is the case in the inner and outer solution, that the derivative of U and V normal to the interfaces is at most $\mathcal{O}(1)$, but that the derivatives of U and V in directions tangent to the interfaces are expected to be at most $\mathcal{O}(\epsilon)$, and taking into account that the variables ξ, z have been scaled by ϵ^{-1}, we obtain that $A = \mathcal{O}(\epsilon^{\alpha+\beta})$. Variation in the shape of the interface, which may be roughly estimated via its curvature, has been taken into account here by taking α to be sufficiently small. As for B, we may obtain the rough estimate that $B = \mathcal{O}(\epsilon^{-5/2+\alpha+2\beta})$. Assuming that $\mu = \mathcal{O}(\epsilon^{1/2})$ and that μ exhibits no rapid variation, we see that $C = \mathcal{O}(\epsilon^{-3/2+\alpha+2\beta})$. Similar considerations to those used in estimating A yield that $D = \mathcal{O}(\epsilon^{\alpha+\beta})$. Thus,

$$\int_{\partial \widetilde{P}_{sides}} \Big\{[F - \mu U + \frac{1}{2}(U_\zeta^2 + V_\zeta^2) - \frac{1}{2}(U_\xi^2 + V_\xi^2)]\hat{e}_\xi - (U_\zeta U_\xi + V_\zeta V_\xi)\hat{e}_\zeta\Big\} \cdot \hat{n}\, dS = \mathcal{O}(\epsilon^{-5/2+\alpha+2\beta}). \tag{5.1.6}$$

Let $G = G(\zeta,\, \xi,\, z)$ denote the integrand in the integral in (5.1.6). Taylor expanding,

$$G(\zeta,\, \xi,\, z) = G(\zeta,\, \xi,\, 0) + zG_z(\zeta,\, \xi,\, \hat{z}(\zeta,\, \xi)).$$

Therefore for $z \in (-\epsilon^{\alpha-1},\, \epsilon^{\alpha-1})$, under the assumption that the variation in the z direction is $\mathcal{O}(\epsilon)$,

$$G(\zeta,\, \xi,\, z) = G(\zeta,\, \xi,\, 0)(1 + \mathcal{O}(\epsilon^\alpha)).$$

Returning to (5.1.6), we find that

$$\epsilon^{\alpha-1}(1 + \mathcal{O}(\epsilon^\alpha)) \int_{\partial \widetilde{T}} \Big\{[F - \mu U + \frac{1}{2}(U_\zeta^2 + V_\zeta^2) - \frac{1}{2}(U_\xi^2 + V_\xi^2)]\hat{e}_\xi - (U_\zeta U_\xi + V_\zeta V_\xi)\hat{e}_\zeta\Big\} \cdot \hat{n}\, dS$$
$$= \mathcal{O}(\epsilon^{-5/2+\alpha+2\beta}), \tag{5.1.7}$$

where $\partial \widetilde{T}$ denotes the perimeter of the isosceles triangle lying in the median plane of $\widetilde{P}$.

Note now that the integral on the left hand side of the above equation is precisely of the form of the integral treated in [26, 3], hence in order to implement the analysis there, it remains only to show than the integral of the left hand side is significantly larger that the error estimate on the right hand side. However note that the gradient term $(U_\xi^2 + V_\xi^2)$ can be expected to be $\mathcal{O}(1)$ throughout the inner regions, so this term yields a contribution which is $\mathcal{O}(1)$. This estimate is corroborated by the analysis in [26] which implies that this is precisely the size of the integral on the left. In fact we can divide through both sides of (5.1.7) by $\epsilon^{\alpha-1}(1+\mathcal{O}(\epsilon^{\alpha}))$ to obtain an overall error term of $\mathcal{O}(\epsilon^{1/4})$ if we take $7/8 < \beta < 1$ so as to guarantee that $1/4 < (\alpha + 2\beta - 5/2) - (\alpha - 1)$. In fact we can obtain $\mathcal{O}(\epsilon^{1/2-\tilde{\delta}})$ accuracy for any $0 < \tilde{\delta} << 1$ by taking $1 - \tilde{\delta}/2 < \beta < 1$. We remark that if we were to make a slightly stronger (and not unreasonable) assumption on the size of B earlier, $\mathcal{O}(\epsilon^{1/2})$ accuracy would be guaranteed.

We may now follow the steps in the analysis in [26] to conclude that to within the accuracy cited above, Young's law holds; i.e.,

$$\frac{\sin\phi_1}{\sigma_1} = \frac{\sin\phi_2}{\sigma_2} = \frac{\sin\phi_3}{\sigma_3}, \tag{5.1.8}$$

where for $i = 1, 2, 3$, ϕ_i denotes the angle opposite interface Γ_i and

$$\sigma_i := \int_{-\infty}^{\infty} [(U_i^0)_\rho^2 + (V_i^0)_\rho^2]\, d\rho, \tag{5.1.9}$$

where σ_i denotes the surface energy of Γ_i. In (5.1.9) $(U_i^0(\rho),\, V_i^0(\rho))$ denotes the leading order approximations to the inner solution along Γ_i. See Figure 3.

5.2. **Balance of fluxes.** We shall reduce the present analysis to the analysis which appears in [26], employing the prisms P and $\widetilde{P}$ and the variables η, $U(\eta)$, $V(\eta)$ which were introduced in §5.1. In terms of these variables, we obtain as in [26] that

$$\epsilon^{5/2}(U_t - \epsilon^{-1} m_t \cdot \nabla_\eta U) = \nabla_\eta \cdot \vec{J}.$$

Making the same scaling assumptions as in §5.1, integrating over $\widetilde{P}$, and using the divergence theorem,

$$\int_{\partial\widetilde{P}} \hat{n}\cdot\vec{J} = \mathcal{O}(\epsilon^{\alpha+2\beta-3/2}). \tag{5.2.1}$$

Estimates similar to those which we made for A in §5.1 yield that

$$\int_{\partial\widetilde{P}_{top}} \hat{n}\cdot\vec{J} + \int_{\partial\widetilde{P}_{bottom}} \hat{n}\cdot\vec{J} = \mathcal{O}(\epsilon^{\alpha+\beta+1/2}). \tag{5.2.2}$$

Using (5.2.2) and Taylor expanding about $z = 0$ as in §5.1, we may conclude that

$$\epsilon^{\alpha-1}(1+\mathcal{O}(\epsilon^{\alpha})) \int_{\partial\widetilde{T}} \hat{n}\cdot\vec{J}\, dS = \mathcal{O}(\epsilon^{\alpha+2\beta-3/2}),$$

where $\partial\widetilde{T}$ denotes the perimeter of the isosceles triangle which lies in the median plane of $\widetilde{P}$. Dividing both side of the above equation by $\epsilon^{\alpha-1}(1+\mathcal{O}(\epsilon^{\alpha}))$, the analysis has been reduced to that which appears in §5.2 of [26]. By considering the overall error estimate given here and the steps undertaken in [26], this implies that for $7/8 < \beta < 1$ to within $\mathcal{O}(\epsilon^{1/2})$ accuracy,

$$0 = \sum_{i=1}^{3} M_i \tau_i \cdot \nabla \mu_i^{1/2}. \tag{5.2.3}$$

In (5.2.3), $\mu_i^{1/2}$ denotes the coefficient of $\epsilon^{1/2}$ in the perturbation expansion for μ along Γ_i and τ_i denotes a unit tangent to Γ_i at $m(t)$ pointing outwards from the triple junction which lies in the median plane of P, and

$$M_i := \int_{-l(\epsilon)}^{l(\epsilon)} Q(U_i^0(\rho),\, V_i^0(\rho))\, d\rho,$$

Figure 4. A curve along which an IBP or an ABP intersects the exterior boundary of the domain, $\partial\Omega$.

Figure 5. The intersection of a rectangle with Ω, in the plane normal to the curve of intersections described in Figure 4

where $l(\epsilon)$ is any algebraically large function of ϵ which is $o(\epsilon^{-1})$ and $(U_i^0(\rho),\, V_i^0(\rho))$ is again the leading order approximation to the inner solution along Γ_i.

5.3. **Continuity of the chemical potential.** If we wish to consider solutions with some minimal regularity requirements, then it is physically reasonable to consider solutions for which the chemical potential is continuous (Note, however, that continuity of the chemical potential does not follow immediately even in one space dimension from the results in [10].). Continuity of the chemical potential implies equality of the chemical potentials as evaluated on two IPBs which meet at a triple junction line. More specifically, referring to (4.1.5), (4.1.20), and proceeding as in [26], this means that

$$H^{-1/2}|_{IPB_1} + H^{-1/2}|_{IPB_2} = \mathcal{O}(\epsilon^{1/2}), \tag{5.3.1}$$

where IPB_1 and IPB_2 denote two IPBs meeting along a triple junction line and $H^{-1/2}|_{IPB_1}$, $H^{-1/2}|_{IPB_2}$ refer to their (scaled) mean curvatures.

6. Conditions at the exterior boundary

We consider here the conditions which hold along a line of intersections where an interface Γ, which may be either an IPB or an APB, intersects $\partial\Gamma$. The analysis here completely parallels that which appears in §5 except that instead of a prism construction, we shall construct a parallelopiped whose cross sectional dimensions are proportional to ϵ^β and whose height is given by ϵ^α. See Figure 4. We may assume as in §5 that $7/8 < \beta < 1$ and $\alpha = 2\beta$. We shall take the median plane of the parallelopiped to be normal to the line of intersections. Moreover, we shall assume that the midpoint of one of the sides of the parallelopiped is tangent to the line of intersections, and we denote this point of tangency by $m(t)$. The majority of the parallelopiped will be taken to lie within Ω, and we denote by R its intersection with Ω. See Figure 5. Let us introduce the stretched variable $\eta = \frac{x-m(t)}{\epsilon}$ and the coordinates $\eta = (\zeta,\, \xi)$, where ξ is parallel to Γ and points outwards from Ω.

We proceed now as in §5.1, working first with the first two equations in (2.9), except that now instead of multiplying by $(U_\xi,\, V_\xi)$, we multiply by $(\partial_\tau U,\, \partial_\tau V)$. Making estimates which parallel those given in §5, we find that

$$\phi = \frac{\pi}{2} \tag{6.0.1}$$

to within the same accuracy as was obtained in §5.1.

Afterwards we consider the third equation in (2.9). By working with R and η and taking steps which parallel those in §5.2 and those in §6.1 of [26], we may conclude that to within an $\mathcal{O}(\epsilon^{1/2})$ error,

$$\hat{n} \cdot \nabla \mu^{1/2} = 0, \tag{6.0.2}$$

where $\hat{n}$ denotes the unit exterior normal to $\partial\Omega$ at $m(t)$ which lies in the median plane of R, and $\mu^{1/2}$ denotes the coefficient of $\epsilon^{1/2}$ in the perturbation expansion for the chemical potential along Γ. Recalling (4.1.20), we see that along $IPBs$, (6.0.2) may also be expressed as

$$\hat{n} \cdot \nabla H^{-1/2} = 0, \tag{6.0.3}$$

where $H^{-1/2}$ is the coefficient of $\epsilon^{-1/2}$ in the perturbation expansion for the mean curvature H of the IPB.

7. Discussion

In this paper we have undertaken asymptotics for the AC/CH system in a bounded domain $\Omega \subset R^3$ based on the assumptions that $\Theta = \epsilon^{1/2}$, $1/2 - \bar{u} = \mathcal{O}(\epsilon^{3/2}$, and that the mean curvature of the IPBs and APBs are respectively $\mathcal{O}(\epsilon^{-1/2})$ and $\mathcal{O}(\epsilon^{3/2})$. The results of our asymptotic analysis are summarized in Figure 6.

Figure 6. A schematic summary of the limiting equations of motion, to leading order.

In the outer region, according to our analysis, u and v are T.S.T. close to the global minimizers of the homogeneous free energy, the mass flux $\vec{j}$ and the mobility Q are T.S.T., and the chemical potential, μ, and F_u, F_v have regular perturbation expansions in terms of $\epsilon^{1/2}$.

To obtain an evolution equation for IPB motion, asymptotics were undertaken at levels $\mathcal{O}(\epsilon^{-1})$ through $\mathcal{O}(\epsilon^{3/2})$. To leading order IPBs move by surface diffusion. Stated more precisely, the normal velocity of the IPB is proportional to minus the Laplace-Beltrami operator acting on $H^{-1/2}$, where $H^{-1/2} = H\epsilon^{1/2} + o(\epsilon^{1/2})$ is the leading order coefficient in the expansion for the mean curvature of the IPB. See (4.1.26). The precise choice of the location of the mid-surface of the inner region does not influence the equation of motion for IPBs to leading order.

To obtain an evolution equation for the APBs, asymptotics were undertaken at levels $\mathcal{O}(\epsilon^{-1})$ through $\mathcal{O}(\epsilon^{5/2})$, and the mid-surface of the inner region was defined via symmetry considerations. Our calculations gave that APBs move according to motion by mean curvature. In other words, the normal velocity of the APB is proportional to $H^{3/2}$ where $H^{3/2} = H\epsilon^{-3/2} + o(\epsilon^{-3/2})$ is the leading order coefficient in the expansion for the mean curvature of the APB. Moreover, $\triangle_s \mu = 0$ to $\mathcal{O}(\epsilon^{3/2})$ accuracy. See (4.2.41) and (4.2.42).

At triple junction lines, we found in that Young's law holds to $\mathcal{O}(\epsilon^{1/2-\tilde{\delta}})$ accuracy, for any $0 < \tilde{\delta} << 1$. See (5.1.8). We also obtain that to $\mathcal{O}(\epsilon^{1/2})$ accuracy, a balance of mass flux condition holds and that continuity of the chemical potential implies that the mean curvatures of two IPBs joining along a triple junction line should be equal and of opposite sign. See (5.2.3) and (5.3.1).

When an IPB or an APB intersect with the exterior boundary of the domain $\partial\Omega$, we found that to within $\mathcal{O}(\epsilon^{1/2-\tilde{\delta}})$ accuracy for any $0 < \tilde{\delta} << 1$, the intersections are normal and that to within $\mathcal{O}(\epsilon^{1/2})$ a no-flux condition holds. See (6.0.1) and (6.0.2),(6.0.3).

Analytical and qualitative properties for the limiting equations of motion will be discussed in future publications.

I. Appendix

Let us consider the equations

$$\begin{aligned} F_{UU}\widetilde{U} + F_{UV}\widetilde{V} - \widetilde{U}_{\rho\rho} &= G_U, \\ F_{UV}\widetilde{U} + F_{VV}\widetilde{V} - \widetilde{V}_{\rho\rho} &= G_V, \end{aligned} \tag{I.1}$$

where $F_{UU} := F_{UU}(U^0, V^0)$, $F_{UV} := F_{UV}(U^0, V^0)$, and $F_{VV} := F_{VV}(U^0, V^0)$, where (U^0, V^0) denotes either of the heteroclinic orbits referred to within the text with regard to APBs, and $G_U(\rho)$ and $G_V(\rho)$ are arbitrary functions which belong to $\mathcal{C}(-\infty, \infty)$ with finite limits at $\pm\infty$. Note now that if we look for classical solutions to (I.1) with finite limits at $\pm\infty$, this implies that at $+\infty$,

$$\begin{aligned} F_{UU}(\infty)\widetilde{U}(\infty) + F_{UV}(\infty)\widetilde{V}(\infty) &= G_U(\infty), \\ F_{UV}(\infty)\widetilde{U}(\infty) + F_{UU}(\infty)\widetilde{V}(\infty) &= G_V(\infty). \end{aligned} \tag{I.2}$$

Since matching implies that in the notation of §2, $F_{UU}(\infty) = F^0_{UU}$, $F_{UV}(\infty) = F^0_{UV}$, and $F_{VV}(\infty) = F^0_{VV}$, and since $F^0_{UU}F^0_{VV} - (F^0_{UV})^2 > 0$ by (2.7), (I.2) may be solved to yield:

$$\widetilde{U}(\infty) = \frac{F^0_{VV}G_U(\infty) - F^0_{UV}G_V(\infty)}{F^0_{UU}F^0_{VV} - (F^0_{UV})^2} \quad \text{and} \quad \widetilde{V}(\infty) = \frac{-F^0_{UV}G_U(\infty) + F^0_{VV}G_V(\infty)}{F^0_{UU}F^0_{VV} - (F^0_{UV})^2}. \tag{I.3}$$

Remark I.1. *Since it is readily verified that F^0_{UU}, F^0_{UV}, and F^0_{VV} are all $\mathcal{O}(e^{c/\sqrt{\epsilon}})$, it follows from (I.3) that if $G_U(\infty)$ and $G_V(\infty)$ are $\mathcal{O}(1)$, then $\widetilde{U}(\infty)$ and $\widetilde{V}(\infty)$ are $\mathcal{O}(e^{-c/\sqrt{\epsilon}})$. A similar argument demonstrates that $\widetilde{U}(-\infty)$ and $\widetilde{V}(-\infty)$ are $\mathcal{O}(e^{-c/\sqrt{\epsilon}})$. This, in conjunction with matching reaffirms self-consistency of the asymptotics within the framework of the assumptions made on u and v in the outer solution.*

It follows from Theorem 2.2 and Lemma 5.1 in [31, Section 2] and (2.7) that we may rely on the Fredholm alternative to conclude that there exists a unique classical solution to (I.1),(I.3) which is orthogonal to the solutions of the null adjoint equation, which in the present context may be taken as

$$\begin{aligned} F_{UU}\widetilde{U} + F_{UV}\widetilde{V} - \widetilde{U}_{\rho\rho} &= 0, \\ F_{UV}\widetilde{U} + F_{VV}\widetilde{V} - \widetilde{V}_{\rho\rho} &= 0, \end{aligned} \tag{I.4}$$

in conjunction with the boundary conditions:

$$\widetilde{U}_\rho(\pm\infty) = \widetilde{V}_\rho(\pm\infty) = 0. \tag{I.5}$$

It is readily verified that (U^0_ρ, V^0_ρ) constitutes a solution to (I.4)-(I.5), and it is not difficult to demonstrate that there are no further solutions to (I.4)-(I.5) which are linearly independent of (U^0_ρ, V^0_ρ).

Claim I.2. *Let (U^0, V^0) denote the heteroclinic orbit which connects the two ordered variants, and let us assume that G_U is even and G_V is odd. Then the unique solution $(\widetilde{U}, \widetilde{V})$ to (I.1)-(I.3) which is orthogonal to (U^0_ρ, V^0_ρ) satisfies*

$$\widetilde{U}(\rho) = \widetilde{U}(-\rho), \quad \widetilde{V}(\rho) = -\widetilde{V}(-\rho), \quad \textit{for all} \quad \rho \in (-\infty, \infty).$$

Proof. Let us decompose $\widetilde{U}$ and $\widetilde{V}$ into their even (symmetric) and odd (anti-symmetric) parts

$$\begin{aligned} \widetilde{U} &= \widetilde{U}^S + \widetilde{U}^A, \\ \widetilde{V} &= \widetilde{V}^S + \widetilde{V}^A, \end{aligned}$$

and write $(\widetilde{U},\,\widetilde{V})$ as

$$(\widetilde{U},\,\widetilde{V}) = (\widetilde{U}^S,\,\widetilde{V}^A) + (\widetilde{U}^A,\,\widetilde{V}^S).$$

Recalling that if $(U^0,\,V^0)$ denotes the heteroclinic orbit connecting two ordered variants, then (see remarks below (4.2.15)) $F_{UU}(\rho)$ and $F_{VV}(\rho)$ are symmetric and $F_{UV}(\rho)$ is antisymmetric, the equations to be satisfied by $(\widetilde{U}^S,\,\widetilde{V}^A)$ can be found by separating out the appropriate even and odd parts of (I.1)-(I.3). Namely,

$$\begin{aligned} F_{UU}\widetilde{U}^S + F_{UV}\widetilde{V}^A - \widetilde{U}^S_{\rho\rho} &= G_U, \\ F_{UV}\widetilde{U}^S + F_{VV}\widetilde{V}^A - \widetilde{V}^A_{\rho\rho} &= G_V, \end{aligned} \tag{I.6}$$

in conjunction with the boundary conditions:

$$\widetilde{U}^S(\pm\infty) = \widetilde{U}(\pm\infty), \quad \widetilde{V}^A(\pm\infty) = \widetilde{V}(\pm\infty). \tag{I.7}$$

But noting that the systems (I.1),(I.3) and (I.6)-(I.7) are in fact identical, it follows from the Fredholm alternative that

$$\widetilde{U} = \widetilde{U}^S + kU^0_\rho \ \text{ and } \ \widetilde{V} = \widetilde{V}^A + kV^0_\rho.$$

Since U^0 is even and V^0 is odd, it follows that U^0_ρ is odd and V^0_ρ is even. Therefore, implementing the orthogonality normalization condition $(\widetilde{U},\,\widetilde{V}) \perp (U^0_\rho,\,V^0_\rho)$ (*c.f.* §4.1), we find that k must vanish, which proves the Claim. □

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I. Figure Captions

Figure 1. The region $B := \{(u, v) \in R^2 : 0 < u + v < 1, 0 < u - v < 1\}$.

Figure 2. A line of triple-junctions where two IPBs and one APB meet.

Figure 3. An isosceles triangle in the plane normal to the line of triple-junctions.

Figure 4. A curve along which an IBP or an ABP intersects the exterior boundary of the domain, $\partial\Omega$.

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