

Approximation of motion of interface junctions using a vector-valued distance function

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Abstract

We review the research regarding the analysis of junction motion due to mean curvature flow and give a suggestion for a possible future direction of dealing with general topological changes in interface network motion. We present a related numerical scheme using a vector-valued signed distance function and provide its formal analysis.

1 Motivation

The ultimate goal of the present research is to provide a mathematical understanding for the phenomenon of moving droplets and bubbles attached to surfaces, including a clarification of the dynamics of contact angle, which is still not fully understood.

In previous papers ([20], [12], etc.), we have developed a scalar model for this kind of droplet motion and studied its mathematical properties. In the scalar setting we assume that the shape of the droplet can be described by the graph of a scalar function $u : \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R}$ and base the model equation on the surface energy for the considered system.

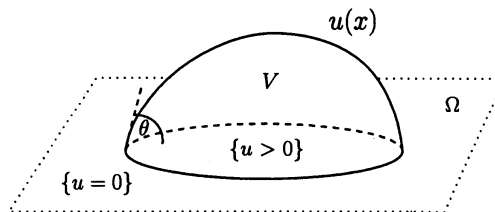


Figure 1: Scalar setting of the moving droplet problem.

The surface energy after scaling can be written in the form

$$E(u) = \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + \gamma \chi_{u>0} \right) dx,$$

where γ depends on the surface tensions of the present surfaces and $\chi_{u>0}$ is the characteristic function of the set $\{x \in \Omega : u(t, x) > 0\}$. The candidates for the shape of the droplet are restricted by the constraint

$$\int_{\Omega} u \chi_{u>0} dx = V,$$

which expresses the volume conservation of the fluid surrounded by the graph of u .

One can either consider the gradient flow for E , which yields the model equation

$$\begin{aligned} u_t &= \Delta u + \chi_{u>0} \lambda(u) && \text{in } \{u > 0\} \\ |\nabla u|^2 &= 2\gamma && \text{on } \partial\{u > 0\}, \end{aligned}$$

or apply Hamilton's principle on the action integral corresponding to E , which gives the model equation

$$\begin{aligned} \chi_{u>0} u_{tt} &= \Delta u + \chi_{u>0} \lambda(u) && \text{in } \{u > 0\} \\ |\nabla u|^2 - u_t^2 &= 2\gamma && \text{on } \partial\{u > 0\}. \end{aligned}$$

Here, λ is a function of t only, a nonlocal term depending on u , that can be interpreted as the Lagrange multiplier for the volume constraint.

The second identity in the above models is an additional condition necessary to determine the position of the unknown free boundary $\partial\{u > 0\}$. It is a certain approximation of the Young's law for the considered scalar setting. Notice that for the parabolic problem the contact angle at the free boundary is fixed during the motion, while in the hyperbolic model it depends on the evolution. Moreover, it is important to take into account that the contact angle condition in this model is not a priori prescribed but naturally follows from the variation of the energy (or action integral).

The above approach allows for some mathematical analysis but physically it provides only an approximation of the motion in the sense that the surface energy is simplified to the Dirichlet functional and in fact permits only vertical motions of the droplet's surface. Moreover, the scalar formulation can deal only with contact angles that are less or equal to $\pi/2$, which is not always the case in reality. Therefore, we extend the scalar setting to the motion of hypersurfaces in $\mathbb{R}^n$ due to reduction of their exact surface energy. In addition, to incorporate the contact angle dynamics, we generalize the setting to the multiphase problem, where the hypersurfaces represent interfaces between more than two phase regions, and thus form junctions. A more precise formulation of the problem is given in the following section.

2 The multiphase problem

In this section, we derive the governing equations for a network of interfaces moving according to the gradient flow of surface energy. Consider a partition of $\mathbb{R}^N = P_1 \cup P_2 \cup \dots \cup P_k$ into k mutually exclusive phase regions $P_i \subset \mathbb{R}^N$ ($i = 1, 2, \dots, k$). Let $\Gamma := \bigcup \{\gamma_{ij} : i, j = 1, 2, \dots, k\}$, where $\gamma_{ij} = \gamma_{ji}$ denotes the interface between phases P_i and P_j .

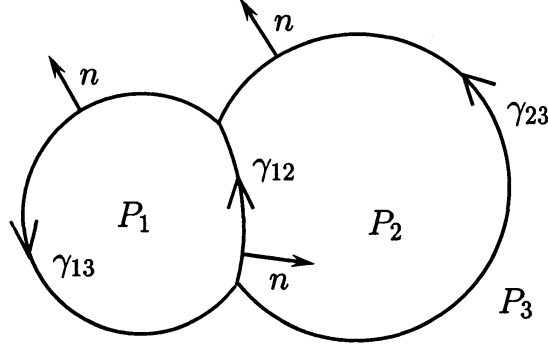


Figure 2: An example of multiphase configuration.

To make the derivation transparent, we consider a special case of three evolving interfaces $\gamma_i(s)$, $s \in [p_i, q_i]$, $i = 1, 2, 3$, inside a fixed smooth region Ω of $\mathbf{R}^2$, that meet the outer boundary $\partial\Omega$ at a right angle and get together at a triple junction $J = \gamma_i(q_i)$, $i = 1, 2, 3$. In general, each interface has different surface tension σ_i .

Then the total surface energy is given by

$$E(\Gamma) = \sum_{i=1}^3 \int_{\gamma_i} \sigma_i dl = \sum_{i=1}^3 \int_{p_i}^{q_i} \sigma_i |\gamma'_i(s)| ds.$$

The gradient flow of the surface energy can be found from its variation. Define the tangential vector t_i , curvature κ_i and outer normal n_i of curve γ_i by

$$t_i = \frac{\gamma'_i}{|\gamma'_i|}, \quad \kappa_i = \frac{\gamma'_{ix}\gamma''_{iy} - \gamma'_{iy}\gamma''_{ix}}{|\gamma'_i|^3}, \quad n_i = \frac{1}{|\gamma'_i|}(\gamma'_{iy}, -\gamma'_{ix}).$$

Then for a smooth vector field φ vanishing near the boundary $\partial\Omega$,

$$\begin{aligned} \frac{d}{d\varepsilon} L(\Gamma + \varepsilon\varphi(\Gamma))|_{\varepsilon=0} &= \sum_{i=1}^3 \int_{p_i}^{q_i} \sigma_i t_i \cdot \frac{d}{ds}(\varphi(\gamma_i)) ds \\ &= - \sum_{i=1}^3 \left(\int_{p_i}^{q_i} \sigma_i t'_i \varphi(\gamma_i) ds - \sigma_i t_i \cdot \varphi(J) \right) \\ &= \sum_{i=1}^3 \left(\int_{\gamma_i} (\sigma_i \kappa_i n_i) \cdot \varphi dl + \sigma_i t_i \cdot \varphi(J) \right). \end{aligned}$$

Hence, the gradient flow of triple junctions leads to normal velocities of points on interfaces

$$v_i = -\sigma_i \kappa_i,$$

and the condition at the triple junction

$$\sum_{i=1}^3 \sigma_i t_i = 0.$$

The above junction condition represents the balance of forces which is known to be equivalent to the Young's law

$$\frac{\sin \theta_1}{\sigma_1} = \frac{\sin \theta_2}{\sigma_2} = \frac{\sin \theta_3}{\sigma_3},$$

where θ_i is the angle formed by the phase P_i at the junction.

The above derivation addresses a special case of three interfaces in a plane but it is easy to see that it can be extended to arbitrary interface networks in $\mathbb{R}^n$. In the sequel, we deal only with interface networks that have the same surface tension for all interfaces. Then the normal velocity for any interface can be set as $v = -\kappa$, where κ is the mean curvature. The balance of forces at triple junctions in a plane then reduces to the Herring condition imposing symmetric junctions with 120° angles. The junction condition for quadruple and higher junctions has the same form but does not prescribe a unique angle configuration. In the following we avoid such mathematical and technical complications by confining ourselves to the case of triple junctions of curves in a plane.

There are several works dealing with the analysis of triple junctions. [2] derived curvature motion and junction condition from a vector-valued Ginzburg-Landau equation and showed short-time existence by employing linearization around the initial condition and a fixed point argument. [14] gave global existence of planar network close to equilibrium. [5] studied exponential stability for area-preserving mean curvature flow. [9] deals with global existence, local uniqueness and nonlinear stability, while [4] extends the local existence to general dimension. [15] showed that no singularity can occur for a triod unless the length of one curve goes to zero. There exist also rare results within the rigorous geometric measure theory, e.g., [13] analyzes the regularity for weak varifold solutions. Moreover, the recent paper [11] provides local regularity for general networks with several multiple junctions.

3 Level set approach

The most difficult aspect of such a network evolution from both the mathematical and numerical point of view are topological changes related to attaching, merging or pinching of interfaces, or to merging or splitting of junctions. One example of such topological change from [17], computed by the method presented in this paper, is shown below.

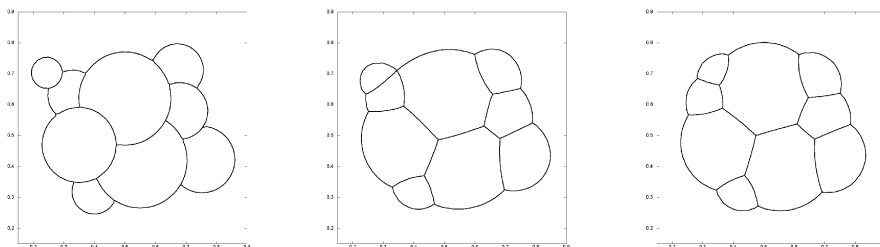


Figure 3: Initial 10-phase configuration (left); its evolution after some time, forming a quadruple junction (center); and its stable configuration, where the quadruple junction has split into two triple junctions (right).

For the two phase case, i.e., one interface separating two phase regions, this problem was solved by the level-set method. The idea of this method is to express the interface as the level set of a smooth function $u(t, x)$ and write the equation for the evolution of u , which corresponds to the mean curvature flow of the interface. It is found that the governing equation is of the type

$$\frac{\partial u}{\partial t} - |\nabla u| \operatorname{div} \left(\frac{\nabla u}{|\nabla u|} \right) = 0.$$

This equation is degenerate and nonlinear but enjoys the comparison principle. Thanks to this fact, the authors of [3], [8] succeeded in introducing a notion of its solution in the viscosity sense. This immediately leads to a rigorous definition of mean curvature flow including topological changes since such changes are naturally handled by the level set function.

Since the level set equation is hard to deal with in practice, several methods for its approximation were developed. One of them is the phase-field method solving instead of the nonlinear equation the Allen-Cahn PDE

$$u_t = \varepsilon \Delta u - \frac{1}{\varepsilon} f'(u),$$

where ε is a small positive parameter and f is a double-well potential. The solution of this equation develops transition layers which approximate the mean curvature motion in the sense of the level set equation. The phase-field method has been extended to the vector-valued setting to treat the multiphase problem and the analysis of its convergence for triple junctions has been started by the paper [2].

Another method, called the BMO method ([16]), is based on a splitting scheme for the phase-field method. In particular, it iterates short-time solution of the heat equation and subsequently of the equation $u_t = -\frac{1}{\varepsilon} f'(u)$, which has the effect of dividing the solution into two regions with values corresponding to the positions of the wells of f . Thus one obtains the following algorithm for evolving the boundary ∂P of a region P by mean curvature flow:

1. Given a region P , set χ to be its characteristic function.
2. Solve the heat equation with initial condition χ :

$$\begin{aligned} u_t(t, x) &= \Delta u(t, x) && \text{for } (t, x) \in (0, \Delta t] \times \Omega, \\ \frac{\partial u}{\partial n}(t, x) &= 0 && \text{on } (0, \Delta t] \times \partial\Omega, \\ u(0, x) &= \chi(x) && \text{in } \Omega. \end{aligned}$$

3. Update χ as the $\frac{1}{2}$ -level set of $u(\Delta t, \cdot)$:

$$\chi(x) = \begin{cases} 1 & \text{if } u(\Delta t, x) > \frac{1}{2}, \\ 0 & \text{if } u(\Delta t, x) \leq \frac{1}{2}. \end{cases}$$

The evolved interface is now the boundary of the set $\{x \in \Omega; \chi(x) = 1\}$.

4. Go back to step 2 to proceed with the computation for the next time step.

This algorithm is very attractive because of its simplicity (it requires only the solution of the heat equation), its ability to naturally treat topological changes and the possibility of its usage in general dimension and under constraints (see [19]). It has been shown, in a general framework including topological changes, that this algorithm converges to motion by mean curvature as $\Delta t \rightarrow 0$ [1, 7, 10]. Extension to the multiphase case was given already in the original paper [16] and a vector-valued approach that is able to include volume constraint is explained in [19].

Regarding the design of a rigorous definition of multiphase mean curvature flow, neither the level set approach, nor its derivatives (phase-field method and BMO method) succeeded until now in finding the way. However, there exists an interesting result by [18], which states that if the signed distance function to an interface satisfies the heat equation (in viscosity sense), then the interface moves by mean-curvature flow in the sense of the corresponding level set equation. This idea was used in the proof of the convergence of the BMO algorithm by the signed distance approach in [10]. Our goal is to extend the notion of signed distance function to interface networks and generalize the result by [18] in order to obtain a definition of multiphase mean curvature flow in the level set viscosity sense. As the first step, we designed a corresponding numerical method and carried out its formal analysis.

4 Vector valued signed distance function

In this section we propose a form of the signed distance function suitable for network analysis and present the corresponding BMO algorithm. There are two reasons for introducing the signed distance function. One of them was mentioned in the previous section – we aim at giving a rigorous definition and analysis of multiphase motion including topological changes. The other reason is related to numerical computations, where it is known that the original BMO algorithm using characteristic functions suffers from restrictions on the time step for uniform meshes. The employment of signed distance function alleviates these restrictions, as was shown in [17].

To define the multiphase version of signed distance function, consider again the partition of $\mathbb{R}^N = P_1 \cup P_2 \cup \dots \cup P_k$ into k mutually exclusive phase regions $P_i \subset \mathbb{R}^N$ ($i = 1, 2, \dots, k$). Let $\Gamma := \bigcup \{\gamma_{ij} : i, j = 1, 2, \dots, k\}$, where $\gamma_{ij} = \gamma_{ji}$ denotes the interface between phases P_i and P_j . Set up reference vectors $\mathbf{p}_i$ corresponding to each phase P_i as unit vectors of dimension $k - 1$ pointing from the centroid of a standard k -simplex to its vertices ([19]). Note that this choice of reference vectors imposes symmetry.

Definition 1. For $\varepsilon > 0$, we define the **signed distance vector** $\delta_\varepsilon : \mathbb{R}^N \rightarrow \mathbb{R}^{k-1}$ by:

$$\delta_\varepsilon(x) := \sum_{i=1}^k \left[1 - \min \left(1, \frac{d_i(x)}{\varepsilon} \right) \right] \mathbf{p}_i,$$

where $d_i := \text{dist}(x, P_i)$ denotes the distance of point x to phase P_i .

One can readily verify that for any point $x \in \Omega$, the following is true for any pair of reference vectors $\mathbf{p}_i$ and $\mathbf{p}_j$:

1. If $B(x, \varepsilon) \cap (P_i \cup P_j) = \emptyset$, then $\delta_\varepsilon(x) \cdot (\mathbf{p}_i - \mathbf{p}_j) = 0$.
2. If $B(x, \varepsilon) \cap (P_i \cup P_j) \neq \emptyset$, then

$$\delta_\varepsilon(x) \cdot (\mathbf{p}_i - \mathbf{p}_j) = \frac{k}{\varepsilon(k-1)} \begin{cases} \varepsilon - d_i(x), & B(x, \varepsilon) \cap P_j = \emptyset \\ d_j(x) - \varepsilon, & B(x, \varepsilon) \cap P_i = \emptyset \\ d_j(x) - d_i(x), & \text{otherwise.} \end{cases}$$

where $B(x, \varepsilon)$ denotes ε -neighborhood of x .

In view of the last identity, the vector-valued δ_ε can be interpreted as a multiphase extension of the scalar signed distance function. Moreover, we note that on interface γ_{ij} , the signed distance vector δ_ε is defined as the sum of reference vectors $\mathbf{p}_i$ and $\mathbf{p}_j$; while on regions away from the ε -tubular neighborhood of interface Γ , δ_ε reduces to the reference vector $\mathbf{p}_i$ corresponding to its phase location i .

The multiphase BMO algorithm using signed distance function ([19], [17]) reads now as follows:

Algorithm 1 (Signed Distance Scheme). Given an initial interface network $\Gamma_0 := \bigcup \{\gamma_{ij} : i, j = 1, 2, \dots, k\}$ and a time step size $\Delta t > 0$, we obtain its mean curvature flow approximation by generating a sequence of time discrete interface networks $\{\Gamma_m\}_{m=1}^M$ at times $t = m\Delta t$ ($m = 1, \dots, M$), as follows:

1. **INITIALIZATION.** Construct δ_ε with respect to Γ_{m-1} .
2. **DIFFUSION STEP.** Solve the vector-valued heat equation until time Δt :

$$\begin{cases} \mathbf{u}_t(t, x) = \Delta \mathbf{u}(t, x) & \text{in } (0, \infty) \times \mathbb{R}^N, \\ \mathbf{u}(0, x) = \delta_\varepsilon(x) & \text{on } \{t=0\} \times \mathbb{R}^N. \end{cases} \quad (1)$$

3. **PROJECTION STEP.** For each x , identify the reference vector $\mathbf{p}_i$ closest to the solution $\mathbf{u}(\Delta t, x)$, that is,

$$\mathbf{p}_i \cdot \mathbf{u}(\Delta t, x) = \max_{j=1,2,\dots,k} \mathbf{p}_j \cdot \mathbf{u}(\Delta t, x). \quad (2)$$

This redistribution of reference vectors determines the approximate new phase regions after time Δt , which in turn, defines the new interface network Γ_m .

5 Formal analysis

In this section, we estimate the normal velocity of an interface subjected to our algorithm and show that indeed, it evolves according to mean curvature flow. Moreover, we give a stability analysis of triple junction under the proposed scheme.

5.1 Interface velocity

Theorem 2. Let $x \in \Gamma := \bigcup \{\gamma_{ij} : i, j = 1, 2, \dots, k\} \subset \mathbb{R}^N$ such that there exists a unique pair (i, j) for which $x \in \gamma_{ij}$. Then, the normal velocity v of interface Γ at x evolving via SD (signed distance) method is

$$v(x) = -\kappa + O(\Delta t), \quad \text{as } \Delta t \rightarrow 0,$$

where κ is $(N - 1)$ -times the mean curvature of Γ at x .

Proof. For simplicity, consider $N = 2$. Fix $\varepsilon > 0$ and select an arbitrary point $x \in \mathbb{R}^2$ on the interface. Without loss of generality, assume $x \in \gamma_{ij}$. Now, rotate and translate the coordinate system so that $x = 0$ in the new coordinate system and its outer normal $\mathbf{n}$ lies in the positive x_2 -direction.

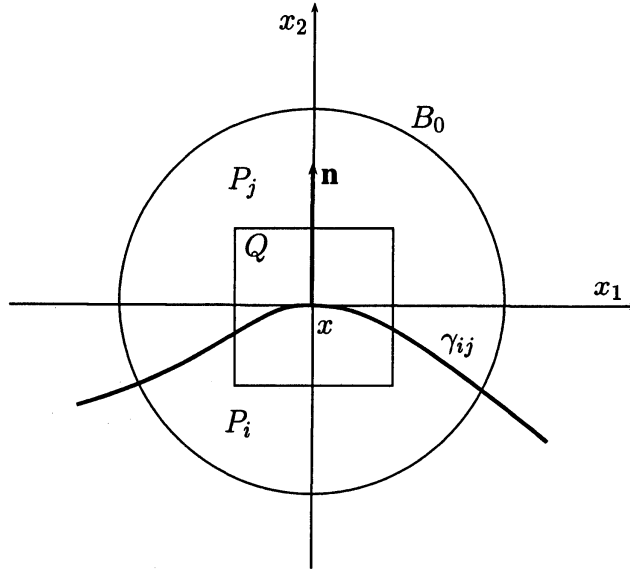


Figure 4: Diagram of the interface for the velocity derivation.

Choose $\tau > 0$, small enough so that the open ball $B_0 := B(0, 2\sqrt{2}\tau)$ contains only phases P_i and P_j . Assume that there exists a smooth function $f : \mathbb{R} \rightarrow \mathbb{R}$ whose graph $(x_1, f(x_1))$ describes interface γ_{ij} inside the ball B_0 . Hence, if $\kappa := \kappa(x_1, f(x_1))$ defines the curvature of the interface γ_{ij} at point $x := (x_1, f(x_1))$, then

$$\begin{aligned} f(0) &= 0 \\ f'(0) &= 0 \\ f''(0) &= -\kappa(0) =: -\kappa \end{aligned}$$

Consider $Q := [-\tau, \tau] \times [-\tau, \tau]$. Assume further that every ε -ball in Q contains a portion of interface γ_{ij} , that is, $\forall x \in Q$, we have $B(x, \varepsilon) \cap Q \cap P_i \neq \emptyset$ and $B(x, \varepsilon) \cap Q \cap P_j \neq \emptyset$, such

that

$$\begin{aligned} d_i(x) &= \text{dist}(x, \gamma_{ij} \cap Q), & \text{if } x \in Q \cap P_j, \\ d_j(x) &= \text{dist}(x, \gamma_{ij} \cap Q), & \text{if } x \in Q \cap P_i. \end{aligned}$$

In this setup, we see that a suitable choice for $\tau < \frac{\varepsilon}{\sqrt{2}}$.

Let $\mathbf{u}$ be the solution of the vector-type heat equation

$$\begin{cases} \mathbf{u}_t(t, x) = \Delta \mathbf{u}(t, x) & \text{in } (0, \infty) \times \mathbb{R}^N, \\ \mathbf{u}(0, x) = \mathbf{u}_0(x) & \text{on } \{t = 0\} \times \mathbb{R}^N. \end{cases}$$

For simplicity, denote $t = \Delta t$. Then, the normal velocity v of interface γ_{ij} at point $x = 0$ obtained from SD method can be found from the relation

$$\mathbf{u}(t, 0, vt) \cdot (\mathbf{p}_i - \mathbf{p}_j) = 0.$$

Hence,

$$0 = \frac{1}{4\pi t} \int_Q + \int_{\mathbb{R}^2 \setminus Q} \delta_\varepsilon(x) \cdot (\mathbf{p}_i - \mathbf{p}_j) e^{-\frac{|x - (0, vt)|^2}{4t}} dx =: I + II.$$

Using the remarks on definition 1, we show that the second integral II is exponentially small:

$$\begin{aligned} |II| &\leq \frac{1}{4\pi t} \int_{\mathbb{R}^2 \setminus Q} |\delta_\varepsilon(x) \cdot (\mathbf{p}_i - \mathbf{p}_j)| e^{-\frac{|x - (0, vt)|^2}{4t}} dx \\ &\leq \frac{k}{k-1} \frac{1}{4\pi t} \int_{\mathbb{R}} \int_{\mathbb{R} \setminus (-\tau, \tau)} + \int_{\mathbb{R} \setminus (-\tau, \tau)} \int_{\mathbb{R}} e^{-\frac{x_1^2 + (x_2 - vt)^2}{4t}} dx_2 dx_1 \\ &\leq C \left[\int_{\frac{\tau - vt}{2\sqrt{t}}}^{\infty} + \int_{\frac{\tau + vt}{2\sqrt{t}}}^{\infty} e^{-x_2^2} dx_2 + 2 \int_{\frac{\tau}{2\sqrt{t}}}^{\infty} e^{-x_1^2} dx_1 \right] \\ &\leq C e^{-\frac{\tau^2}{4t}}. \end{aligned} \tag{3}$$

Some of the estimates used in this proof are shown at the end of this section. On the other hand, since the ε -neighborhood of every point $x \in Q$ contains both phase P_i and P_j , it follows from the second remark of definition 1 that

$$\begin{aligned} I &= \frac{1}{4\pi t} \int_Q \frac{k}{k-1} \left(\frac{d_j(x)}{\varepsilon} - \frac{d_i(x)}{\varepsilon} \right) e^{-\frac{|x - (0, vt)|^2}{4t}} dx \\ &= \frac{k}{\varepsilon(k-1)} \frac{1}{4\pi t} \int_{Q \cap P_i} - \int_{Q \cap P_j} \text{dist}(x, \gamma_{ij} \cap Q) e^{-\frac{|x - (0, vt)|^2}{4t}} dx \\ &= \frac{k}{\varepsilon(k-1)} \frac{1}{4\pi t} \int_Q d(x) e^{-\frac{|x - (0, vt)|^2}{4t}} dx, \end{aligned} \tag{4}$$

where $d : \mathbb{R}^2 \rightarrow \mathbb{R}$ is the scalar signed distance. Now, applying the Taylor expansion of the scalar signed distance (cf. [6]) at $x = 0$, equation (4) becomes

$$\begin{aligned} I &= \frac{k}{\varepsilon(k-1)} \frac{1}{4\pi t} \int_Q \left[(x_2 + \frac{1}{2}\kappa x_1^2) + (\frac{1}{6}\kappa x_1^3 - \frac{1}{2}\kappa^2 x_1^2 x_2) + O(|x|^4) \right] e^{-\frac{|x - (0, vt)|^2}{4t}} dx \\ &=: \frac{k}{\varepsilon(k-1)} [I_1 + I_2 + I_3]. \end{aligned}$$

Note that for $n = 1, 2, \dots$, integrating by parts yields

$$\frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R} \setminus (-\tau, \tau)} x_1^n e^{-\frac{x_1^2}{4t}} dx_1 = O\left(\sqrt{t}(\tau + \sqrt{t})^{n-1} e^{-\frac{\tau^2}{4t}}\right)$$

and

$$\frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R} \setminus (-\tau, \tau)} x_2^n e^{-\frac{(x_2 - vt)^2}{4t}} dx_2 = O\left(\sqrt{t}(\tau + \sqrt{t})^{n-1} e^{-\frac{\tau^2}{4t}}\right).$$

We use these bounds to estimate the first integral I , as exhibited in the following claims:

Claim 1. $I_1 = (v + \kappa)t + O\left((1 + \tau + \sqrt{t})\sqrt{t}e^{-\frac{\tau^2}{4t}}\right)$, as $t \rightarrow 0$.

Indeed,

$$\begin{aligned} \frac{1}{4\pi t} \int_{\mathbb{R}^2} \left(x_2 + \frac{1}{2}\kappa x_1^2\right) e^{-\frac{|x - (0, vt)|^2}{4t}} dx &= \frac{1}{2\sqrt{\pi t}} \int_{\mathbb{R}} x_2 e^{-\frac{(x_2 - vt)^2}{4t}} dx_2 + \frac{\kappa}{2\sqrt{\pi t}} \int_0^\infty x_1^2 e^{-\frac{x_1^2}{4t}} dx_1 \\ &= \frac{1}{2\sqrt{\pi t}} \int_{\mathbb{R}} (x_2 + vt) e^{-\frac{x_2^2}{4t}} dx_2 + \kappa t = vt + \kappa t. \end{aligned}$$

Moreover,

$$\begin{aligned} \left| \frac{1}{4\pi t} \int_{\mathbb{R}^2 \setminus Q} x_2 e^{-\frac{|x - (0, vt)|^2}{4t}} dx \right| &\leq \frac{1}{4\pi t} \left| \int_{\mathbb{R}} e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_{\mathbb{R} \setminus (-\tau, \tau)} x_2 e^{-\frac{(x_2 - vt)^2}{4t}} dx_2 \right. \\ &\quad \left. + \int_{\mathbb{R} \setminus (-\tau, \tau)} e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_{\mathbb{R}} x_2 e^{-\frac{(x_2 - vt)^2}{4t}} dx_2 \right| \\ &\leq 1 \cdot \sqrt{t} e^{-\frac{\tau^2}{4t}} + e^{-\frac{\tau^2}{4t}} \cdot |v|t \\ &\leq C\left(\sqrt{t} + t\right) e^{-\frac{\tau^2}{4t}}, \end{aligned}$$

and

$$\begin{aligned} \left| \frac{1}{4\pi t} \int_{\mathbb{R}^2 \setminus Q} \frac{1}{2}\kappa x_1^2 e^{-\frac{|x - (0, vt)|^2}{4t}} dx \right| &\leq \frac{\kappa}{4\pi t} \left[\int_0^\infty x_1^2 e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_{\mathbb{R} \setminus (-\tau, \tau)} e^{-\frac{(x_2 - vt)^2}{4t}} dx_2 \right. \\ &\quad \left. + \int_{\mathbb{R} \setminus (-\tau, \tau)} x_1^2 e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_0^\infty e^{-\frac{(x_2 - vt)^2}{4t}} dx_2 \right] \\ &\leq \kappa \left[t \cdot e^{-\frac{\tau^2}{4t}} + \sqrt{t}(\tau + \sqrt{t}) e^{-\frac{\tau^2}{4t}} \cdot \frac{1}{2} \right] \\ &\leq C\sqrt{t}(\tau + \sqrt{t}) e^{-\frac{\tau^2}{4t}}, \end{aligned}$$

which proves the claim.

Claim 2. $I_2 = -v\kappa^2 t^2 + O\left(\sqrt{t}(\tau + \sqrt{t})^2 e^{-\frac{\tau^2}{4t}}\right)$, as $t \rightarrow 0$.

Indeed,

$$\begin{aligned} \frac{1}{4\pi t} \int_{\mathbb{R}^2} \left(\frac{1}{6}\kappa x_1^3 - \frac{1}{2}\kappa^2 x_1^2 x_2\right) e^{-\frac{|x - (0, vt)|^2}{4t}} dx &= -\frac{\kappa^2}{4\pi t} \int_0^\infty x_1^2 e^{-\frac{x_1^2}{4t}} dx_1 \int_{\mathbb{R}} x_2 e^{-\frac{(x_2 - vt)^2}{4t}} dx_2 \\ &= -\frac{\kappa^2 t}{2\sqrt{\pi t}} \int_{\mathbb{R}} (x_2 + vt) e^{-\frac{x_2^2}{4t}} dx_2 = -v\kappa^2 t^2. \end{aligned}$$

Moreover,

$$\begin{aligned}
\left| \frac{1}{4\pi t} \int_{\mathbb{R}^2 \setminus Q} \frac{1}{6} \kappa_x x_1^3 e^{-\frac{|x-(0,vt)|^2}{4t}} dx \right| &\leq \frac{C}{4\pi t} \left| \int_{\mathbb{R}} x_1^3 e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_{\mathbb{R} \setminus (-\tau, \tau)} e^{-\frac{(x_2-vt)^2}{4t}} dx_2 \right. \\
&\quad \left. + \int_{\mathbb{R} \setminus (-\tau, \tau)} x_1^3 e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_{\mathbb{R}} e^{-\frac{(x_2-vt)^2}{4t}} dx_2 \right| \\
&\leq C\sqrt{t} \left(\tau + \sqrt{t} \right)^2 e^{-\frac{\tau^2}{4t}},
\end{aligned}$$

and

$$\begin{aligned}
\left| \frac{1}{4\pi t} \int_{\mathbb{R}^2 \setminus Q} -\frac{1}{2} \kappa^2 x_1^2 x_2 e^{-\frac{|x-(0,vt)|^2}{4t}} dx \right| &\leq \frac{C}{4\pi t} \left| \int_0^\infty x_1^2 e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_{\mathbb{R} \setminus (-\tau, \tau)} x_2 e^{-\frac{(x_2-vt)^2}{4t}} dx_2 \right. \\
&\quad \left. + \int_{\mathbb{R} \setminus (-\tau, \tau)} x_1^2 e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_{\mathbb{R}} x_2 e^{-\frac{(x_2-vt)^2}{4t}} dx_2 \right| \\
&\leq C \left[t \cdot \sqrt{t} e^{-\frac{\tau^2}{4t}} + \sqrt{t} \left(\tau + \sqrt{t} \right) e^{-\frac{\tau^2}{4t}} \cdot |v|t \right] \\
&\leq Ct\sqrt{t} \left(\tau + \sqrt{t} \right) e^{-\frac{\tau^2}{4t}},
\end{aligned}$$

which proves the claim.

Claim 3. $I_3 = O(t^2)$, as $t \rightarrow 0$.

Indeed,

$$\begin{aligned}
|I_3| &\leq \frac{C}{4\pi t} \int_Q |x_1^2 + x_2^2|^2 e^{-\frac{x_1^2 + (x_2-vt)^2}{4t}} dx \\
&\leq \frac{C}{4\pi t} \left[\int_0^\infty x_1^4 e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_{\mathbb{R}} e^{-\frac{(x_2-vt)^2}{4t}} dx_2 + \int_{\mathbb{R}} e^{-\frac{x_1^2}{4t}} dx_1 \cdot \int_0^\infty x_2^4 e^{-\frac{(x_2-vt)^2}{4t}} dx_2 \right] \\
&\leq Ct^2 \left[\int_0^\infty x_1^4 e^{-x_1^2} dx_1 + \int_0^\infty \left(|x_2| + \sqrt{t} \right)^4 e^{-x_2^2} dx_2 \right].
\end{aligned}$$

Hence, $|I_3| \leq Ct^2$; thereby, proving the claim.

Finally, it follows from equation (3) and all three claims that

$$0 = I + II = \frac{k}{\varepsilon(k-1)} \left[(v + \kappa) t + O\left((1 + \tau + \sqrt{t}) \sqrt{t} e^{-\frac{\tau^2}{4t}} \right) + O(t^2) \right] + O(e^{-\frac{\tau^2}{4t}}).$$

This gives

$$v = -\kappa + O\left(t + \left(\frac{\varepsilon}{t} + \frac{\tau+1}{\sqrt{t}} + 1 \right) e^{-\frac{\tau^2}{4t}} \right),$$

as $t \rightarrow 0$. □

§ Some useful estimates

We now prove the estimates used in the proof above.

Lemma 3. For any $\alpha \geq 0$, we have

$$\int_{\alpha}^{\infty} e^{-x^2} dx \leq \frac{1}{2} \sqrt{\pi} e^{-\alpha^2}.$$

Proof. Note that $x \geq \alpha \geq 0$. Then, $x^2 = (x - \alpha)^2 + 2\alpha x - \alpha^2 \geq (x - \alpha)^2 + \alpha^2$. Hence,

$$\int_{\alpha}^{\infty} e^{-x^2} dx \leq e^{-\alpha^2} \int_{\alpha}^{\infty} e^{-(x-\alpha)^2} dx = \frac{1}{2} \sqrt{\pi} e^{-\alpha^2}.$$

□

Lemma 4. For any $\varepsilon > 0$,

$$\frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R} \setminus (-\tau, \tau)} e^{-\frac{(x-vt)^2}{4t}} dx = O\left(e^{-\frac{\tau^2}{4t}}\right),$$

as $t \rightarrow 0$.

Proof. Applying lemma 3 yields

$$\begin{aligned} \left| \frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R} \setminus (-\tau, \tau)} e^{-\frac{(x-vt)^2}{4t}} dx \right| &= \frac{1}{\sqrt{\pi}} \int_{\frac{\tau-vt}{2\sqrt{t}}}^{\infty} e^{-x^2} dx + \int_{\frac{\tau+vt}{2\sqrt{t}}}^{\infty} e^{-x^2} dx \\ &\leq \frac{1}{2} \left[e^{-\frac{(\tau-vt)^2}{4t}} + e^{-\frac{(\tau+vt)^2}{4t}} \right] \leq C e^{-\frac{\tau^2}{4t}}. \end{aligned}$$

□

Lemma 5. For any $\varepsilon > 0$ and $n = 1, 2, \dots$,

1. $\frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R} \setminus (-\tau, \tau)} x^n e^{-\frac{x^2}{4t}} dx = O\left(\sqrt{t}(\tau + \sqrt{t})^{n-1} e^{-\frac{\tau^2}{4t}}\right),$
2. $\frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R} \setminus (-\tau, \tau)} x^n e^{-\frac{(x-vt)^2}{4t}} dx = O\left(\sqrt{t}(\tau + \sqrt{t})^{n-1} e^{-\frac{\tau^2}{4t}}\right),$

as $t \rightarrow 0$.

Proof. For $n = 1, 2, \dots$, we have

$$I := \left| \frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R} \setminus (-\tau, \tau)} x^n e^{-\frac{x^2}{4t}} dx \right| \leq C(\sqrt{t})^n \int_{\frac{\tau}{2\sqrt{t}}}^{\infty} |x|^n e^{-x^2} dx \quad (5)$$

Applying integration by parts and lemma 3, we have for $\alpha = \frac{\tau}{2\sqrt{t}}$,

$$\begin{aligned}
\int_{\alpha}^{\infty} x^n e^{-x^2} dx &= \frac{1}{2} \alpha^{n-1} e^{-\alpha^2} + \sum_{i=1}^k \frac{(n-1)(n-3)\cdots(n-2i+1)}{2^{i+1}} \alpha^{n-2i-1} e^{-\alpha^2} \\
&\quad + \begin{cases} \int_{\alpha}^{\infty} e^{-x^2} dx, & n, \text{ even}, \\ e^{-\alpha^2}, & n, \text{ odd}. \end{cases} \\
&= \frac{1}{2} \alpha^{n-1} e^{-\alpha^2} \left[1 + \sum_{i=1}^k \frac{(n-1)(n-3)\cdots(n-2i+1)}{2^i \alpha^{2i}} \right] + \begin{cases} \int_{\alpha}^{\infty} e^{-x^2} dx, & n, \text{ even}, \\ e^{-\alpha^2}, & n, \text{ odd}. \end{cases} \\
&\leq C [\alpha^{n-1} + \alpha^{n-3} + \cdots + \alpha^{n-2k-1} + 1] e^{-\alpha^2}
\end{aligned}$$

where $k = \frac{n-2}{2}$ when n is even and $\frac{n-3}{2}$, otherwise. Thus,

$$\begin{aligned}
I &\leq C \left[\tau^{n-1} \sqrt{t} + \tau^{n-3} (\sqrt{t})^3 + \cdots + \tau^{n-2k-1} (\sqrt{t})^{2k-1} + (\sqrt{t})^n \right] e^{-\alpha^2} \\
&\leq C \sqrt{t} (\tau + \sqrt{t})^{n-1} e^{-\frac{\tau^2}{4t}}, \tag{6}
\end{aligned}$$

as $t \rightarrow 0$. The second estimate is shown in a similar fashion. $\square$

5.2 Junction stability

In this section, we establish that the SDV (signed distance vector) scheme preserves the symmetric (120°) Herring angle conditions at the triple junction. We utilize a similar argument as in [6], as follows:

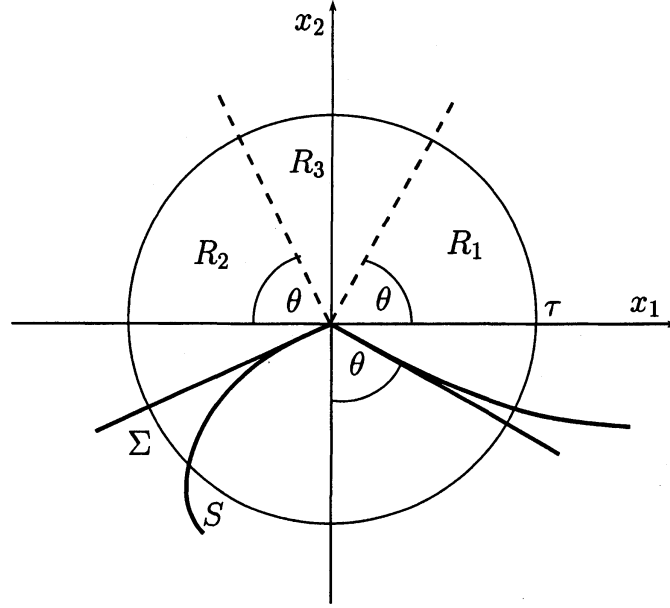
1. Assume a triple junction at the origin and evolve the configuration via SD method until time t .
2. Locate the triple junction after time t and denote this by z .
3. Determine the junction angles at the new junction location z to establish its stability.

We proceed throughout the whole section in this manner. To establish the stability of the triple junction, we first need to write down the Taylor expansion of the convolution

$$F^S(z) := \int_{B(0,\tau)} d_S(x) \Phi_t(z-x) dx$$

of phase distance d_S with the heat kernel $\Phi_t(x, t) := \frac{1}{4\pi t} e^{-\frac{|x|^2}{4t}}$, when restricted to some neighborhood $B(0, \tau)$ of the triple junction.

Consider a phase region $S \subset \mathbb{R} \times (-\infty, 0]$ bounded by two interfaces γ_1, γ_2 intersecting at the origin (triple junction). Assume that the tangents at the origin form a wedge Σ with an opening angle $2\theta < \pi$ and symmetric with respect to the negative x_2 -axis.

Figure 5: Distance to a wedge-like set S .

Let $d_\Sigma : \mathbb{R}^2 \rightarrow \mathbb{R}^+ \cup \{0\}$, be the distance to the tangent wedge Σ . Hence,

$$d_\Sigma(x) = \begin{cases} x_1 \cos \theta + x_2 \sin \theta, & \text{in } R_1 := \{x : -x_1 \cot \theta \leq x_2 \leq x_1 \tan \theta\} \\ -x_1 \cos \theta + x_2 \sin \theta, & \text{in } R_2 := \{x : x_1 \cot \theta \leq x_2 \leq -x_1 \tan \theta\} \\ |x|, & \text{in } R_3 := \{x : x_2 \geq |x_1| \tan \theta\} \\ 0, & \text{otherwise} \end{cases}$$

Remark. We list down some integrals necessary to compute the convolution:

1. $\int_{R_1} x_1 \Phi_t(x) dx = \frac{\sqrt{t}}{2\sqrt{\pi}} (\sin \theta + \cos \theta)$
2. $\int_{R_1} x_2 \Phi_t(x) dx = \frac{\sqrt{t}}{2\sqrt{\pi}} (\sin \theta - \cos \theta)$
3. $\int_{R_1} x_1 x_2 \Phi_t(x) dx = -\frac{t}{\pi} \cos 2\theta$
4. $\int_{R_1} x_2^2 \Phi_t(x) dx = t \left(\frac{1}{2} - \frac{1}{\pi} \sin 2\theta \right)$
5. $\int_{R_1} x_1^3 \Phi_t(x) dx = \frac{t\sqrt{t}}{\sqrt{\pi}} (\sin \theta + \cos \theta) (2 + \sin \theta \cos \theta)$
6. $\int_{R_1} x_2^3 \Phi_t(x) dx = \frac{t\sqrt{t}}{\sqrt{\pi}} (\sin \theta - \cos \theta) (2 - \sin \theta \cos \theta)$

$$7. \int_{R_1} x_1^2 x_2 \Phi_t(x) dx = \frac{t\sqrt{t}}{\sqrt{\pi}} (\sin \theta - \cos \theta) (1 + \sin \theta \cos \theta)$$

$$8. \int_{R_1} x_1 x_2^2 \Phi_t(x) dx = \frac{t\sqrt{t}}{\sqrt{\pi}} (\sin \theta + \cos \theta) (1 - \sin \theta \cos \theta)$$

Using these integrals, we arrive at the following formula.

Lemma 6. *The convolution of distance d_Σ to the tangent wedge Σ with the heat kernel Φ_t , restricted to some open ball $B(0, \tau)$ has the following Taylor expansion at the origin:*

$$\begin{aligned} F^\Sigma(z) &= \frac{\sqrt{t}}{\sqrt{\pi}} \left(\frac{\pi}{2} + 1 - \theta \right) + \frac{1}{\pi} \left(\frac{\pi}{2} \sin \theta + \cos \theta \right) z_2 + (1 + z_2) C_1(t) + (z_1^2 + z_2^2) C_2(t) \\ &\quad + \frac{4 \cos^2 \theta + \sin 2\theta + \pi - 2\theta}{16\sqrt{\pi t}} z_1^2 + \frac{4 \sin^2 \theta - \sin 2\theta + \pi - 2\theta}{16\sqrt{\pi t}} z_2^2 + O(t^{-1}|z|^3) \end{aligned}$$

where $C_1(t) = O\left(e^{-\frac{\tau^2}{4t}}\right)$ and $C_2(t) = O\left(\frac{(\tau+\sqrt{t})^3}{t^2} e^{-\frac{\tau^2}{4t}}\right)$, as $t \rightarrow 0$.

Proof. Note that by the above remark, we get

$$\begin{aligned} \int_{R_1 \cup R_2} d_\Sigma(x) \Phi_t(x) dx &= 2 \cos \theta \int_{R_1} x_1 \Phi_t(x) dx + 2 \sin \theta \int_{R_1} x_2 \Phi_t(x) dx \\ &= \frac{\sqrt{t}}{\sqrt{\pi}} [\cos \theta (\sin \theta + \cos \theta) + \sin \theta (\sin \theta - \cos \theta)] = \frac{\sqrt{t}}{\sqrt{\pi}}, \end{aligned}$$

and

$$\int_{R_3} d_\Sigma(x) \Phi_t(x) dx = \frac{1}{4\pi t} \int_\theta^{\pi-\theta} \int_0^\infty r^2 e^{-\frac{r^2}{4t}} dr d\phi = \frac{t}{\sqrt{4\pi t}} \int_\theta^{\pi-\theta} d\phi = \frac{\sqrt{t}}{2\sqrt{\pi}} (\pi - 2\theta).$$

Moreover, since $d_\Sigma(x) \leq |x|$, then we have

$$\begin{aligned} \left| \int_{\mathbb{R}^2 \setminus Q} d_\Sigma(x) \Phi_t(x) dx \right| &\leq \frac{1}{4\pi t} \int_0^{2\pi} \int_\tau^\infty r^2 e^{-\frac{r^2}{4t}} dr d\phi \\ &\leq C\sqrt{t} \int_{\frac{\tau}{2\sqrt{t}}}^\infty r^2 e^{-r^2} dr \\ &= C\sqrt{t} \left[-\frac{1}{2} r e^{-r^2} \Big|_{\frac{\tau}{2\sqrt{t}}}^\infty + \frac{1}{2} \int_{\frac{\tau}{2\sqrt{t}}}^\infty e^{-r^2} dr \right] \\ &\leq C(\tau + \sqrt{t}) e^{-\frac{\tau^2}{4t}}. \end{aligned}$$

Thus, $F^\Sigma(0) = \frac{\sqrt{t}}{\sqrt{\pi}} \left(\frac{\pi}{2} + 1 - \theta \right) + O\left(\tau e^{-\frac{\tau^2}{4t}}\right)$, as $t \rightarrow 0$.

Since d_Σ and Φ_t are symmetric with respect to $x_1 = 0$, then

$$\int_{\mathbb{R}^2} d_\Sigma(x) \frac{\partial}{\partial z_2} \Phi_t(z - x) \Big|_{z=0} dx = \frac{1}{2t} \int_{\mathbb{R}^2} x_1 d_\Sigma(x) \Phi_t(x) dx = 0,$$

hence, the partial derivative $F_1^\Sigma(0) = O(e^{-\frac{r^2}{4t}})$, as $t \rightarrow 0$.

On the other hand, we see that

$$\begin{aligned} \int_{R_1 \cup R_2} d_\Sigma(x) \frac{\partial}{\partial z_2} \Phi_t(z-x) \Big|_{z=0} dx &= \frac{1}{t} \int_{R_1} x_2 (x_1 \cos \theta + x_2 \sin \theta) \Phi_t(x) dx \\ &= -\frac{1}{\pi} \cos \theta \cos 2\theta + \sin \theta \left(\frac{1}{2} - \frac{1}{\pi} \sin 2\theta \right) \\ &= \frac{1}{2} \sin \theta - \frac{1}{\pi} \cos \theta \end{aligned}$$

and

$$\begin{aligned} \int_{R_3} d_\Sigma(x) \frac{\partial}{\partial z_2} \Phi_t(z-x) \Big|_{z=0} dx &= \frac{1}{2t} \int_{R_3} d_\Sigma(x) \Phi_t(x) dx \\ &= \frac{1}{2t} \int_\theta^{\pi-\theta} \sin \phi d\phi \frac{1}{4\pi t} \int_0^\infty r^3 e^{-\frac{r^2}{4\pi t}} dr \\ &= \frac{2}{\pi} [\cos \theta - \cos(\pi - \theta)] \cdot \int_0^\infty r^3 e^{-r^2} dr = \frac{2}{\pi} \cos \theta. \end{aligned}$$

Similarly,

$$\left| \int_{\mathbb{R}^2 \setminus Q} d_\Sigma(x) \frac{\partial}{\partial z_2} \Phi_t(z-x) \Big|_{z=0} dx \right| \leq \frac{1}{2t} \frac{1}{4\pi t} \int_0^{2\pi} \int_\tau^\infty r^2 \sin \phi e^{-\frac{r^2}{4t}} r dr d\phi = O(e^{-\frac{r^2}{4t}}).$$

Hence, the partial derivative $F_2^\Sigma(0) = \frac{1}{2} \sin \theta + \frac{1}{\pi} \cos \theta + O(e^{-\frac{r^2}{4t}})$, as $t \rightarrow 0$.

Continuing with the quadratic terms, we have

$$\begin{aligned} \int_{R_1 \cup R_2} d_\Sigma(x) \frac{\partial^2}{\partial z_1^2} \Phi_t(z-x) \Big|_{z=0} dx &= \frac{1}{t} \int_{R_1} d_\Sigma(x) \left(\frac{x_1^2}{2t} - 1 \right) \Phi_t(x) dx \\ &= \frac{1}{2t^2} \int_{R_1} x_1^2 (x_1 \cos \theta + x_2 \sin \theta) \Phi_t(x) dx - \frac{1}{t} \int_{R_1} d_\Sigma(x) \Phi_t(x) dx \\ &= \frac{1}{2\sqrt{\pi t}} (\sin 2\theta + \cos^2 \theta), \end{aligned}$$

and

$$\begin{aligned} \int_{R_3} d_\Sigma(x) \frac{\partial^2}{\partial z_1^2} \Phi_t(z-x) \Big|_{z=0} dx &= \frac{1}{4t^2} \int_{R_3} |x| (x_1^2 - 2t) \Phi_t(x) dx \\ &= \frac{1}{2t} \frac{1}{4\pi t} \int_0^\infty \int_\theta^{\pi-\theta} r^2 (r^2 \cos^2 \phi - 2t) e^{-\frac{r^2}{4\pi t}} d\phi dr \\ &= \frac{1}{16\pi t^3} \left[\int_0^\infty r^4 e^{-\frac{r^2}{4\pi t}} dr \cdot \int_\theta^{\pi-\theta} \cos^2 \phi d\phi - 2t(\pi - \theta) \int_0^\infty r^2 e^{-\frac{r^2}{4\pi t}} dr \right] \\ &= \frac{1}{8\sqrt{\pi t}} [\pi - 2\theta - 3 \sin 2\theta]. \end{aligned}$$

Moreover,

$$\begin{aligned}
\left| \int_{\mathbb{R}^2 \setminus Q} d_{\Sigma}(x) \frac{\partial^2}{\partial z_1^2} \Phi_t(z-x) \Big|_{z=0} dx \right| &\leq \frac{1}{4\pi t} \int_{\mathbb{R}^2 \setminus Q} |x| \left| \frac{x_1^2}{4t^2} - \frac{1}{2t} \right| e^{-\frac{|x|^2}{4t}} dx \\
&\leq \frac{C}{t} \int_{\tau}^{\infty} r^2 \left(\frac{r^2}{t^2} + \frac{1}{t} \right) e^{-\frac{r^2}{4t}} dr \\
&\leq \frac{C}{\sqrt{t}} \int_{\frac{\tau}{2\sqrt{t}}}^{\infty} (r^4 + r^2) e^{-r^2} dr \\
&\leq \frac{C}{\sqrt{t}} \left[(r^3 + r) e^{-r^2} \Big|_{\frac{\tau}{2\sqrt{t}}}^{\infty} + \int_{\frac{\tau}{2\sqrt{t}}}^{\infty} e^{-r^2} dr \right] \\
&\leq C \left(\frac{\tau^3}{t^2} + \frac{\tau}{t} + \frac{1}{\sqrt{t}} \right) e^{-\frac{\tau^2}{4t}}.
\end{aligned}$$

Hence, the second partial derivative

$$F_{11}^{\Sigma}(0) = \frac{1}{8\sqrt{\pi t}} (4 \cos^2 \theta + \sin 2\theta + \pi - 2\theta) + O\left(t^{-2}(\tau + \sqrt{t})^3 e^{-\frac{\tau^2}{4t}}\right), \quad \text{as } t \rightarrow 0.$$

Similarly, we get $F_{22}^{\Sigma}(0) = \frac{1}{8\sqrt{\pi t}} (4 \sin^2 \theta - \sin 2\theta + \pi - 2\theta) + O\left(t^{-2}(\tau + \sqrt{t})^3 e^{-\frac{\tau^2}{4t}}\right)$, as $t \rightarrow 0$. In addition, since

$$\frac{\partial}{\partial z_2 \partial z_1} \Phi_t(z-x) \Big|_{z=0} = \frac{x_1 x_2}{4t^2} \Phi_t(x),$$

then by a similar symmetry argument, we have $F_{12}^{\Sigma}(0) = 0$.

Finally, since d_{Σ} is 1-Lipschitz, then for $k \geq 3$, we have

$$\begin{aligned}
|F_{i_1 i_2 \dots i_k}(0)| &= \left| \int_Q d_{\Sigma}(x) \frac{\partial^k}{\partial x_{i_1} \partial x_{i_2} \dots \partial x_{i_k}} \Phi_t(x) dx \right| \\
&\leq \int_{\mathbb{R}^2} \left| \frac{\partial}{\partial x_{i_k}} d_{\Sigma}(x) \right| \left| \frac{\partial^{k-1}}{\partial x_{i_1} \partial x_{i_2} \dots \partial x_{i_{k-1}}} \Phi_t(x) \right| dx \\
&\leq C \frac{1}{\sqrt{4\pi t}} \int_0^{\infty} \left(\frac{x_1}{2t} \right)^{k-1} e^{-\frac{x_1^2}{4t}} dx_1 \\
&\leq C t^{\frac{1-k}{2}} \int_0^{\infty} x_1^{k-1} e^{-x_1^2} dx_1 \leq C t^{\frac{1-k}{2}},
\end{aligned}$$

for some constant $C > 0$. Finally, putting these values together yields the desired Taylor expansion at the origin

$$F^{\Sigma}(z) = F^{\Sigma}(0) + F_1^{\Sigma}(0)z_1 + F_2^{\Sigma}(0)z_2 + \frac{1}{2}F_{11}^{\Sigma}(0)z_1^2 + F_{12}^{\Sigma}(0)z_1z_2 + \frac{1}{2}F_{22}^{\Sigma}(0)z_2^2 + O\left(\frac{|z|^3}{t}\right),$$

as $t \rightarrow 0$. □

We are now ready to set up the convolution of the phase distance.

Proposition 7. *The convolution of phase distance d_S with the heat kernel Φ_t , restricted to some open ball $B(0, \tau)$ satisfies the following Taylor expansion at the origin:*

$$F^S(z) = \frac{\sqrt{t}}{\sqrt{\pi}} \left(\frac{\pi}{2} + 1 - \theta + C(t) \right) + C(t)z_1 + \frac{1}{\pi} \left(\frac{\pi}{2} \sin \theta + \cos \theta + C(t) \right) z_2 + \frac{1}{\sqrt{t}} C(t) z_1 z_2 \\ + \frac{4 \cos^2 \theta + \sin 2\theta + \pi - 2\theta + C(t)}{16\sqrt{\pi t}} z_1^2 + \frac{4 \sin^2 \theta - \sin 2\theta + \pi - 2\theta + C(t)}{16\sqrt{\pi t}} z_2^2 + O\left(\frac{|z|^3}{t}\right),$$

where $C(t) = O(\sqrt{t})$, as $t \rightarrow 0$.

Proof. We can assume that

$$|d_S(x) - d_\Sigma(x)| \leq \mathcal{H}(\partial S \cap B(0, |x|), \partial \Sigma \cap B(0, |x|)) \leq C|x|^2,$$

as $x \rightarrow 0$. It follows that

$$|F^S(0) - F^\Sigma(0)| \leq \int_Q |d_S(x) - d_\Sigma(x)| \Phi_t(x) dx \\ \leq C \int_{\mathbb{R}^2} |x|^2 \Phi_t(z - x) dx \leq \frac{C}{4\pi t} \int_0^\infty r^3 e^{-\frac{r^2}{4t}} dr \leq Ct,$$

as $t \rightarrow 0$. Similarly, for $k \geq 1$, we have

$$|F_{i_1 i_2 \dots i_k}^S(0) - F_{i_1 i_2 \dots i_k}^\Sigma(0)| = \int_Q |d_S(x) - d_\Sigma(x)| \left| \frac{\partial^k}{\partial x_{i_1} \partial x_{i_2} \dots \partial x_{i_k}} \Phi_t(x) \right| dx \\ \leq C \int_{\mathbb{R}^2} |x|^2 \left| \frac{\partial^k}{\partial x_{i_1} \partial x_{i_2} \dots \partial x_{i_k}} \Phi_t(x) \right| dx \\ \leq \frac{C}{t^{k+1}} \int_0^\infty r^{k+3} e^{-\frac{r^2}{4t}} dr \leq Ct^{\frac{2-k}{2}},$$

as $t \rightarrow 0$. Finally, adjusting Lemma 6 to the above estimates yields the desired result. $\square$

For simplicity, take $N = 2$. Consider a triple junction of a k -phase network where three interfaces meet, say γ_{12} , γ_{13} and γ_{23} . Let $2\theta_i$ be the interior angle of phase region P_i ($i = 1, 2, 3$) at the triple junction. Without loss of generality, translate and rotate the whole plane $\mathbb{R}^2$ so that the junction is at the origin and P_1 -boundary interfaces γ_{12} and γ_{13} make an angle of $\theta_1 \in (0, \frac{\pi}{2})$ with the negative x_2 axis. Choose $\tau > 0$, small enough so that $P_1 \cap B(0, \tau)$ is in the lower half plane with

$$B(0, \tau) \subset \{x \in P_1 \cup P_2 \cup P_3 : B(x, \varepsilon) \cap P_i \neq \emptyset \ (i = 1, 2, 3)\}$$

and such that for any $x \in P_i \cap B(0, \tau)$ ($i = 1, 2, 3$), the distance to phase region P_j ($j \neq i$) satisfies $d_j(x) = \text{dist}(x, \gamma_{ij} \cap B(0, \tau))$.

We then perform one step of the SD method with time step t . At time t , we determine the location z of the triple junction by solving

$$\begin{cases} \mathbf{u}(t, z) \cdot (\mathbf{p}_1 - \mathbf{p}_2) = 0 \\ \mathbf{u}(t, z) \cdot (\mathbf{p}_1 - \mathbf{p}_3) = 0 \end{cases} \quad (7)$$

where u solves the vector-type heat equation (1), that is,

$$u(t, z) = \int_{B(0, \tau)} + \int_{\mathbb{R}^2 \setminus B(0, \tau)} \delta_\varepsilon(x) \Phi_t(x - z) dx =: I + II.$$

For any distinct $i, j \in \{1, 2, 3\}$, we have by the remark on Definition 1,

$$\begin{aligned} |II \cdot (\mathbf{p}_i - \mathbf{p}_j)| &\leq \frac{k}{k-1} \frac{1}{4\pi t} \int_\tau^\infty \int_0^{2\pi} r e^{-\frac{r^2 - 2rs \cos(\theta - \omega) + s^2}{4t}} d\theta dr \\ &\leq \frac{C}{t} \int_{\tau-s}^\infty (r+s) e^{-\frac{r^2}{4t}} dr \leq C \frac{1}{\sqrt{t}} e^{-\frac{\tau^2}{4t}}. \end{aligned} \quad (8)$$

where z is written as (s, ω) in polar coordinates. Moreover,

$$I \cdot (\mathbf{p}_i - \mathbf{p}_j) = \frac{k}{\varepsilon(k-1)} \int_{B(0, \tau)} [d_j(x) - d_i(x)] \Phi_t(x - z) dx = \frac{k}{\varepsilon(k-1)} [F^j(z) - F^i(z)]. \quad (9)$$

By Lemma 7, we have

$$\begin{aligned} F^1(z) &= A(\theta_1) \sqrt{t} + B(\theta_1) z_2 + \frac{1}{\sqrt{t}} D(\theta_1) z_1^2 + \frac{1}{\sqrt{t}} E(\theta_1) z_2^2 \\ &\quad + \psi(t) (\sqrt{t} + z_1 + z_2 + \frac{1}{\sqrt{t}} z_1 z_2) + O(t^{-1} |z|^3) =: \beta(\theta_1, z_1, z_2) \\ F^2(z) &= \beta(\theta_2, -\cos \theta_3 z_1 - \sin \theta_3 z_2, \sin \theta_3 z_1 - \cos \theta_3 z_2) \\ F^3(z) &= \beta(\theta_3, \cos \theta_2 z_1 - \sin \theta_2 z_2, -\sin \theta_2 z_1 - \cos \theta_2 z_2), \end{aligned} \quad (10)$$

where

$$\begin{aligned} A(\theta) &= \frac{1}{\sqrt{\pi}} \left(\frac{\pi}{2} + 1 - \theta \right) & D(\theta) &= \frac{1}{16\sqrt{\pi}} (4 \cos^2 \theta + \sin 2\theta + \pi - 2\theta) \\ B(\theta) &= \frac{1}{\pi} \left(\frac{\pi}{2} \sin \theta + \cos \theta \right) & E(\theta) &= \frac{1}{16\sqrt{\pi}} (4 \sin^2 \theta - \sin 2\theta + \pi - 2\theta) \end{aligned}$$

and $\psi(t) = O(\sqrt{t})$, as $t \rightarrow 0$. The expansions for F^2 and F^3 are obtained from F^1 by $(\theta_1 + \theta_2)$ -counterclockwise and $(\theta_1 + \theta_3)$ -clockwise rotations, respectively.

Remark. From (7), (8), (9) and (10), we deduce the following:

1. If $\theta_i = \frac{\pi}{3}$ ($i = 1, 2, 3$), then z moves with a speed of at most $O(1)$.
2. If $\theta_i = \frac{\pi}{3} + O(1)$ ($i = 1, 2, 3$), then z moves with a speed of at least $O(\frac{1}{\sqrt{t}})$.

Lemma 8. *After time t , the triple junction moves via SD method from the origin to the point $z = (z_1, z_2)$:*

$$\begin{aligned} z_1 &= \frac{4\sqrt{\pi t}}{3\pi + 2\sqrt{3}} (2\theta_2 + \theta_1 - \pi) + O(\delta\sqrt{t} + t) \\ z_2 &= \frac{4\sqrt{\pi t}}{2 + \pi\sqrt{3}} \left(\theta_1 - \frac{\pi}{3} \right) + O(\delta\sqrt{t} + t), \end{aligned}$$

where $\delta = \max(\theta_1 - \frac{\pi}{3}, \theta_2 - \frac{\pi}{3})$.

Proof. Using expansions (10) and relations (8) and (9), we rewrite equation (7) in terms of $\xi_i := \frac{1}{\sqrt{t}}z_i$, as follows:

$$\begin{aligned} 0 &= a_0 + b_0\xi_1 - c_0\xi_2 + O(\sqrt{t} + |\xi|^2) \\ 0 &= a_1 - b_1\xi_1 - c_1\xi_2 + O(\sqrt{t} + |\xi|^2) \end{aligned}$$

where $a_i = \frac{1}{\sqrt{\pi}}(\theta_1 - \theta_{i+2})$, $b_i = B(\theta_{i+2}) \sin \theta_{3-i}$, and $c_i = B(\theta_{i+2}) \cos \theta_{3-i} + B(\theta_1)$ for $i = 0, 1$. Note that

$$\begin{aligned} b_0c_1 + b_1c_0 &= \frac{3\sqrt{3}}{2}B\left(\frac{\pi}{3}\right)B\left(\frac{\pi}{3}\right) + O(\delta) \\ c_0a_1 - a_0c_1 &= \frac{3}{2\sqrt{\pi}}B\left(\frac{\pi}{3}\right)(2\theta_2 + \theta_1 - \pi) + O(\delta^2) \\ a_0b_1 + a_1b_0 &= \frac{3\sqrt{3}}{2\sqrt{\pi}}B\left(\frac{\pi}{3}\right)\left(\theta_1 - \frac{\pi}{3}\right) + O(\delta^2), \end{aligned}$$

where $\delta = \max(\theta_1 - \frac{\pi}{3}, \theta_2 - \frac{\pi}{3})$. Thus, we get

$$\begin{aligned} \xi_1 &= \frac{c_0a_1 - a_0c_1}{b_0c_1 + b_1c_0} + O(\sqrt{t}) = \frac{2\theta_2 + \theta_1 - \pi}{\sqrt{3\pi}B\left(\frac{\pi}{3}\right)} + O(\delta + \sqrt{t}), \quad \text{as } t \rightarrow 0 \\ \xi_2 &= \frac{a_0b_1 + a_1b_0}{b_0c_1 + b_1c_0} + O(\sqrt{t}) = \frac{\theta_1 - \frac{\pi}{3}}{\sqrt{\pi}B\left(\frac{\pi}{3}\right)} + O(\delta + \sqrt{t}), \quad \text{as } t \rightarrow 0. \end{aligned}$$

□

Next, we look at the effect of the evolution after time t on the phase interior angles of the triple junction located at point $z := z(\theta_1, \theta_2)$ given by Lemma 8. Consider the map $\Theta : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ which defines the junction angles at time t as follows:

$$\Theta(\theta_1, \theta_2) = \frac{1}{2} \left(\cos^{-1} \left(\frac{N_{31} \cdot N_{12}}{\|N_{31}\| \|N_{12}\|} \right), \cos^{-1} \left(\frac{N_{12} \cdot N_{23}}{\|N_{12}\| \|N_{23}\|} \right) \right),$$

where the normal N^{ij} to interface $\gamma_{ij}(i, j = 1, 2, 3)$ is defined by

$$\begin{aligned} N^{ij}(z) &:= \nabla (\mathbf{u}(t, z) \cdot (\mathbf{p}_i - \mathbf{p}_j)) \\ &= \frac{k}{\varepsilon(k-1)} (F_1^j(z) - F_1^i(z), F_2^j(z) - F_2^i(z)) + O(e^{-\frac{r^2}{4t}}), \quad t \rightarrow 0. \end{aligned}$$

Here, the partial derivatives of F^i are computed from expansions (10) as follows:

$$\begin{aligned} F_{z_1}^1(z) &= \frac{2}{\sqrt{t}}D(\theta_1)z_1 + C_1(z, t) \\ F_{z_2}^1(z) &= B(\theta_1) + \frac{2}{\sqrt{t}}E(\theta_1)z_2 + C_2(z, t) \\ F_{z_1}^2(z) &= B(\theta_2) \sin \theta_3 + \frac{2}{\sqrt{t}}[H(\theta_2) \cos^2 \theta_3 + E(\theta_2)]z_1 + \frac{1}{\sqrt{t}}H(\theta_2) \sin 2\theta_3 z_2 + C_1(z, t) \\ F_{z_2}^2(z) &= -B(\theta_2) \cos \theta_3 + \frac{1}{\sqrt{t}}H(\theta_2) \sin 2\theta_3 z_1 + \frac{2}{\sqrt{t}}[H(\theta_2) \sin^2 \theta_3 + E(\theta_2)]z_2 + C_2(z, t) \\ F_{z_1}^3(z) &= -B(\theta_3) \sin \theta_2 + \frac{2}{\sqrt{t}}[D(\theta_3) - H(\theta_3) \sin^2 \theta_2]z_1 - \frac{1}{\sqrt{t}}H(\theta_3) \sin 2\theta_2 z_2 + C_1(z, t) \\ F_{z_2}^3(z) &= -B(\theta_3) \cos \theta_2 - \frac{1}{\sqrt{t}}H(\theta_3) \sin 2\theta_2 z_1 + \frac{2}{\sqrt{t}}[D(\theta_3) - H(\theta_3) \cos^2 \theta_2]z_2 + C_2(z, t), \end{aligned} \tag{11}$$

where $H(\theta) := D(\theta) - E(\theta)$ and $C_i(z, t) := O(\sqrt{t} + |z|t^{-1})$, as $t \rightarrow 0$.

We now establish the stability of triple junction in the following theorem:

Theorem 9. Let $(\hat{\theta}_1, \hat{\theta}_2) := \Theta(\theta_1, \theta_2)$, be the junction angles after time step Δt . Then, there exists a 2×2 matrix M whose largest singular value $\sigma < 1$ such that

$$\begin{bmatrix} \hat{\theta}_1 - \frac{\pi}{3} \\ \hat{\theta}_2 - \frac{\pi}{3} \end{bmatrix} = M \begin{bmatrix} \theta_1 - \frac{\pi}{3} \\ \theta_2 - \frac{\pi}{3} \end{bmatrix} + O(\delta^2 + \sqrt{\Delta t}), \quad (12)$$

as $\Delta t \rightarrow 0$. Here, $\delta = \max(\theta_1 - \frac{\pi}{3}, \theta_2 - \frac{\pi}{3})$.

Proof. For convenience, we write t instead of Δt . Using the Taylor expansions (10), we see that at point $z := z(\frac{\pi}{3}, \frac{\pi}{3})$, we have

$$\|N^{12}\| = \|N^{23}\| = \|N^{31}\| = \frac{k\sqrt{3}}{\varepsilon(k-1)} B(\frac{\pi}{3}) + O(\sqrt{t})$$

and

$$N^{31} \cdot N^{12} = N^{12} \cdot N^{23} = -\frac{1}{2} \left(\frac{k\sqrt{3}}{\varepsilon(k-1)} B(\frac{\pi}{3}) \right)^2 + O(\sqrt{t}),$$

as $t \rightarrow 0$. Hence, $\Theta(\frac{\pi}{3}, \frac{\pi}{3}) = (\frac{\pi}{3}, \frac{\pi}{3}) + O(\sqrt{t})$, as $t \rightarrow 0$.

On the other hand, write $\Theta := (\frac{1}{2} \cos^{-1} \Psi^1, \frac{1}{2} \cos^{-1} \Psi^2)$. Hence, $\Psi^i(\frac{\pi}{3}, \frac{\pi}{3}) = -\frac{1}{2}$, for $i = 1, 2$. Now, using expansions (10) and Lemma 8, we arrive at the following partial derivatives:

$$\begin{aligned} \Psi_{\theta_1}^1(\frac{\pi}{3}, \frac{\pi}{3}) &= \|N^{12}\|^{-2} [(N^{31} - \Psi^1 N^{12}) \cdot N_{\theta_1}^{12}(\frac{\pi}{3}, \frac{\pi}{3}) + (N^{12} - \Psi^1 N^{31}) \cdot N_{\theta_1}^{31}(\frac{\pi}{3}, \frac{\pi}{3})] \\ &= -\frac{\sqrt{3}}{4} \left[1 + \sqrt{3} \frac{B'(\frac{\pi}{3})}{B(\frac{\pi}{3})} + \frac{2\sqrt{3}}{\sqrt{\pi}} \frac{E(\frac{\pi}{3}) - D(\frac{\pi}{3})}{B(\frac{\pi}{3})^2} \right] + O(\sqrt{t}) =: \alpha + O(\sqrt{t}), \end{aligned}$$

as $t \rightarrow 0$. In a similar fashion, we get $\Psi_{\theta_2}^1(\frac{\pi}{3}, \frac{\pi}{3}) = O(\sqrt{t})$, $\Psi_{\theta_1}^2(\frac{\pi}{3}, \frac{\pi}{3}) = O(\sqrt{t})$, and $\Psi_{\theta_2}^2(\frac{\pi}{3}, \frac{\pi}{3}) = \alpha + O(\sqrt{t})$, as $t \rightarrow 0$. It follows that

$$D\Theta(\frac{\pi}{3}, \frac{\pi}{3}) = -\frac{\sqrt{3}}{3} \begin{bmatrix} \alpha & 0 \\ 0 & \alpha \end{bmatrix} + O(\sqrt{t}),$$

as $t \rightarrow 0$. Take $M := -\frac{\sqrt{3}}{3} \alpha \mathbf{I}_2$ whose singular value $\sigma = \frac{\sqrt{3}}{3} \alpha \approx 0.2451 < 1$. Finally, equation (12) follows from the Taylor expansion of Θ near $(\frac{\pi}{3}, \frac{\pi}{3})$. $\square$

The above theorem guarantees that at every time step of SDV algorithm 1, the phase interior angles at the triple junction that are initially close to the symmetric configuration will always tend to get closer to $\frac{2\pi}{3}$ with an error of order $\sqrt{\Delta t}$. In particular, $\hat{\theta}_i = \frac{\pi}{3} + O(\delta + \sqrt{\Delta t})$. Thus, we see that it stably imposes the symmetric Herring condition at the triple junction.

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