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Loss of convexity for a modified Mullins-Sekerka model arising in diblock copolymer melts†

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Abstract

This modified (two-sided) Mullins-Sekerka model is a nonlocal evolution model for closed hypersurfaces, which appears as a singular limit of a modified Cahn-Hilliard equation describing micro-phase separation of diblock copolymer. Under this evolution the propagating interfaces maintain the enclosed volumes of the two phases. We will show by means of an example that this model does not preserve convexity in two space dimensions.

1 Introduction

Recently, a modified Cahn–Hilliard equation was proposed in [12] to study micro-phase separation of diblock copolymer, see also [13, 14] for more material-scientific background. Introducing an appropriate scaling, the corresponding formal singular limit leads to a modified two-sided Mullins–Sekerka model in which, as the new feature, two nonlocal inhomogeneous terms appear in the equations for the phases, cf. (1) below.

The existence of a unique classical (short-term) solution of this modified Mullins–Sekerka model was established recently in [2]. Moreover, it is shown in [2] that this flow preserves volume, but unlike for the usual Mullins–Sekerka model [1, 3, 4, 11], the flow generated by (1) does not decrease the area of the interface and generally rules out that Euclidean spheres be equilibrium points.

In this paper we show that the flow given through (1) in the plane does not preserve convexity. This agrees with the usual Mullins-Sekerka flow [9, 10] and with the surface diffusion flow [6], but is in contrast to the averaged mean curvature flow [5, 8].

2 The modified two-sided Mullins-Sekerka model

We look at a closed simple curve Γ_0 contained in a fixed domain $\Omega \subset \mathbb{R}^2$, and we consider the free boundary problem governed by the evolution law given by

$$\left.\begin{array}{rcll} -\Delta v_\pm &=& \pm 1 - f & \text{in } \Omega \setminus \Gamma_t\,, \\ \dfrac{\partial v_+}{\partial n} &=& 0 & \text{on } \partial\Omega\,, \\ v_\pm &=& C\kappa & \text{on } \Gamma_t\,, \\ V &=& \dfrac{1}{2}\left[\dfrac{\partial v}{\partial n}\right] & \text{on } \Gamma_t\,. \end{array}\right\} \tag{1}$$

In the equations above, n is the outer unit normal to Γ_t and to $\partial\Omega$, while V and κ are the normal velocity and the curvature of Γ_t, respectively, and C is a positive constant. The signs are chosen in such a way that a circle has positive curvature and a shrinking curve has negative velocity. The expression on the right-hand side of the equation for V denotes the jump of the normal derivative of v across Γ_t, that is $\left[\frac{\partial v}{\partial n}\right] = \frac{\partial v_+}{\partial n} - \frac{\partial v_-}{\partial n}$, where the subscripts $+$ and $-$ indicate the regions outside and inside of Γ_t. We define $n_+ = n$ and $n_- = -n$, which are the inner unit normals to the outside region Ω_+ and to the inside region Ω_- of Γ_t, and then we rewrite the equation for the normal velocity as

$$V = \frac{1}{2}\Big(\frac{\partial v_+}{\partial n_+} + \frac{\partial v_-}{\partial n_-}\Big)\,.$$

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Finally, if $|A|$ denotes the area of any given measurable set A, then

$$f = \frac{1}{|\Omega|}\Big(|\Omega_+| - |\Omega_-|\Big).$$

It has been shown in [2] that for smooth solutions to (1) this quantity is in fact constant in time, as the motion preserves both $|\Omega_+|$ and $|\Omega_-|$.

The principal idea is to consider an initial curve Γ_0 for which one can make qualitative statements about the initial velocity, and then to use continuity to forecast the shape of the evolving curves. We look at a shape given by a straight tube with two almost semi-circular end-caps, connected with a sufficiently smooth transition. We will show that for a long straight part the inner normal derivative $\frac{\partial v_-}{\partial n_-}$ is negative near the center of the straight part of the figure, and has bigger magnitude at the center. We will also show that the signed quantity $\frac{\partial v_+}{\partial n_+}$ is decreasing towards the center, and is of smaller magnitude than the contribution by the normal derivative of v_-. This shows that first of all V is negative near the center of the straight parts, and secondly, that the magnitude of V decreases towards the center of the straight part. Thus the figure will become non-convex.

3 The inside of the curve

First we consider only the region Ω_- inside of the curve. We choose Γ_0 the same way as in a previous paper by the first author [9]. That is, Γ_0 contains the two line segments $\{(x, \pm y_0) : -L \leq x \leq L\}$ for some $y_0 > 0$ and $L > 0$, closed off with two almost semi-circular end-caps, one to the left and one to the right. To be precise, the end-caps are circular arcs connected with a short transitional curve to the straight lines. They are chosen so that Γ_0 is of class C^∞, is convex, and is symmetric to the origin, to the x-axis, and to the y-axis. Define

$$w(x, y) = \frac{1+f}{2}(y^2 - y_0^2),$$

then $\Delta w = 1 + f$ in $\mathbb{R}^2$. We define

$$u(x, y) = v_-(x, y) - w(x, y), \quad (x, y) \in \Omega_-,$$

so that $\Delta u = 0$ in Ω_-. Note that

$$\frac{\partial w}{\partial n_-}(x, \pm y_0) = \mp\frac{\partial w}{\partial y}(x, \pm y_0) = -(1 + f)y_0 = \text{const.} < 0,$$

for $(x, \pm y_0) \in \Gamma_0$. Hence, if we want to investigate the chance of the normal derivative of v_- on the straight parts of Γ_0, it suffices to investigate the change of the normal derivative of u instead. We note that $w \equiv 0$ on the straight parts.

The statement made in the introduction about $\frac{\partial v_-}{\partial n_-}$ follows from repeated applications of the maximum principle to u, the precise argument is similar to one presented in the already mentioned paper [9]. Let $(x(s), y(s), C\kappa(s))$ be a parameterization of the curve formed in three-space by the graph of the curvature over Γ_0. It has been shown in [9] (for the case $C = 1$) that the projection of this curve onto the plane $x = 0$ is concave downwards, it looks like an upside-down letter U. The function w is independent of the variable x, and hence also has a well-defined projection on the plane $x = 0$, which is a downwards opening parabola. From this follows that the curve $(x(s), y(s), u(x(s), y(s))) = (x(s), y(s), C\kappa(s) - w((x(s), y(s)))$ also has a well-defined projection onto the plane $x = 0$. This curve is the difference of a concave-down curve minus a concave-up curve, hence is concave down. From this we can conclude that at each point $(0, y(s_1), u(s_1))$ with $-y_0 < y(s_1) < y_0$ we have a (unique) tangent line lying above the curve with an equation of the form $z = my + b$. This equation defines a plane in three-space which touches the curve (x, y, u) at exactly the two points $(\pm x(s_1), y(s_1), u(x(s_1), y(s_1))$, and the plane is above the curve (x, y, u) at all other points. With the maximum principle for harmonic functions, we can now conclude that the graph of u lies below this plane.

We restrict our attention to the right half of the figure. The argument from above shows that $u_x > 0$ on the curved part of the boundary. On the straight part we have $u_x \equiv 0$, as $u = v - w$ is identically zero there. We also have $u_x \equiv 0$ on the y-axis by the symmetry of v and w, and hence of u. We conclude $u_x > 0$ in the interior of the right half of Ω_- by the maximum principle.

As $u_x \equiv 0$ on the upper straight part, we must have $\frac{\partial}{\partial n} u_x = u_{xy} < 0$ on the right half of it by another application of the maximum principle. As $w \leq 0$ for $|y| \leq y_0$, we have $u = v - w \geq 0$ on Γ_0. Yet another application of the maximum principle for the function u itself tells us that $\frac{\partial u}{\partial n} = u_y < 0$ on the upper straight line. Therefore on the right half of the upper line the quantity $\frac{\partial u}{\partial n_-} = |u_y|$ decreases towards the center. By symmetry the same effect happens on the left half of the curve. Hence the same is true for $\frac{\partial v_-}{\partial n_-}$, that is the (signed) inward normal derivative is smaller at the center than towards the ends of the straight parts. Thus the inner function v_- contributes in such a way to the normal velocity V as to break convexity.

Notice that no statement has been made about the sign of the normal derivative of v_-. The longer the straight part of Γ_0, by unchanged radius of the end-caps, the smaller the normal derivative of u is on any bounded piece of the straight part. This is easily seen with the maximum principle and comparing with suitable harmonic barrier functions. To be precise, let κ_M be the maximum of the curvature of Γ_0 and set

$$\hat{u} = C_1((x - x_0)^2 - y^2 + y_0^2) \quad \text{with } C_1 = \frac{4(y_0^2 + C\kappa_M)}{L^2},$$

for some fixed $0 < x_0 < L/2$. Obviously $\hat{u}$ is harmonic, $\hat{u}(x_0, \pm y_0) = 0 = u(x_0, \pm y_0)$, and $\hat{u}(x, \pm y_0) \geq 0 = u(x, y_0)$ on the straight parts of Γ_0. Using $1 + f \leq 2$ and that for (x, y) on the curved part of Γ_0 one has $(x - x_0)^2 \geq (L/2)^2$ and $y^2 \leq y_0^2$, direct calculations shows also $\hat{u} \geq u$ on the curved part of Γ_0, hence on all of Γ_0, and by the weak maximum principle on all of Ω_-. With the strong maximum principle one concludes for the minimum point (x_0, y_0) of the function $\hat{u} - u$ that

$$0 < \frac{\partial u}{\partial n_-}(x_0, y_0) < \frac{\partial \hat{u}}{\partial n_-}(x_0, y_0) = -\frac{\partial \hat{u}}{\partial y}(x_0, y_0) = 2y_0 C_1 = \frac{8y_0(y_0^2 + C\kappa_M)}{L^2}.$$

Hence for large L the magnitude of the normal derivative of v_- on the middle half of the straight parts of Γ_0 is roughly given by the magnitude of the normal derivative of w,

$$\frac{\partial v_-}{\partial n_-} = -(1 + f)y_0 + O\Big(\frac{y_0^3 + y_0\kappa_M}{L^2}\Big), \quad L \to \infty. \tag{2}$$

Changing the length of Γ_0 does also change the normal derivative of w because it changes the constant f, however, if one keeps $1 + f$ away from zero by making the container Ω big enough, there is a negative upper bound on the inward normal derivative of w. With this argument one sees that for a sufficiently long Γ_0 the inward normal derivative of v_- will be negative near the center of the straight part. In this case then, the contribution of the inner function v_- is to push the straight parts inwards, and more so at the center.

4 The outside of the curve

4.1 Reduction to problems about harmonic functions

Define

$$w(x, y) = \frac{-1 + f}{4}(x^2 + y^2),$$

then $\Delta w = -1 + f$ in $\mathbb{R}^2$, so that $\Delta(v_+ - w) = 0$ in Ω_+. The function w is obviously radially symmetric, hence we can compute its normal derivative on $\partial\Omega = \partial B_R(0)$ by taking the (radial) derivative of $w(r) = \frac{-1+f}{4} r^2$, that is

$$\frac{\partial w}{\partial n} = w'(R) = \frac{-1 + f}{2} R \quad \text{on } \partial\Omega.$$

Let φ be a suitable multiple of the fundamental solution of the Laplacian to balance this nonzero normal derivative, that is

$$\varphi(r) = \beta \log r, \quad r = |(x, y)|,$$

defined for $(x, y) \in \Omega_+$. Then

$$\frac{\partial \varphi}{\partial n} = \varphi'(R) = \frac{\beta}{R} \quad \text{on } \partial\Omega,$$

so that the constant

$$\beta = \frac{-1 + f}{2} R^2$$

results in

$$\frac{\partial\varphi}{\partial n} = \frac{\beta}{R} = \frac{\partial w}{\partial n} = \frac{-1+f}{2}R \quad \text{on } \partial\Omega\,.$$

Finally, define

$$u = v_+ - (w - \varphi) \quad \text{in } \Omega_+\,,$$

then u satisfies the following:

$$\left.\begin{array}{rcll} \Delta u &=& 0 & \text{in } \Omega_+\,, \\ \dfrac{\partial u}{\partial n} &=& 0 & \text{on } \partial\Omega\,, \\ u &=& C\kappa - w + \varphi & \text{on } \Gamma_0\,. \end{array}\right\} \tag{3}$$

We will split u once more and write it as $u = Cu_{MS} + U$, where u_{MS} is the outer function occurring in the standard Mullins-Sekerka problem, that is u_{MS} satisfies

$$\left.\begin{array}{rcll} \Delta u_{MS} &=& 0 & \text{in } \Omega_+\,, \\ \dfrac{\partial u_{MS}}{\partial n} &=& 0 & \text{on } \partial\Omega\,, \\ u_{MS} &=& \kappa & \text{on } \Gamma_0\,. \end{array}\right\} \tag{4}$$

The remainder U then satisfies

$$\left.\begin{array}{rcll} \Delta U &=& 0 & \text{in } \Omega_+\,, \\ \dfrac{\partial U}{\partial n} &=& 0 & \text{on } \partial\Omega\,, \\ U &=& \varphi - w & \text{on } \Gamma_0\,. \end{array}\right\} \tag{5}$$

Hence we have the following decomposition of v_+,

$$v_+ = Cu_{MS} + U + w - \varphi \quad \text{in } \Omega_+\,. \tag{6}$$

Notice that a-priori both w and φ depend on R. However, somewhat surprisingly, it turns out that the constant β is in fact independent of R. To see this, compute

$$f = \frac{1}{|\Omega|}\Big(|\Omega| - 2|\Omega_-|\Big) = \frac{1}{\pi R^2}\Big(\pi R^2 - 2|\Omega_-|\Big)\,,$$

so that

$$\beta = \frac{-1+f}{2}R^2 = -\frac{|\Omega_-|}{\pi}\,.$$

We now compute the normal derivatives of w and φ on the straight parts of Γ_0,

$$\frac{\partial w}{\partial n}(x, \pm y_0) = \frac{-1+f}{2}y_0 = \text{const.}\,, \tag{7}$$

and

$$-\frac{\partial\varphi}{\partial n}(x, \pm y_0) = \frac{|\Omega_-|}{\pi}\cdot\frac{y_0}{x^2+y_0^2}\,, \tag{8}$$

which unfortunately decreases in x for $x > 0$. Hence the contribution of $-\varphi$ is such as to maintain convexity by pushing the center of the straight piece out stronger than the ends. Our goal below will be to show that the other two functions compensate for this effect.

4.2 The limiting problem as $R \to \infty$

This problem will enable us to make qualitative statements about the behavior of U near the center of the straight parts. It arises as one lets $R \to \infty$ in equation (5), and hence $f \to 1$, and it reads as

$$\left.\begin{array}{rcll} \Delta U &=& 0 & \text{in } \Omega_+\,, \\ |U| &=& O(1) & \text{as } |(x,y)| \to \infty\,, \\ U &=& -\frac{|\Omega_-|}{\pi}\log|(x,y)| & \text{on } \Gamma_0\,. \end{array}\right\} \tag{9}$$

Hence in the previous notation one has $\Omega = \mathbb{R}^2$. Notice that this limiting problem does not trivially drop out of equation (1) if one takes there $\Omega = \mathbb{R}^2$ and $f = 1$, because it is not clear what to ask of the function v_+ at infinity.

As mentioned before, we will place the curve Γ_0 into a Cartesian coordinate system. We can use Poisson's formula to represent the harmonic function U in the half plane $y > y_0$ if we know its restriction to the line $y = y_0$,

$$U(x,y) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{y-y_0}{(x-\xi)^2+(y-y_0)^2}\, U(\xi,y_0)\, d\xi\,.$$

As the upper straight part of the curve is on the line $y = y_0$, we know that

$$U(\xi,y_0) = -\frac{|\Omega_-|}{2\pi}\log(\xi^2+y_0^2)$$

on this part of the line $y = y_0$, that is on the interval $[-L, L] \times \{y_0\}$. We will split the Poisson integral into three parts,

$$\begin{aligned} U(x,y) \quad = \quad & -\frac{|\Omega_-|}{2\pi^2}\int_{-L}^{L} \frac{y-y_0}{(x-\xi)^2+(y-y_0)^2}\log(\xi^2+y_0^2)\, d\xi \\ & +\frac{1}{\pi}\int_{L}^{\infty} \frac{y-y_0}{(x-\xi)^2+(y-y_0)^2} U(\xi,y_0)\, d\xi \\ & +\frac{1}{\pi}\int_{-\infty}^{-L} \frac{y-y_0}{(x-\xi)^2+(y-y_0)^2} U(\xi,y_0)\, d\xi\,. \end{aligned} \tag{10}$$

Straightforward calculation yields for the kernel

$$k(\xi,x,y) = \frac{y-y_0}{(x-\xi)^2+(y-y_0)^2}$$

the equality

$$\int_{L}^{\infty} |k_{xy}(\xi,x,y_0) + k_{xy}(-\xi,x,y_0)|\, d\xi = \frac{4Lx}{(L^2-x^2)^2}$$

for $0 < x < L$.

By construction all points of Γ_0 have a distance of at least y_0 to the origin. We choose $y_0 \geq 1$, so that in particular

$$U \leq -\frac{|\Omega_-|}{\pi}\log(y_0) \leq 0$$

on the curve Γ_0. Furthermore, let d be the combined x-extension of the transitional part and the circular end-cap. If we had no transitional part and only a semi-circle as an end-cap, the we would have $d = y_0$. From this we see that by making the transitional part sufficiently short, we may assume $d \leq 2y_0$. Hence all the points on Γ_0 have an x-coordinate less than or equal to $L + 2y_0$. As the boundary data of U on Γ_0 is a radial function, and as the enclosing circle of Γ_0 touches Γ_0 at the leftmost and rightmost points of Γ_0, we get the simple estimate

$$U \geq -\frac{|\Omega_-|}{\pi}\log(L+2y_0)$$

on the curve Γ_0. The last two inequalities and the maximum principle imply

$$0 > U > -\frac{|\Omega_-|}{\pi}\log(L+2y_0)$$

on all of Ω_+. Using that U is symmetric and combining this estimate with the computation for the kernel one obtains immediately the following estimate for the mixed second derivative of the sum of the second and third integrals in (10),

$$\left|\frac{\partial^2}{\partial x\partial y}\frac{1}{\pi}\int_{L}^{\infty}(k(\xi,x,y)+k(-\xi,x,y))U(\xi,y_0)\, d\xi\Big|_{y=y_0}\right| < \frac{4L|\Omega_-|\log(L+2y_0)}{\pi^2(L^2-x^2)^2}x\,. \tag{11}$$

The behavior of the first integral in (10) is stated in the following lemma.

Lemma 1 *Fix $y_0 \geq 1$ and let I be the Poisson integral of $\log(x^2+y^2)$ for $y > y_0$ restricted to the interval $[-L, L] \times \{y_0\}$, that is*

$$I(x,y) = \frac{1}{\pi}\int_{-L}^{L} \frac{y-y_0}{(x-\xi)^2+(y-y_0)^2}\log(\xi^2+y_0^2)\, d\xi\,, \quad x \in \mathbb{R}\,,\ y > y_0\,.$$

Then for $L \geq 4y_0$ and sufficiently small $\varepsilon = \varepsilon(L, y_0) > 0$ one has

$$\frac{\partial^2}{\partial x \partial y} I(x, y_0) - \frac{\partial^2}{\partial x \partial y} \log(x^2 + y^2)\Big|_{y=y_0} < -\Big(\frac{4\log(L^2 + y_0^2)}{\pi L^3} + \frac{7L}{3\pi(L^2 + y_0^2)^2}\Big)x$$

for $0 < x < \varepsilon$.

Proof. This is the technical crux of the paper. The computations are tedious, and we defer them to the Appendix. □

We now apply the Lemma to the first integral in (10) and obtain in combination with (11),

$$\begin{aligned}
&\frac{\partial^2}{\partial x \partial y} U(x, y_0) - \frac{\partial^2}{\partial x \partial y} \varphi(x^2 + y^2)\Big|_{y=y_0} \\
&\quad > \frac{2|\Omega_-|}{\pi^2 L^3}\Big(\log(L^2 + y_0^2) + \frac{7L^4}{12(L^2 + y_0^2)^2} - \frac{L^4 \log((L + 2y_0)^2)}{(L^2 - x^2)^2}\Big)x \\
&\quad = \frac{2|\Omega_-|}{\pi^2 L^3}\Big(\log\Big(\frac{L^2 + y_0^2}{(L + 2y_0)^2}\Big) + \frac{7L^4}{12(L^2 + y_0^2)^2} - \log((L + 2y_0)^2)\Big(\frac{L^4}{(L^2 - x^2)^2} - 1\Big)\Big)x\,. \qquad (12)
\end{aligned}$$

This estimate holds for $0 < x < \varepsilon$ with $\varepsilon = \varepsilon(L, y_0) > 0$ from Lemma 1.

We set $L = ty_0$ in the first two terms inside of the parentheses, and define the resulting function as

$$F(t) = \log\Big(\frac{t^2 + 1}{(t + 2)^2}\Big) + \frac{7t^4}{12(t^2 + 1)^2}\,.$$

By taking the derivative it is easily seen that F is an increasing function for, say, $t > 1$, and one computes $F(6) = 0.0042\ldots > 0$. By going back to inequality (12), we have that the sum of the first two terms inside of the parentheses on the right-hand side is positive provided $L \geq 6y_0$. For any such fixed L and y_0 the third term inside of the parentheses tends to zero as $x \to 0$, hence, after possibly shrinking ε, we may assume that for $0 < x < \varepsilon$ this term is less than the sum of the first two, and the sum of the three terms is positive. Summarizing the result of this section, we obtain for all $L \geq 6y_0$ and with some constant $c = c(L, y_0, \delta) > 0$ for the solution U of equation (9) the estimate

$$\frac{\partial^2}{\partial x \partial y} U(x, y_0) > \frac{\partial^2}{\partial x \partial y} \varphi(x^2 + y^2)\Big|_{y=y_0} + c\,, \qquad (13)$$

valid for $\delta < x < \varepsilon$ where $\varepsilon = \varepsilon(L, y_0) > 0$ and $0 < \delta < \varepsilon$.

4.3 The problem on a finite ball

Now we need a lemma like the following to be able to connect the solution of the limiting case $R \to \infty$ with the solutions for finite R.

Lemma 2 *Let Γ be a simple smooth closed curve in $\mathbb{R}^2$, and let Ω_R be the region inside of the ball $B_R(0)$ and outside of Γ. Let $\psi_R : \Gamma \to \mathbb{R}$ be smooth, and $\psi_R \to \psi$ uniformly as $R \to \infty$. Let u_R be the solution to*

$$\left.\begin{array}{rcll}
\Delta u_R &=& 0 & \text{in } \Omega_R\,, \\
\dfrac{\partial u_R}{\partial n} &=& 0 & \text{on } \partial B_R(0)\,, \\
u_R &=& \psi_R & \text{on } \Gamma\,,
\end{array}\right\}$$

and let $\overline{u}$ be the solution to

$$\left.\begin{array}{rcll}
\Delta \overline{u} &=& 0 & \text{in } \Omega_+\,, \\
|\overline{u}| &=& O(1) & \text{as } |(x, y)| \to \infty\,, \\
\overline{u} &=& \psi & \text{on } \Gamma\,.
\end{array}\right\}$$

Finally let K be any fixed compact subset of $\Omega_R \cup \Gamma$ for R sufficiently large. Then for any $\eta > 0$ the estimate

$$|\overline{u} - u_R|_{2+\alpha;K} \leq \eta\,,$$

holds, provided R is sufficiently large. The indicated norm is the usual Hölder norm.

The proof of this lemma is similar to the proof of Lemma 6.5 in [7], and is omitted here.

Now let $\overline{u}$ be the solution to equation (9), that is, the solution obtained from the limiting case $R \to \infty$. Let u_R be the solution to equation (5). Set ψ equal to the right-hand side of the third equation in (9), that is $\psi(x,y) = \varphi(|(x,y)|)$. Similarly, set ψ_R equal to the right-hand side of the third equation in (5), so that

$$\psi_R(x,y) = -\frac{-1+f}{4}(x^2+y^2) + \varphi(|(x,y)|)\,.$$

As $f \to 1$ for $R \to \infty$, we are in the setting to use Lemma 2 with $\eta = c/2$ for the constant c from estimate (13), and K being the interval from (13) as well, that is, the set $[\delta,\varepsilon] \times \{y_0\}$. We conclude that there is a (big) ball $B_R(0)$ containing Γ_0 so that for the solution u_R we have the estimate

$$\frac{\partial^2}{\partial x \partial y} u_R(x,y_0) > \frac{\partial^2}{\partial x \partial y}\varphi(|(x,y)|)\Big|_{y=y_0} + c/2\,, \tag{14}$$

again valid on the same interval K. Using the results from [10] we also have a sign for the mixed derivative of the outer harmonic function u_{MS} connected with the unmodified Mullins-Sekerka problem,

$$\frac{\partial^2}{\partial x \partial y} u_{MS}(x,y_0) > 0\,, \tag{15}$$

valid for $\delta < x < \varepsilon - \delta$ for any $0 < \varepsilon < L/2$ and $0 < \delta < \varepsilon/2$, provided R is large enough.

Coming back to the previous notation, we fix this R and have $U = u_R$. By equation (6) we have

$$\frac{\partial v_+}{\partial n} = C\frac{\partial u_{MS}}{\partial n} + \frac{\partial U}{\partial n} + \frac{\partial w}{\partial n} - \frac{\partial \varphi}{\partial n}\,. \tag{16}$$

Recall the computations of the normal derivatives of w and φ in equations (7) and (8). As stated earlier, $-\frac{\partial \varphi}{\partial n}$ decreases in x for $x > 0$. That is the reason why we had to work so hard to find an estimate for the mixed derivative of U, so we can balance this term, which is exactly what (14) does for us because $\frac{\partial}{\partial n} = \frac{\partial}{\partial y}$ and $U = u_R$. Combining (7), (8), (14), (15), and (16), we conclude that the normal derivative of v_+ does in fact grow towards the right, for L sufficiently large, and for $\delta < x < \varepsilon - \delta$.

In the final paragraph of this section we want to show that the normal derivative of v_+ is small, as least for L and R sufficiently large. To achieve this, we use once more the decomposition (16). We have already computed the normal derivatives of w and φ in equations (7) and (8), respectively. Similarly to how we compared for sufficiently large L and R the mixed derivative of U with the mixed derivative of $-\varphi$ near the center of the straight piece of Γ_0, one can show that the normal derivative of U is almost equal to the normal derivative of $-\varphi$. The computations are in fact easier as one has to take only one derivative; the details are omitted here. The normal derivative of u_{MS} is small, provided L is sufficiently large. This is once again seen with the use of the strong maximum principle and suitable harmonic barrier functions on Ω_+, here

$$\hat{u}(x,y) = C_2(\log((x-x_0)^2+y^2) - \log(y_0^2)) \quad \text{with } C_2 = \frac{\kappa_M}{\log((L/2y_0)^2)}\,,$$

the argument being a slight modification of the one at the end of Section 3, the difference being that $\partial\Omega_+$ has two components, namely Γ_0 and $\partial B_R(0)$. As before one checks with direct calculation that $\hat{u} \geq u$ on Γ_0, and now also that $\frac{\partial \hat{u}}{\partial n} > \frac{\partial u}{\partial n}$ on $\partial B_R(0)$, so that with the strong maximum principle one concludes $\hat{u} > u$ in Ω_+. Now one finishes the argument exactly as before. Finally, the normal derivative of w can be made small because $f \to 1$ as $R \to \infty$. Notice that the smallness of the contribution of $\frac{\partial v_+}{\partial n}$ to the normal velocity is not enough to conclude a break of convexity, one does in fact need an estimate on the change of the normal derivative, as computed above.

5 The conclusion

We have shown in the previous sections that the two inner normal derivatives making up the normal velocity grow as we go away from the center (where we start a distance $\delta > 0$ away from the center), and hence so does the normal velocity, which is their average. A loss of convexity can thus be concluded, regardless of the sign of the normal velocity. Two cases arise.

(a) The normal velocity is negative near the center of the straight parts. Since the signed normal velocity grows as we go away from the center, it is less negative away from the center, and we get a loss

of convexity because the curve moves in faster near the center of the straight parts as compared to the movement further away from the center.
(b) The normal velocity is nonnegative near the center of the straight parts. Since the signed normal velocity grows as we go away from the center, it is more positive away from the center, and we get a loss of convexity because the curve moves out slower near the center of the straight parts as compared to the movement further away from the center.

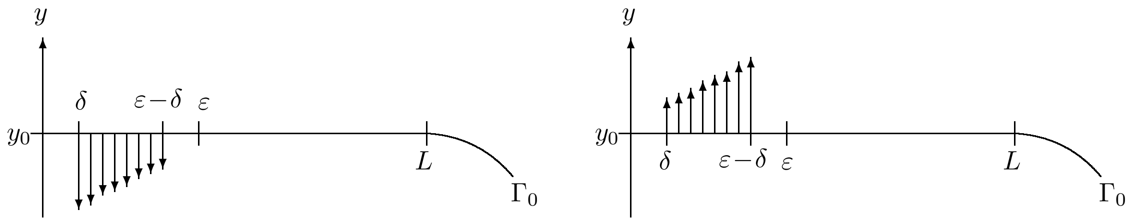

Figure 1: A schematic sketch of the initial normal velocity of the interval K belonging to the straight part of Γ_0. Part(a) on the left shows the case of negative normal velocity; Part (b) on the right shows the case of positive normal velocity. Not drawn to scale.

As mentioned in the introduction, the existence of smooth solutions for this modified Mullins-Sekerka flow on a bounded domain has been established recently [2]. In fact, as follows from the proofs in [2], the solution constitutes a semi-flow on a space of curves (in two dimensions) parameterized over a reference curve, and one has continuous dependence of the solution on the initial data, measured in the $C^{2+\alpha}$ norm. The example presented herein that leads to a loss of convexity can therefore be slightly perturbed, and it will still evolve into a nonconvex shape. In particular we can perturb it in such a fashion that the resulting initial curve is strictly convex.

Finally we notice that the condition $y_0 \geq 1$ is in fact only a technical condition used to simplify the proofs above. In fact, $y_0 \geq 1$ can always be achieved through rescaling of the original problem. This only changes the constant C in (1).

Theorem 1 *There are strictly convex smooth initial configurations that will evolve into nonconvex curves under the modified two-sided Mullins-Sekerka flow on a large disk. In particular one can choose a strictly convex small smooth perturbation of a curve consisting of a straight tube of length at least six times its diameter, closed off with two almost semi-circular end caps.*

Using the computations from the end of Sections 3 and 4, we can conclude that the normal velocity is negative near the center of the straight part, provided the initial curve Γ_0 is sufficiently long, and the containing ball Ω is sufficiently large. This is so because under these circumstances the contribution of the inner function v_- to the normal velocity is negative, and the one from the outer function v_+ can be made arbitrarily small. Hence the center moves in, and faster than the ends do. That is, we are in case (a) from above, see also Figure 1. This is contrary to the behavior of solutions to the unmodified Mullins-Sekerka model, where convexity is always broken while the center of the curve moves out, see [10].

Corollary 1 *If the curve from the Theorem has a sufficiently long straight part and is placed into a sufficiently large ball, then it will lose its convexity by moving inwards near the center of the straight parts.*

Appendix: The proof of Lemma 1

For this proof let us fix some notation first,

$$\begin{aligned} k(\xi, x, y) &= \frac{y - y_0}{(x-\xi)^2 + (y-y_0)^2}, \\ g(\xi) &= \log(\xi^2 + y_0^2), \\ I(x, y) &= \frac{1}{\pi} \int_{-L}^{L} k(\xi, x, y) g(\xi)\, d\xi. \end{aligned}$$

Because of $k_x = -k_\xi$ and because g is even, we get using integration by parts

$$\begin{aligned} I_x(x,y) &= \frac{1}{\pi}\int_{-L}^{L} k_x(\xi,x,y)g(\xi)\,d\xi \\ &= \frac{g(L)}{\pi}[k(-L,x,y)-k(L,x,y)] + \frac{1}{\pi}\int_{-L}^{L} k(\xi,x,y)g'(\xi)\,d\xi\,. \end{aligned} \tag{17}$$

Hence we obtain

$$I_{xy}(x,y) = \frac{g(L)}{\pi}[k_y(-L,x,y)-k_y(L,x,y)] + \frac{1}{\pi}\int_{-L}^{L} k_y(\xi,x,y)g'(\xi)\,d\xi\,. \tag{18}$$

Let

$$K(\xi,x,y) = \frac{x-\xi}{(x-\xi)^2+(y-y_0)^2}\,,$$

then

$$K_\xi(\xi,x,y) = \frac{(x-\xi)^2-(y-y_0)^2}{((x-\xi)^2+(y-y_0)^2)^2} = k_y(\xi,x,y)\,. \tag{19}$$

Using this relationship, integration by parts, and that g' is odd, we obtain from (18) the formula

$$\begin{aligned} I_{xy}(x,y) &= \frac{g(L)}{\pi}[k_y(-L,x,y)-k_y(L,x,y)] + \frac{g'(L)}{\pi}[K(-L,x,y)+K(L,x,y)] \\ &\quad -\frac{1}{\pi}\int_{-L}^{L} K(\xi,x,y)g''(\xi)\,d\xi\,. \end{aligned} \tag{20}$$

We now proceed to compute the first two terms in this formula for $y=y_0$ and using (19) for k_y,

$$\begin{aligned} \frac{g(L)}{\pi}[k_y(-L,x,y_0)-k_y(L,x,y_0)] &= -\frac{4L\log(L^2+y_0^2)}{\pi(L^2-x^2)^2}x \\ &= -\frac{4\log(L^2+y_0^2)}{\pi L^3}x + o(x)\,, \quad x\to 0\,, \end{aligned} \tag{21}$$

and

$$\begin{aligned} \frac{g'(L)}{\pi}[K(-L,x,y_0)+K(L,x,y_0)] &= -\frac{4L}{\pi(L^2-x^2)(L^2+y_0^2)}x \\ &= -\frac{4}{\pi L(L^2+y_0^2)}x + o(x)\,, \quad x\to 0\,. \end{aligned} \tag{22}$$

It remains to treat the integral in (20),

$$\begin{aligned} I_2(x,y) &:= -\frac{1}{\pi}\int_{-L}^{L} K(\xi,x,y)g''(\xi)\,d\xi \\ &= -\frac{g''(x)}{\pi}\int_{-L}^{L} K(\xi,x,y)\,d\xi - \frac{1}{\pi}\int_{-L}^{L} K(\xi,x,y)(g''(\xi)-g''(x))\,d\xi \\ &= \frac{g''(x)}{2\pi}\log((\xi-x)^2+(y-y_0)^2)\Big|_{-L}^{L} + \frac{1}{\pi}\int_{-L}^{L}\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi \\ &\quad -(y-y_0)\frac{1}{\pi}\int_{-L}^{L}\frac{y-y_0}{(x-\xi)^2+(y-y_0)^2}\cdot\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi\,. \end{aligned} \tag{23}$$

The last integral in (23) without the factor $(y-y_0)$ is the Poisson integral of the function

$$h(\xi) = \begin{cases} \dfrac{g''(\xi)-g''(x)}{\xi-x} & \text{for } -L<\xi<L\,,\ \xi\neq x\,, \\ g'''(x) & \text{for } \xi = x\,, \\ 0 & \text{for } |\xi|\geq L\,. \end{cases}$$

As h is continuous on $(-L,L)$ the limit of this integral as $y\to y_0^+$ exists, and equals $h(x)$. The factor $(y-y_0)$ in front of the integral therefore forces the contribution of this integral to be zero in the limit, and we have

$$I_2(x,y_0)=\lim_{y\to y_0^+} I_2(x,y)=\frac{g''(x)}{2\pi}\log\frac{L-x}{L+x}+\frac{1}{\pi}\int_{-L}^{L}\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi\,.$$

As $\log\dfrac{L-x}{L+x}=-\dfrac{2}{L}x+o(x)$ and $g''(x)=2\dfrac{y_0^2-x^2}{(x^2+y_0^2)^2}=\dfrac{2}{y_0^2}+o(1)$, both for $x\to 0$, we get

$$I_2(x,y_0)=-\frac{4}{\pi L y_0^2}x+o(x)+\frac{1}{\pi}\int_{-L}^{L}\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi\,,\quad x\to 0\,. \tag{24}$$

Let $I_3(x,y_0)$ be the integral in the previous formula. We split it into three parts, and we substitute $z=x-\xi$ in the second integral and $z=\xi-x$ in the third integral below,

$$\begin{aligned} I_3(x,y_0) &= \frac{1}{\pi}\int_{-L}^{-L+2x}\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi+\frac{1}{\pi}\int_{-L+2x}^{x}\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi+\frac{1}{\pi}\int_{x}^{L}\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi \\ &= \frac{1}{\pi}\int_{-L}^{-L+2x}\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi+\frac{1}{\pi}\int_{0}^{L-x}\frac{g''(x+z)-g''(x-z)}{z}\,dz\,. \end{aligned} \tag{25}$$

Let $I_4(x,y_0)$ and $I_5(x,y_0)$, respectively, denote the last two integrals in the previous formula. We proceed to compute $I_4(x,y_0)$ first,

$$\begin{aligned} I_4(x,y_0) &= \frac{2}{\pi}\left(\frac{1}{2x}\int_{-L}^{-L+2x}\frac{g''(\xi)-g''(x)}{\xi-x}\,d\xi\right)x \\ &= \frac{2}{\pi}\cdot\frac{g''(-L)-g''(x)}{-L}x+o(x) \\ &= -\frac{4}{\pi L}\Big(\frac{y_0^2-L^2}{(L^2+y_0^2)^2}-\frac{1}{y_0^2}\Big)x+o(x)\,,\quad x\to 0\,. \end{aligned} \tag{26}$$

In the above we used the Mean Value Theorem for integrals to get the second equality. Integral $I_5(x,y_0)$ we split a last time,

$$I_5(x,y_0)=\frac{1}{\pi}\int_{0}^{L}\frac{g''(x+z)-g''(x-z)}{z}\,dz-\frac{1}{\pi}\int_{L-x}^{L}\frac{g''(x+z)-g''(x-z)}{z}\,dz\,. \tag{27}$$

We call the first integral above $I_6(x,y_0)$, and we compute the second integral using the Mean Value Theorem,

$$\frac{1}{\pi}\Big(\frac{1}{x}\int_{L-x}^{L}\frac{g''(x+z)-g''(x-z)}{z}\,dz\Big)x=\frac{1}{\pi}\frac{g''(L)-g''(-L)}{L}x+o(x)=o(x)\,,\quad x\to 0\,,$$

where for the last equality we have used that g'' is even. This shows that

$$I_5(x,y_0)=I_6(x,y_0)+o(x)\,,\quad x\to 0\,. \tag{28}$$

Finally, as $g''(\xi)=2\dfrac{y_0^2-\xi^2}{(\xi^2+y_0^2)^2}$ is a rational function, so is $\dfrac{g''(x+z)-g''(x-z)}{z}$. Expanding in powers of x and z we obtain

$$\begin{aligned} I_6(x,y_0) &= \Big(\frac{1}{\pi}\int_0^L\frac{-16y_0^2z^2-24y_0^4+8z^4}{(z^2+y_0^2)^4}\,dz\Big)x+o(x) \\ &= -\frac{8}{\pi}\Big(\frac{L}{(L^2+y_0^2)^2}+\frac{L}{(L^2+y_0^2)y_0^2}+\frac{1}{y_0^3}\arctan\big(\frac{L}{y_0}\big)\Big)x+o(x)\,,\quad x\to 0\,. \end{aligned} \tag{29}$$

Finally we combine all terms, and we obtain

$$\begin{aligned} I_{xy}(x,y_0) &= -\frac{1}{\pi}\Big(\frac{4\log(L^2+y_0^2)}{L^3}+\frac{8y_0^2}{L(L^2+y_0^2)^2}+\frac{8L}{(L^2+y_0^2)^2} \\ &\qquad +\frac{8L}{(L^2+y_0^2)y_0^2}+\frac{8}{y_0^3}\arctan\big(\frac{L}{y_0}\big)\Big)x+o(x)\,,\quad x\to 0\,. \end{aligned} \tag{30}$$

Ultimately we want to compare this to the mixed derivative of $\log(x^2+y^2)$, that is, to

$$\frac{\partial^2}{\partial x \partial y} \log(x^2+y^2)\Big|_{y=y_0} = -\frac{4xy_0}{(x^2+y_0^2)^2} = -\frac{4}{y_0^3}x + o(x)\,, \quad x \to 0\,. \tag{31}$$

Hence we rewrite (30) in a form more suitable to this comparison,

$$\begin{aligned} I_{xy}(x,y_0) \;=\; & -\frac{4}{y_0^3}\Big(\frac{y_0^3\log(L^2+y_0^2)}{\pi L^3} + \frac{2y_0^5}{\pi L(L^2+y_0^2)^2} + \frac{2Ly_0^3}{\pi(L^2+y_0^2)^2} \\ & + \frac{2Ly_0}{\pi(L^2+y_0^2)} + \frac{2}{\pi}\arctan(L/y_0)\Big)x + o(x)\,, \quad x \to 0\,. \end{aligned} \tag{32}$$

We set $t = L/y_0$ and let $G(t)$ be the sum of parts of the third term plus the last two terms inside of the parentheses above, more precisely,

$$G(t) = \frac{17t}{12\pi(t^2+1)^2} + \frac{2t}{\pi(t^2+1)} + \frac{2}{\pi}\arctan(t)\,.$$

With methods from elementary calculus we see that $G'(\pm\sqrt{65/3}) = 0$, and that there are no other critical points. Since $G(4) = 1.00007\ldots > 1$, since the maximum of G at $t = \sqrt{65/3}$ is to the right of $t = 4$, and since $\lim_{t\to\infty} G(t) = 1$, we see that $G(t) > 1$ for $t \geq 4$. This implies

$$I_{xy}(x,y_0) \;<\; -\frac{4}{y_0^3}\Big(\frac{\log(L^2+y_0^2)}{\pi(L/y_0)^3} + \frac{2y_0^5}{\pi L(L^2+y_0^2)^2} + \frac{7Ly_0^3}{12\pi(L^2+y_0^2)^2} + 1\Big)x + o(x)\,, \quad x \to 0\,, \tag{33}$$

valid for $L \geq 4y_0$. Recalling (31), we can after fixing L and y_0 find an $\varepsilon > 0$ so that for $0 < x < \varepsilon$ the following holds,

$$I_{xy}(x,y_0) < \frac{\partial^2}{\partial x \partial y}\log(x^2+y^2)\Big|_{y=y_0} - \Big(\frac{4\log(L^2+y_0^2)}{\pi L^3} + \frac{7L}{3\pi(L^2+y_0^2)^2}\Big)x\,,$$

which is exactly the assertion of Lemma 1. □

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