A gradient flow approach to a free boundary droplet model

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Abstract

We consider a quasi-static droplet motion based on contact angle dynamics on a planar surface. Based on a gradient flow structure of the problem we derive a natural time–discretization using the JKO–scheme, and discuss convergence in the continuum limit. The time discrete interface motion is described in comparison with *barrier* functions, which are classical sub- and super-solutions in a local neighborhood. This barrier property is different from standard viscosity solutions since there is no comparison principle for our problem. In the continuum limit the barrier properties still hold in a modified sense.

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1 Introduction

The motion of liquid drops on a planar surface is a widely studied topic. We consider a *quasi–stationary* free boundary model, derived in [8], [10] and [12]. The model is contact angle driven, i.e. the motion of the boundary of the wetted region is due to a deviation of the contact angle from the ideal contact angle. It is also quasi–stationary in the sense that the actual profile of the drop adjusts itself to the wetted region by minimizing a "surface energy" under a volume constraint.

We derive a natural time discretization by exploiting a formal gradient flow structure of the model. The time-discrete solutions satisfy barrier properties similar to standard viscosity solutions. These barrier properties stay valid in a modified sense as the time step size goes to zero.

Let us begin by a formal introduction of the model. The profile of the droplet is given by the height function $u : \mathbb{R}^N \times (0,T) \to \mathbb{R}$ with $N = 2$, the *positive phase* $\{u > 0\}$ denotes the wetted region and the free boundary $\partial\{u > 0\}$ denotes the contact line between drop, air and surface. It should be pointed out that our analysis is performed in general space dimension N. Throughout the paper we denote the spatial derivative of u by Du. The motion of the droplet is described by contact angle dynamics - the free boundary $\partial\{u > 0\}$ evolves by a relationship between the outward normal velocity V and the *contact angle* $|Du|$ of the droplet with the surface. In this paper the normal velocity is given by

$$V = |Du|^2 - 1 \qquad \text{on } \partial\{u > 0\}.$$

The square of the contact angle in the velocity law seems natural, as it is the only power for which we directly have a gradient flow structure like the one considered in this paper. For discussion of the contact angle dynamics in form of more general free boundary velocities we refer to [19].

On the other hand the shape of the drop adjusts to the wetted region by obeying two constraints: First the volume in each component ω_i of the drop is kept constant over time. Secondly the liquid/vapor interface is minimal in the sense that it minimizes the Dirichlet integral, leading to the Euler–Lagrange equation $-\Delta u(\cdot,t) \equiv \lambda$. This equation, a simplification of minimal surface equation, defines the shape of a quasi-static droplet. By choosing a suitable Lagrange multiplier $\lambda = \lambda_i(t)$, the volume of droplets in each component can be preserved.

Summarizing above discussion we arrive at the following free boundary problem:

$$(P) \qquad \begin{cases} -\Delta u(\cdot,t) = \lambda_i(t) & \text{in} \quad \omega_i(t); \\ \\ V = |Du|^2 - 1 & \text{on} \quad \partial\omega_i(t); \\ \\ \int_{\omega_i(t)} u(\cdot,t)\,dx \equiv c_i, \end{cases}$$

where, as mentioned above, V is the outward normal velocity of the connected component of the support of the drop $\omega_i(t)$.

Several serious challenges arise in developing a global notion of solutions for the model described above:

Firstly, (P) *does not satisfy the comparison principle* between solutions, even in the case of single components. In particular the viscosity solutions approach applied to mean curvature flow (see [7] for example) does not apply here, even if we assume that there is no topology change. Observe that if λ is independent of time then standard viscosity solution theory as in [14] applies. Based on this observation a discrete-time approximation with fixed λ in each time step was carried out in [9]. This way a unique weak solution is obtained for star-shaped initial data, for short times (as long as the wet region stays star-shaped). However approximating (P) with fixed λ in small time intervals (apparently) does not work well with topology changes.

Secondly, finite-time singularities such as *topology changes* seem unavoidable. *Splitting* of droplets into multiple components is generic for non-convex droplets, even if we start the evolution with a simply connected droplet. *Merging* of different parts of the droplet also naturally occurs. (Recall that our model is quasi-stationary. This means that the dynamics inside the liquid phase is not modeled. In some sense when a topology change occurs we "fast forward" the time so that the droplet becomes quasi-stationary again.) In addition to the topological changes, we expect corner or cusp formation on the interface, due to merging, splitting, and also shrinking of droplets (see [9]).

Lastly, there is a bifurcation *(non-uniqueness)* of solutions in the event of merging.

More precisely, two stationary drops touching each other at exactly one point can either decide to stay as they are, or see each other and develop into one big drop. Similar bifurcation has been previously observed, for solutions of a flame propagation model ([18]).

Our goal is to introduce a global-time notion of weak solution which describes (P) past topological changes and singularities. We take a variational approach, based on the following observation. Formally speaking the droplet evolution (P) is a gradient flow for the energy

$$E(\omega) := \int_\omega |Du_\omega|^2\, dx \; + \; |\omega|, \tag{1.1}$$

where $|\omega|$ denotes the (Lebesgue) measure of ω. The gradient flow takes place on the manifold of possible supports of the droplet. The droplet height u itself is then part of a tangent bundle above the manifold. We refer to Section 2 for detailed discussion of this structure: there a modified energy is introduced to ensure that the supports of the droplets lies in the space of Caccioppoli sets in $I\!R^N$.

In Section 3 we approximate the solution (P) by a time-discrete gradient flow (JKO) scheme, originated by [13]. This scheme defines the solution in the next time step as a minimizer of a composited functional. This functional consists partly of the energy and partly of the distance to the previous time step. See Section 3 for details. Such approach was taken before by Almgren,Taylor and Wang [1] and Luckhaus and Sturzenhecker [15] for crystalline mean curvature motion. Luckhaus and Sturzenhecker also take a similar approach for the Mullins–Sekerka problem. In [4] it was shown that a particular selection of the discrete scheme in [1] converges to viscosity solution of the mean curvature flow in the sense of [7].

As mentioned before our problem lacks the comparison property (see Remark 5.6) even in simple settings, which prevents us to develop any connection to standard viscosity solutions approach. However it is still possible to describe the evolution of solutions by *barrier properties* (Proposition 4.1 and 4.2) of the time-discrete weak solutions. Roughly speaking this means that the time-discrete solutions evolve with the free boundary velocity given by (P), at “regular” points of the interface. This is shown in Section 4.

In the continuum limit the discrete solutions converge weakly in H^1 – see the beginning paragraph of Section 5. As of now we are only able to describe limiting free boundary behavior in terms of the liminf and limsup of the time-discrete solutions (see Theorem 5.5). We refer to Section 5 for definition of weak solutions and precise convergence results. Lastly the paper ends with section 6, where further questions are presented with discussions.

2 Formal gradient flow structure of the droplet model

The gradient flow structure of (P)**.** For technical reasons explained below we approximate (P) by

$$
(P_\epsilon) \qquad \begin{cases} -\Delta u(\cdot,t) = \lambda_i(t) & \text{in} \quad \omega_i(t); \\ V = |Du|^2 - 1 - \epsilon\kappa & \text{on} \quad \partial\omega_i(t); \\ \int_{\omega_i(t)} u(\cdot,t)\,dx \equiv c_i, & \end{cases}
$$

for some small $\epsilon > 0$ where $\kappa = -\nabla \cdot (\frac{Du}{|Du|})$ denotes the mean curvature of the interface, positive if the positive phase $\{u(\cdot,t) > 0\}$ is convex. As the evolution (P) is formally a gradient flow for the energy (1.1) on the"manifold" of sets with finite perimeter, so is (P_ϵ) for the energy (2.1), see below. Let us start with the definitions:

Definition 2.1 *(a) Let us define the set of Caccioppoli sets*

$$Cacc := \{\omega \subset I\!R^N\,;\ \omega \text{ is a closed set with finite perimeter}\}.$$

(b) For any $\omega \in Cacc$ and any volume c

$$u_{\omega,c} := \operatorname{argmin}\left\{\int_\omega |Du|^2\,dx : \quad u \in H^1(I\!R^N), \quad \operatorname{supp} u = \omega, \quad \int_\omega u\,dx = c\right\}.$$

With this notation problem (P_ϵ) is a gradient flow on $Cacc$ for the energy

$$E_\epsilon(\omega) := \int_\omega |Du_{\omega,1}|^2\,dx + |\omega| + \epsilon|\partial\omega|, \tag{2.1}$$

where $|\omega|$ and $|\partial\omega|$ respectively denote the Lebesgue measure and the perimeter of ω.

Remark 2.2 *Note that the minimizer $u_{\omega,c}$ exists: a minimizing sequence of the Dirichlet integral is bounded in $H^1(I\!R^N)$ and therefore converges strongly in $L^2(I\!R^N)$. Also the Dirichlet integral is lower semi continuous.*

Furthermore, if $u_{\omega,c} \in C^2(interior(\omega))$ then the Euler–Lagrange equation of the Dirichlet integral is

$$- \Delta u_{\omega,c} = \lambda \tag{2.2}$$

for a constant λ. Thus, a time evolution of $u_{\omega,c}$ is a candidate to solve (P_ϵ) or (P). For smooth $u_{\omega,c}$ we also have the equality

$$\int_\omega |Du_{\omega,c}|^2 \, dx = \lambda \int_\omega u_{\omega,c} \, dx.$$

We use this intuition to define:

Definition 2.3 *Let $\omega \in Cacc$ then for any volume $c > 0$ we define:*

$$\lambda_c(\omega) := \frac{1}{c} \min \left\{ \int_\omega |Du|^2 \, dx \;\middle|\; \text{supp } u = \omega \,; \int_\omega u \, dx = c \right\}.$$

For $c = 0$ we set $\lambda_0(\omega) = 0$ for all $\omega \in Cacc$.

In the following we suppress the dependence of the energy on the volume in our notation, as it is not essential for one component. To make the description of the gradient flow complete we have to formally equip the set $Cacc$ with a Riemannian structure. For this we choose

$$g_\omega(v, \tilde{v}) := \int_{\partial\omega} v \, \tilde{v} \, dS \qquad \forall v, \tilde{v} \in T_\omega Cacc, \tag{2.3}$$

where the tangent space $T_\omega Cacc$ is the space of normal velocities of ω. Note that the function u_ω is not part of the manifold. It is part of the tangent bundle over $Cacc$. This idea was introduced in [11] for a thin film equation with surfactant. In our case it reflects the quasi–stationary nature of the free boundary problem. Equations (2.1) and (2.3) together define a gradient flow $\partial_t \omega = - \nabla E_\epsilon(\omega)$ on the space $Cacc$ (see e.g. [17]). By definition of ∇E_ϵ this is equivalent to the time evolution following the normal velocity $v_{\nabla E_\epsilon}$:

$$g_\omega \left(v_{\nabla E_\epsilon}, \tilde{v} \right) := - diff \, E_\epsilon(\omega).\tilde{v} \qquad \forall \tilde{v} \in T_\omega Cacc. \tag{2.4}$$

We will now show formally that the time evolution following $v_{\nabla E}$ given by (2.4) is indeed equivalent to the evolution of supp u in (P_ϵ). It suffices to check that

$$v_{\nabla E_\epsilon} = |Du_\omega|^2 - 1 - \epsilon\kappa. \tag{2.5}$$

The evolution of u_ω then solves (P_ϵ) in a weak sense by Definition 2.1, Remark 2.2 and the Euler–Lagrange equation (2.2). To calculate $v_{\nabla E_\epsilon}$ note that for $\tilde{\delta u}$ being the change of u introduced by $\tilde{v}$

$$\begin{aligned} diff\, E_\epsilon(\omega).\tilde{v} \;&=\; \int_\omega 2Du_\omega \cdot\, D\tilde{\delta u}\, dx \;+\; \int_{\partial\omega} (1+|Du_\omega|^2)\,\tilde{v}\, dS \;+\; \int_{\partial\omega} \epsilon\kappa\,\tilde{v}\, dS \\ &=\; -\int_\omega 2\,\Delta u_\omega\,\tilde{\delta u}\, dx \;+\; \int_{\partial\omega} -2\,|Du_\omega|\tilde{\delta u} \;+\; (1+|Du_\omega|^2 \;+\epsilon\kappa)\,\tilde{v}\, dS \\ &=\; \lambda \int_\omega \tilde{\delta u}\, dx + \int_{\partial\omega} \;-2\,|Du_\omega|^2\,\tilde{v} \;+\; (1+|Du_\omega|^2 \;+\; \epsilon\kappa)\,\tilde{v}\, dS \\ &=\; \int_{\partial\omega} (1 \;-\; |Du_\omega|^2 \;+\; \epsilon\kappa)\,\tilde{v}\, dS \end{aligned}$$

by Definition 2.1 and for $\kappa := -\nabla\cdot(\frac{Du}{|Du|})$ the mean curvature of $\partial\omega$ and by the fact that the outward normal $\eta \;=\; -\frac{Du}{|Du|}$. This gives (2.5) by (2.4) and (2.3).

Natural time discretization of a gradient flow, JKO–scheme A gradient flow on a manifold has a natural time discretization. This discretization called the JKO–scheme was introduced in [13]. It coincides with an implicit Euler discretization in Euclidean space, but is adapted to treat the Riemannian structure of the manifold. For this we define the natural distance belonging to the Riemannian structure (2.3) by:

$$dist^2(\omega_0,\omega_1) \;:=\; \inf\left\{\int_0^1 \int_{\partial\omega_t} v(t)^2\, dS\, dt\right\}, \tag{2.6}$$

where the infimum is taken over all time–differentiable paths $\omega(t) \in Cacc$ connecting ω_0 and ω_1 and $v(t)$ is the normal velocity of $\omega(t)$. The time discrete JKO–scheme is then given by finding the state ω^{i+1} given the state ω^i as

$$\omega^{i+1} \;=\; argmin_{\omega\in Cacc}\left\{\frac{1}{2h}\, dist^2(\omega^i\,,\omega) \;+\; E_\epsilon(\omega)\right\} \tag{2.7}$$

where the minimum is taken over all $\omega \in Cacc$.
This time discretization gives two powerful estimates for free. First the energy is non–increasing in each time step, as one would expect for a gradient flow. This holds as ω^{i+1} is a minimizer:

$$E_\epsilon(\omega^i) \;=\; \frac{1}{2h}\, dist^2(\omega^i\,,\omega^i) \;+\; E_\epsilon(\omega^i) \geq \frac{1}{2h}\, dist^2(\omega^i\,,\omega^{i+1}) \;+\; E_\epsilon(\omega^{i+1}) \geq\; E_\epsilon(\omega^{i+1}). \tag{2.8}$$

This estimate gives us convergence in BV–norm of the discrete time supports, as the energy E_ϵ contains the perimeter of the supports. Furthermore, by summing (2.8) up we get the estimate

$$E_\epsilon(\omega^0) \geq \frac{1}{2h} \sum_{i=0}^{N} dist^2(\omega^i, \omega^{i+1}) + E_\epsilon(\omega^{N+1}).$$

We use the formal gradient flow structure to show existence of sub– and super–solutions in the sense of Definitions 5.2 and 5.3 of the droplet model. That is, we construct a time discrete scheme based on the JKO–scheme. In the limit of time step size $h \to 0$ and $\epsilon \to 0$ we show that the resp. $\liminf$ and $\limsup$ of the time discrete solutions are resp. super– and sub–solutions of (P). As the gradient flow construction here is formal, the quantities introduced need some adjustment to make sense in irregular settings and under topology changes.

Merging and splitting of components Until now we described the gradient flow structure for one connected component of supp u. This is valid as long as components do not merge or split. In which case we have to keep track of the volume of the drop in the components. There is in principle two different ways to do that. One would be to keep the overall volume of the drop constant. This would create a model that has features of coarsening, as small drops might loose volume to bigger ones even if they are far away. In this paper we chose another approach, that is, to keep the volume of each connected component fixed. When two components merge the volume adds up. When a component splits the volume of the drop is distributed between the resulting components. Note that for merging and splitting components the droplet u can jump although the evolution of the support is continuous.

3 Construction of a time discrete solution by the JKO–scheme

From here onwards the arguments will be mathematically rigorous. One of the main difficulties in the JKO–scheme is that the state at the next time step is given by two nested minimization, (2.6) and (2.7). We avoid this problem by introducing a different "distance", which was originally introduced in [1] and [15]. It is also used for numerical schemes, see e.g. [5] and [4].

$$\widetilde{dist}^2(\omega_0,\omega_1) \;:=\; \int_{\omega_0\Delta\omega_1} dist(x,\partial\omega_0)\,dx.$$

Here $dist$ is the distance function, and $\omega_0\Delta\omega_1$ denotes the symmetric difference between the two sets. Note that $\widetilde{dist}^2$ is not a (squared) distance function. It lacks symmetry. This could be adjusted by adding a symmetric term, but it introduces unnecessary complications in the following computations. On the other hand $\widetilde{dist}^2$ is an approximation of (2.6) as it uses the same Riemannian structure as in (2.3). To see this take a smooth parameterization $F(s)$ of $\partial\omega_0$ and a small perturbation $F(s)+v(s)\eta(s)$ with outward normal η. Then

$$\widetilde{dist}^2(\omega_0,\omega_1) \;\approx\; \int_{\partial\omega_0}\int_0^{v(s)} dist(F(s),F(s)+y\eta(s))\,dyds \;\approx\; \frac{1}{2}\int_{\partial\omega_0} v^2(s)\,ds.$$

The adjusted JKO–scheme defines ω_h^{i+1} given ω_h^i by

$$\omega_h^{i+1} \;=\; \underset{\omega\in Cacc}{argmin}\left\{\frac{1}{h}\widetilde{dist}^2(\omega_h^i,\omega) \;+\; E_\epsilon(\omega)\right\}.$$

Lemma 3.1 *For fixed $h>0$, fixed volume c and any $\omega^0\in Cacc$ there exists at least one minimizer $\omega_c^{min}\in Cacc$ of*

$$\mathcal{F}(\omega) \;:=\; \frac{1}{h}\widetilde{dist}^2(\omega^0,\omega) \;+\; E_\epsilon(\omega).$$

Note that we do not show uniqueness. We also do not expect uniqueness for (P) or (P_ϵ), see Section 6 for heuristic discussions.

Proof. There exist sets $\omega\subset\mathbb{R}^N$ such that $\mathcal{F}(\omega)<\infty$ (e.g. spheres around ω^0) and $\mathcal{F}(\omega)\geq 0$. Therefore there exists a minimizing sequence $\{\omega_k\}\subset Cacc$ such that

$$\mathcal{F}(\omega_k) \underset{k\to\infty}{\to} \inf\{\mathcal{F}(\omega): \quad \omega\subset\mathbb{R}^N\}.$$

By the definition of $E_\epsilon(\omega)$ we have $|\omega_k|+\epsilon|\partial\omega_k|<C$ and therefore the indicator functions χ_{ω_k} are uniformly bounded in BV–norm. Thus (see e.g. [6], p.176) there exists a subsequence and a function $\chi\in BV(I\!R^N)$ such that

$$\chi_{\omega_k}\to\chi \qquad \text{in } L^1(I\!R^N)$$

Since χ_{ω_k} take values in $\{0,1\}$ so does χ and there exists a set $\tilde{\omega} \subset \mathbb{R}^N$ such that $\chi = \chi_{\tilde{\omega}}$. By definition of $Cacc$ and the boundedness of $E_\epsilon(\tilde{\omega})$ we have

$$\omega_c^{min} := \overline{\text{interior}(\tilde{\omega})} \in Cacc.$$

In this sense $\omega_k \to \omega_c^{min}$. It remains to show that $\mathcal{F}(\omega_c^{min}) \leq \inf \mathcal{F}(\omega_k)$. This is direct for the part of the energy $|\omega_k| + \epsilon|\partial\omega_k|$, by the lower semi continuity of the perimeter. For the remaining part of the energy we have to take into account the convergence of the corresponding droplet with volume c, $u_{\omega,c}$. By the boundedness of the H^1–norm of $u_{\omega_k,c}$

$$u_{\omega_k,c} \to u_c^{min} \qquad \text{in } L^2(I\!R^N).$$

Where $\int u_c^{min} = c$ and supp $u_c^{min} = \omega_c^{min}$ by

$$u_{\omega_k,c} \;=\; u_{\omega_k,c}\,\chi_{\omega_k,c} \;\to u_c^{min}\,\chi_{\omega_c^{min}} \;\; a.e. \text{ in } I\!R^N.$$

Therefore by the lower semi-continuity of H^1–norm and Definition 2.1

$$\inf \int_{\omega_{k,c}} |Du_{\omega_k,c}|^2 \;\geq \int_{\omega_c^{min}} |Du_c^{min}|^2 \;\geq \int_{\omega_c^{min}} |Du_{\omega^{min},c}|^2.$$

On the other hand $\widetilde{dist}^2$ is continuous with respect to the L^1–topology of the indicator functions:

$$\begin{aligned}
\left|\widetilde{dist}^2(\omega^0,\omega) - \widetilde{dist}^2(\omega^0,\bar{\omega})\right| \quad &= \Big|\int_{\omega^0\Delta\omega} dist(x,\partial\omega^0)dx \;-\; \int_{\omega^0\Delta\bar{\omega}} dist(x,\partial\omega^0)dx\Big| \\
&= \Big|\int_{(\omega\Delta\bar{\omega})\Delta\omega^0} dist(x,\partial\omega^0)dx\Big|.
\end{aligned}$$

This vanishes as $\|\chi_\omega - \chi_{\bar{\omega}}\|_{L^1(I\!R^N)} \;=\; |\omega\Delta\bar{\omega}| \to 0$, by the boundedness of the distance function. $\square$

Definition of the time–discrete evolution. We are now in the position to define a time–discrete evolution of the droplets. Loosely speaking we will do the minimization in Lemma 3.1 for each component of the drop separately. If two components merge at the next time step, we will go back and do the same minimization step but for the two components together. Splitting of a component is already taken care of in the minimization in Lemma 3.1, as ω^{min} might have several components. To be more precise: for fixed $h > 0$ and $i \in \mathbb{N}$ take the previous state $\omega_h^i \in Cacc$ with possibly infinitely many connected components $\omega^{i,k} \in Cacc, k \in \mathbb{N}$. For each connected component we have some droplet $u_{\omega^{i,k},c_k}$ by Remark 2.2. Then ω_h^{i+1} is given by

$$\omega_h^{i+1} := \bigcup_k \omega_{c_k}^{min} \qquad \text{if for any } l \neq m: \quad \omega_{c_l}^{min} \cap \omega_{c_m}^{min} = \emptyset, \tag{3.1}$$

where $\omega_{c_k}^{min}$ is the minimizer in Lemma 3.1 for the connected component $\omega^{i,k}$.
If $\omega_{c_l}^{min} \cap \omega_{c_m}^{min} \neq \emptyset$ for only one pair (l, m) and if it does not intersect with other components $(\omega_{c_k}^{min}, k \neq l, m)$, then we define

$$\omega_h^{i+1} := \Big(\bigcup_{k \neq l,m} \omega_{c_k}^{min}\Big) \cup \omega_{c_l+c_k}^{min}.$$

where $\omega_{c_l+c_k}^{min}$ is the minimizer in Lemma 3.1 for initial set $\omega^{i,l} \cup \omega^{i,m}$.
In general the process of sorting out merging components is non-unique: we will prescribe the following process to proceed without ambiguity. Let us first consider the maximal index set I_1 such that each element $\omega_{c_k}^{min}$ with $k \in I_1$ intersects with $\omega_{c_1}^{min}$.
Next take the first element $\omega_{c_k}^{min}$ with $k \notin I_1$ and repeat the process to create the second index set I_2. If I_2 intersects with I_1, then we replace I_1 with $I_1 \cup I_2$. If not, check whether

$$\omega_{I_1}^{min} := \omega_{\Sigma c_k}^{min}, \quad k \in I_1$$

intersects with $\omega_{I_2}^{min}$. If yes then still replace I_1 with $I_1 \cup I_2$. If no, then proceed to create the third index set I_3, and check against $\omega_{I_1}^{min}$ and $\omega_{I_2}^{min}$. This way we end up with a sequence of (disjoint) index sets $I_1, I_2, ...$ such that $\omega_{I_k}^{min}$ are all disjoint. Then

$$\omega_h^{i+1} := \bigcup_k \omega_{I_k}^{min}.$$

Now define

$$u_{I_k} := u_{\omega_{I_k}^{min}, \Sigma_{j \in I_k} c_j}$$

and

$$u_h(\cdot, t) := \sum_k u_{I_k} \qquad \text{for } t \in \big[ih, (i+1)h\big). \tag{3.2}$$

The total volume of u_h at time t is $\int u_h(\cdot, t) dx = \sum_k c_k = 1$.

As the JKO–scheme is constructed to describe a time–discrete gradient flow, we have the energy decrease for free: Suppressing in the notation the dependence of the energy on the volumes in each component, we have:

Lemma 3.2 *The time evolution defined in* (3.1) *and* (3.2) *satisfies*

$$E_\epsilon(\omega_h^i) \ \geq \ \frac{1}{h}\,\widetilde{dist}^{\,2}(\omega_h^i\,, \omega_h^{i+1}) \ + \ E_\epsilon(\omega_h^{i+1}).$$

Proof. ω_h^{i+1} is the minimizer of $\mathcal{F}$ defined in Lemma 3.1, which can be tested with ω_h^i. □

Corollary 3.3 *For fixed $h > 0$ we have that $\lambda_{c_k}(\omega_{c_k}^i) < \infty$ for all $i \geq 0$ and c_k.*

Proof. Due to Lemma 3.2: $\lambda_{c_k}(\omega_{c_k}^i)\, c_k \ \leq \ E_\epsilon(\omega^0)$. But by definition if $c_k = 0$ then $\lambda_{c_k}(\omega) = 0$. □

Unfortunately this does not bound λ uniformly as the volume of the drop might go to zero.

4 The barrier properties for time discrete solutions

In this section we show, that for fixed time step $h > 0$ the discrete–time solution constructed above satisfies the free boundary motion law in time scale h, in the sense that it is comparable to smooth sub– and super–solutions of (P_ϵ) in local neighborhoods. A more precise statement will follow in Propositions 4.1 and 4.2 for which we need the following notation:

Let us denote the *positive phase* of a function $u(x,t) : I\!R^N \times [0,\infty) \to I\!R^+$ and its boundary by:

$$\Omega_t(u) := \{u(\cdot,t) > 0\} \qquad \text{and} \qquad \Gamma_t(u) := \partial\{u(\cdot,t) > 0\},$$

and the positive phase in space–time by:

$$\Omega(u) := \{u > 0\} \subset I\!R^N \times [0,\infty) \qquad \text{and} \qquad \Gamma(u) := \partial\Omega(u).$$

Next we show the barrier properties for the time discrete solutions. We begin with the barrier property for u_h being a super–solution. That is, u_h can be compared to a barrier function ϕ that is below. If ϕ is not fast enough at the boundary and not curved enough in the interior, then the ordering will persist:

Proposition 4.1 (Super–solution barrier property) *Let u_h be defined by (3.2). Consider some ball $B_r(x_0)$ and let*

$$\lambda := \inf\{\lambda(w_i) : w_i \textit{ is a component of either } \Omega_0(u_h) \textit{ or } \Omega_h(u_h) \textit{ intersecting } B_r(x_0)\}.$$

Suppose there exists a smooth function ϕ with $|D\phi| \neq 0$ in $B_r(x_0) \times [0,h]$. Further suppose that for some small $\delta > 0$

$$
\begin{aligned}
-\Delta\phi(\cdot,t) < \lambda - \delta \quad &in \quad B_r(x_0) \times [0,h], \\
\frac{\phi_t}{|D\phi|} - (|D\phi|^2 - 1 - \epsilon\kappa_\phi) < -\delta \quad &on \quad \Gamma(\phi) \cap (B_r(x_0) \times [0,h]),
\end{aligned}
\tag{4.1}
$$

where $\kappa_\phi := -\nabla \cdot (\frac{D\phi}{|D\phi|})$ is the mean curvature of the corresponding level set of ϕ. Then for sufficiently small $h > 0$ – depending on δ, r, the minimum of $|D\phi|$ and the C^2-norm of ϕ in $B_r(x_0) \times [0,h]$ – the following holds:
If $\phi \leq u_h$ on the parabolic boundary of $B_r(x_0) \times [0,h]$, then $\phi(\cdot,h) \leq u_h(\cdot,h)$ in $B_r(x_0)$.

Note that $\frac{\phi_t}{|D\phi|} = V$, where V is the normal velocity of a level set of ϕ. Therefore Proposition 4.1 shows that a function ϕ which is a *sub-solution* of (P_ϵ) can not cross the discrete time solution u_h. Thus u_h is a super–solution. We also mention that a local barrier function like the ones in Proposition 4.1 can always be extended to a global barrier function satisfying (4.1), which is not restricted to a ball B_r.

Proof. Suppose the proposition is not true. Then $\phi(x_0,h) > u_h(x_0,h)$ at some point $x_0 \in \Omega_h(u_h)$. Due to the maximum principle for harmonic functions, this implies that $\Omega_h(\phi) \cap (R^N \backslash \omega_h) \neq \emptyset$ for one of the components ω_h in $\Omega_h(u_h)$. Let ω_0 be a corresponding component in $\Omega_0(u_h)$ which gives rise to ω_h. For notational simplicity, we prove the proposition assuming that ω_h is indeed the only component generated by ω_0, i.e. ω_0 has not splitted into multiple components and ω_h is generated by only one component: the proof for the general case is (almost) identical.
The proof is a contradiction to the minimizing property of ω_h and u_h:

$$
\omega_h := argmin\{\widetilde{dist}^2(\omega_0,\omega) + h\, E_\epsilon(\omega)\}. \tag{4.2}
$$

To this end we will compare ω_h to a set $\tilde{\omega}_h$ which is in principle the unification of $\omega_h \cup \Omega_h(\phi)$. We will show that the new set $\tilde{\omega}_h$ has lower energy plus distance.

To ensure that the unification is a small perturbation of ω_h, we perturb ϕ. We claim that there exists $-h^{1/2} \leq \tau \leq 0$ such that

$$
\varphi(x,t) := (\phi(x,t) + \tau)_+ \leq u_h(x,t) \text{ in } B_r(x_0) \times [0,h]. \tag{4.3}
$$

(*Proof of (4.3)*): Note that $\Omega_t(\varphi) \subset \Omega_t(\phi)$ and for $x \in \Omega_t(\varphi)$ we have that

$$d(x, \Gamma_t(\phi)) \geq C \cdot \tau, \quad C = \inf_{B_r(x_0)\times[0,h]} |D\phi|^{-1}(x,t)$$

by the smoothness of ϕ. So, if we can prove that

$$S := \{x \in (\Omega_0(\phi) \cap B_r(x_0)) : d(x, \Gamma_0(\phi)) \geq Ch^{1/2}\} \subset \omega_h, \tag{4.4}$$

we have proven (4.3). To see this, first observe that (4.4) allows us to choose h small enough such that

$$\{x \in (\Omega_0(\phi) \cap B_r(x_0)) : d(x, \Gamma_0(\varphi)) \geq C_0 h\} \subset \omega_h,$$

where

$$C_0 = \sup_{B_r(x_0)\times[0,h]} \frac{|\phi_t|}{|D\phi|}.$$

As the support of φ changes smoothly and no more than $C_0\, h$ over $t \in [0, h]$ we also have (4.3). It remains to show (4.4): Let $\hat{\omega}_h := \omega_h \cup S$ and $\Sigma := \hat{\omega}_h - \omega_h = S - \omega_h$. Suppose that $|\Sigma| \neq 0$. In this case we claim that

$$\widetilde{dist}^2(\omega_0, \hat{\omega}_h) \,+\, h\, E_\epsilon(\hat{\omega}_h) \,<\, \widetilde{dist}^2(\omega_0, \omega_h) + \, h\, E_\epsilon(\omega_h), \tag{4.5}$$

which would be a contradiction to (4.2). Since $\Omega_0(\phi) \subset \omega_0$, we have by the smoothness of ϕ

$$\widetilde{dist}^2(\omega_0, \hat{\omega}_h) - \widetilde{dist}^2(\omega_0, \omega_h) \leq -C_1 h|\Sigma|.$$

On the other hand, since the Dirichlet energy decreases when the domain increases,

$$\begin{aligned} E(\tilde{\omega}_h) - E(\omega_h) &\leq |\Sigma| + |\partial\hat{\omega}_h| - |\partial\omega_h| \\ &\leq |\Sigma| + |\partial S - \omega_h| - |\partial\omega_h \cap S| \\ &\leq C_2|\Sigma| \end{aligned}$$

where C_2 depends on ϕ. The last inequality follows from

$$\begin{aligned} |\partial S - \omega_h| - |\partial\omega_h \cap S| &\geq \int_{\partial\Sigma} -\frac{D\phi}{|D\phi|}(x,h) \cdot \eta \; dS \\ &= \int_\Sigma \nabla \cdot (\frac{D\phi}{|D\phi|})(x,h)\, dx \\ &= \int_\Sigma -\kappa_\phi \; dx. \end{aligned}$$

Here η is the outward normal vector at $x \in \partial\Sigma$ and κ_ϕ is the mean curvature of the level set of ϕ. As we can choose C_1 bigger than C_2 we can conclude.

$\square$)

Let τ_0 be the supremum of all such τs so that $\Gamma_h(\varphi)$ touches $\partial\omega_h$ in $B_r(x_0)$. Next choosing τ a bit larger than τ_0, we have

$$\big|(\Omega_h(\varphi) - \omega_h) \cap B_r(x_0)\big| \;=\; O(|\tau - \tau_0|) = o(h^2). \tag{4.6}$$

We choose τ and h small enough such that (4.1) still holds for φ. In the following proof we will use φ instead of ϕ.

Let us now define the perturbed set, which is a small perturbation of ω_h:

$$\tilde{\omega}_h = \omega_h \cup \big(\Omega_h(\varphi) \cap B_r(x_0)\big).$$

We claim that

$$\widetilde{dist}^2(\omega_0, \tilde{\omega}_h) \,+\, h\, E_\epsilon(\tilde{\omega}_h) \,<\, \widetilde{dist}^2(\omega_0, \omega_h) + \, h\, E(\omega_h).$$

This yields a contradiction to the minimizing property of ω_h, (4.2). To prove the claim, first observe that

$$\begin{aligned} \widetilde{dist}^2(\omega_0, \tilde{\omega}_h) - \widetilde{dist}^2(\omega_0, \omega_h) \;&=\; \textstyle\int_{\tilde{\omega}_h \Delta \omega_h} signdist(x, \partial\omega_0)dx \\ &\leq\; \textstyle\int_{\tilde{\omega}_h \Delta \omega_h} signdist(x, \Gamma_0(\varphi))dx, \end{aligned}$$

where *signdist* is the signed distance function, that is negative inside the set. Here the first equality is due to straightforward computation, and the inequality is due to the fact that $\Omega_0(\varphi)$ is a subset of ω_0. By construction of φ, for each point $x \in \tilde{\omega}_h \Delta \omega_h$ there exists a time t^* with $0 \leq t^* \leq h + o(h^2)$ such that $x \in \Gamma_{t^*}(\varphi)$. Therefore, as $\frac{\varphi_t}{|D\varphi|}(0, \cdot)$ denotes the outward normal velocity of $\Gamma(\varphi)$,

$$signdist(x, \Gamma_0(\varphi)) \leq h\, \frac{\varphi_t}{|D\varphi|} \,+\, o(h). \tag{4.7}$$

Next we consider the energy difference

$$E_\epsilon(\omega_h) - E_\epsilon(\tilde{\omega}_h) \;=\; I \,+\, II \,+\, III$$

where

$$I = \int |Du_h|(\cdot,h)^2 - \int |D\tilde{u}_h|^2, \qquad II = -\int_{\tilde{\omega}_h \Delta \omega_h} 1\,dx, \qquad III = \epsilon|\partial\omega_h| - \epsilon|\partial\tilde{\omega}_h|.$$

Here $\tilde{u}_h(x)$ solves $-\Delta\tilde{u}_h = \tilde{\lambda}$ with support $\tilde{\omega}_h$, where $\tilde{\lambda}$ is chosen such that $\int \tilde{u}_h dx = \int_{\omega_h} u_h(\cdot,h)dx$. In the next steps we will show that

$$I \geq \int_{\tilde{\omega}_h \Delta \omega_h} |D\varphi|^2(\cdot,h)\ dx \quad \text{ and } \quad III \geq \int_{\tilde{\omega}_h \Delta \omega_h} -\epsilon\kappa_\varphi\ dx$$

This proves our claim by (4.1) and (4.7). Note that (4.1) is strict and therefore extends to a small region inside.

First let us estimate III. Note that, as before,

$$\begin{aligned} |\partial\omega_h| - |\partial\tilde{\omega}_h| &\geq \int_{\partial\omega_h \setminus \partial\tilde{\omega}_h} -\frac{D\varphi}{|D\varphi|}(\cdot,h)\cdot\eta\ dS - \int_{\partial\tilde{\omega}_h \setminus \partial\omega_h} -\frac{D\varphi}{|D\varphi|}(\cdot,h)\cdot\tilde{\eta}\ dS \\ &= \int_{\tilde{\omega}_h \Delta \omega_h} \nabla\cdot(\frac{D\varphi}{|D\varphi|})(\cdot,h)dx \\ &= \int_{\tilde{\omega}_h \Delta \omega_h} -\kappa_\varphi\ dx \end{aligned}$$

where $\tilde{\eta} = -D\varphi/|D\varphi|(x,h)$ is the outward normal vector at $x \in \partial\tilde{\omega}_h$, η is the outward normal vector at $x \in \partial\omega_h$, and κ_φ is the mean curvature of the level sets of φ.

It remains to estimate I. To this end let us define two auxiliary functions, $\bar{u}$ and v:

$$\begin{aligned} -\Delta\bar{u} &= \lambda(w_h) \quad \text{in } \tilde{\omega}_h \text{ with } \operatorname{supp}(\bar{u}) = \tilde{\omega}_h, \\ -\Delta v &= 0 \qquad\quad \text{in } \omega_h \text{ with } v = \varphi_+(\cdot,h) \text{ on } \partial\omega_h. \end{aligned} \tag{4.8}$$

Then we have for $c := \int_{\omega_h} u_h(\cdot,h)$ and $\bar{c} := \int_{\tilde{\omega}_h} \bar{u}$:

$$\begin{aligned} \int_{\omega_h} |Du_h(\cdot,h)|^2 - \int_{\tilde{\omega}_h} |D\tilde{u}_h|^2 &= \lambda \int_{\omega_h} u_h(\cdot,h) \ - \lambda(\tilde{\omega}_h) \int_{\tilde{\omega}_h} \tilde{u} \\ &= \tfrac{c}{\bar{c}}\lambda\,(\int_{\tilde{\omega}_h} \bar{u} \ - \ \int_{\omega_h} u), \end{aligned} \tag{4.9}$$

as $\tilde{u} = \frac{c}{\bar{c}}\bar{u}$. Furthermore $\bar{u} \geq \max(u_h\big|_{\omega_h} + v\,,\,\varphi)(\cdot,h)\}$ since

$$\tilde{\omega}_h = \Omega_h(\max(u_h\big|_{\omega_h} + v\,,\,\varphi)) \text{ and } -\Delta\max(u_h\big|_{\omega_h} + v, \varphi)(\cdot,h) \leq \lambda.$$

For the same reason we have for the inward normal η of ω_h

$$\partial_\eta(u_h(\cdot,h)+v) \geq \partial_\eta \varphi(\cdot,h). \tag{4.10}$$

Thus

$$\begin{aligned}
\lambda\Big(\int_{\tilde\omega_h}\bar u - \int_{\omega_h} u_h(\cdot,h)\Big) &\geq \lambda\int_{\omega_h} v + \lambda\int_{\omega_h\Delta\tilde\omega_h}\varphi(\cdot,h)\\
&\geq -\int_{\omega_h}\Delta(u_h(\cdot,h)+v)\,v - \int_{\omega_h\Delta\tilde\omega_h}(\Delta\varphi\,\varphi)(\cdot,h)\\
&\geq \int_{\omega_h}(D(u_h(\cdot,h)+v))Dv + \int_{\partial\omega_h}\partial_\eta(u_h(\cdot,h)+v)\,v\\
&\quad + \int_{\omega_h\Delta\tilde\omega_h}|D\varphi|^2(\cdot,h) - \int_{\partial\omega_h}(\partial_\eta\varphi\varphi)(\cdot,h)\\
&\geq \int_{\omega_h}|Dv|^2 + \int_{\omega_h\Delta\tilde\omega_h}|D\varphi|^2(\cdot,h),
\end{aligned}$$

by (4.10) and (4.8). Thus together with (4.9) we have

$$I \geq \frac{c}{\bar c}\int_{\omega_h\Delta\tilde\omega_h}|D\varphi|^2(\cdot,h).$$

Lastly, note that as $\tau\to\tau_0$, $\lambda(\tilde\omega_h)$ converges to $\lambda(\omega_h)$, and therefore $\bar c\to c$: this can be checked by using (4.2) - indeed (4.2) yields that $u_h(\cdot,h)$ is the *innerdish* (approximated from outside) solution of $-\Delta u=\lambda(\omega_h)$ in ω_h (see section 5 for definition of innerdish solutions). In particular we can choose $\tau-\tau_0$ given in (4.6) small enough that $\bar c\leq c(1+o(h))$.

$\square$

Similarly u_h can be also compared with barriers which are *super-solutions* of (P_ϵ). Therefore u_h is a sub-solution of (P_ϵ):

Proposition 4.2 (Sub-solution – barrier property) *Let u_h be defined by (3.2) and consider some ball $B_r(x_0)$. Let*

$$\lambda=\sup\{\lambda(w_i): w_i \textit{ is a component of either } \Omega_0(u_h) \textit{ or } \Omega_h(u_h) \textit{ intersecting } B_r(x_0)\}.$$

Suppose there exists a smooth function ϕ with $|D\phi| \neq 0$ in $B_r(x_0) \times [0,h]$. Further suppose that for some small $\delta > 0$

$$-\Delta\phi(\cdot,t) > \lambda + \delta \quad \textit{and} \quad \frac{\phi_t}{|D\phi|} - (|D\phi|^2 - 1 - \epsilon\kappa_\phi) > \delta \qquad \textit{in } B_r(x_0) \times [0,h]. \quad (4.11)$$

Then for sufficiently small $h > 0$ – depending on δ, r, the minimum of $|D\phi|$ and the C^2-norm of ϕ in $B_r(x_0) \times [0,h]$ – the following holds:
If $u_h \leq \phi_+ := \max(\phi, 0)$ on the parabolic boundary of $B_r(x_0) \times [0,h]$, then $u_h(\cdot,h) \leq \phi(\cdot,h)_+$ in $B_r(x_0)$.

Proof. The proof is similar of the proof of Proposition 4.1. We still present the proof here as the estimation of the Dirichlet integral has a non-trivial difference from the previous proof.

Suppose the above proposition is not true. Then $\phi(\cdot,h)$ crosses $u_h(\cdot,h)$ from above at some point in $B_r(x_0)$. As before, the maximum principle for harmonic functions states that then $\Omega_h(\phi) \cap w_h$ is nonempty for a component w_h of $\Omega_h(u_h)$. Set ω_0 be the component of $\Omega_0(u_h)$ which generates ω_h. Again we construct a contradiction to the minimizing property of ω_h and u_h. With a parallel argument from the proof of Proposition 4.1 one can change ϕ to $\varphi := (\phi + \tau)_+$, $0 \leq \tau \leq Ch^{1/2}$ such that $u_h(x,h) \leq (\phi(x,h) + \tau_0)_+$ and

$$\big|(\omega_h - \Omega_h(\varphi)) \cap B_r(x_0)\big| \;=\; O(|\tau - \tau_0|) = o(h^2).$$

This time we denote:

$$\tilde{\omega}_h = ((\omega_h \cap \Omega_h(\varphi)) \cap B_r(x_0)) \cup (\omega_h \cap (I\!R^N - B_r(x_0)).$$

We claim that

$$\widetilde{dist}^2(\omega_0, \tilde{\omega}_h) \;+\; h\, E_\epsilon(\tilde{\omega}_h) \;<\; \widetilde{dist}^2(\omega_0, \omega_h) + \; h\, E_\epsilon(\omega_h).$$

First observe that this time

$$\begin{aligned} \widetilde{dist}^2(\omega_0, \tilde{\omega}_h) - \widetilde{dist}^2(\omega_0, \omega_h) \;&=\; -\textstyle\int_{\tilde{\omega}_h \Delta \omega_h} signdist(x, \partial\omega_0)dx \\ &\leq\; -\textstyle\int_{\tilde{\omega}_h \Delta \omega_h} signdist(x, \Gamma_0(\varphi))dx. \end{aligned}$$

By integration of the velocity of $\Gamma_t(\varphi)$ we have

$$-signdist(x, \Gamma_0(\varphi)) \leq -\,h\,\frac{\varphi_t}{|D\varphi|} \;+\; o(h). \qquad (4.12)$$

Next we consider the energy difference

$$E_\epsilon(\omega_h) - E_\epsilon(\tilde\omega_h) \;=\; I \,+\, II \,+\, III \tag{4.13}$$

where

$$I \;=\; \int |Du_h|^2(\cdot,h) - \int |D\tilde u_h|^2, \qquad II \;=\; \int_{\tilde\omega_h \Delta \omega_h} 1\,dx, \qquad III \;=\; \epsilon|\partial\omega_h| \;-\; \epsilon|\partial\tilde\omega_h|.$$

Here $\tilde u(x)$ solves $-\Delta\tilde u = \tilde\lambda$ with support $\tilde\omega_h$, where $\tilde\lambda$ is chosen such that $\int \tilde u = \int u_h(\cdot,h)$. We will show that

$$I \geq -\int_{\tilde\omega_h\Delta\omega_h} |D\varphi|^2(\cdot,h)\;dx \quad \text{ and } \quad III \geq \int_{\tilde\omega_h\Delta\omega_h} \epsilon\kappa_\varphi\;dx$$

This proves our claim by (4.11), (4.13) and (4.12).

First let us estimate III:

$$\begin{aligned}
|\partial\omega_h| - |\partial\tilde\omega_h| \;&\geq\; \textstyle\int_{\partial\omega_h\setminus\partial\tilde\omega_h} \dfrac{D\varphi}{|D\varphi|}(\cdot,h)\cdot\eta\;dS - \textstyle\int_{\partial\tilde\omega_h\setminus\partial\omega_h} \dfrac{D\varphi}{|D\varphi|}(\cdot,h)\cdot\tilde\eta\;dS \\
&=\; -\textstyle\int_{\tilde\omega_h\Delta\omega_h} \nabla\cdot(\dfrac{D\varphi}{|D\varphi|})(\cdot,h)dx \\
&=\; \textstyle\int_{\tilde\omega_h\Delta\omega_h} \kappa_\varphi\;dx
\end{aligned}$$

where $\tilde\eta = -D\varphi/|D\varphi|(x,h)$ is the outward normal vector at $x\in\partial\tilde\omega_h$, η is the outward normal vector at $x\in\partial\omega_h$, and κ_φ is the mean curvature of the level sets of φ.

It remains to estimate I. We again consider the two auxiliary functions, $\bar u$ and v defined by (4.8). As before we have for $c := \int_{\omega_h} u_h(\cdot,h)$ and $\bar c := \int \bar u$:

$$\textstyle\int_{\omega_h} |Du_h|^2(\cdot,h) - \int_{\tilde\omega_h} |D\tilde u|^2 \;=\; \frac{c}{\bar c}\lambda\,(\int_{\tilde\omega_h}\bar u \;-\; \int_{\omega_h} u_h(\cdot,h)). \tag{4.14}$$

But this time the inequality $(\min[\bar u,\varphi(\cdot,h)] - v)_+ \geq u_h(\cdot,h)\big|_{\omega_h}$ holds, as

$$\omega_h = \text{ supp } (\min[\bar u\,,\,\varphi(\cdot,h)] - v)$$

and

$$-\Delta(\min[\bar u\,,\,\varphi(\cdot,h)] - v) \geq \lambda.$$

For the same reason we have for the outward normal η of $\tilde{\omega}_h$

$$\partial_\eta(u_h(\cdot,h)+v) \ \geq \partial_\eta\, \phi\,(\cdot,h). \tag{4.15}$$

Thus, as $\min(\bar{u},\phi)=\bar{u}$ in $\tilde{\omega}_h$ and $\min(\bar{u},\varphi)=\varphi$ in $\tilde{\omega}_h\Delta\omega_h$, using the smoothness of φ it follows that

$$\begin{aligned}
\lambda\,(\textstyle\int_{\tilde{\omega}_h}\bar{u}-\int_{\omega_h}u_h(\cdot,h)) \ &\geq\ \lambda\textstyle\int_{\tilde{\omega}_h}v-\lambda\int_{\omega_h\Delta\tilde{\omega}_h}\varphi(\cdot,h)\\
&\geq\ -\textstyle\int_{\tilde{\omega}_h}\Delta(u_h(\cdot,h)+v)\,v+\int_{\omega_h\Delta\tilde{\omega}_h}(\Delta\varphi\varphi)(\cdot,h)\\
&\quad+\textstyle\int_{\omega_h\Delta\tilde{\omega}_h}(-\Delta\varphi\,-\lambda)\,\varphi(\cdot,h)\\
&\geq\ \textstyle\int_{\tilde{\omega}_h}(D(u_h(\cdot,h)+v))\,Dv\,-\,\int_{\partial\tilde{\omega}_h}\partial_\eta(u_h(\cdot,h)+v)\,v\\
&\quad-\ \textstyle\int_{\omega_h\Delta\tilde{\omega}_h}|D\varphi|^2(\cdot,h)+\int_{\partial\tilde{\omega}_h}(\partial_\eta\varphi\varphi)(\cdot,h)+\int_{\omega_h\Delta\tilde{\omega}_h}o(h)\\
&\geq\ \textstyle\int_{\omega_h}|Dv|^2\,-\,\int_{\omega_h\Delta\tilde{\omega}_h}|D\varphi|^2(\cdot,h)\,+\,\int_{\omega_h\Delta\tilde{\omega}_h}o(h)
\end{aligned}$$

by (4.15) and (4.8). Thus together with (4.14) we have

$$I\ \geq\frac{c}{\bar{c}}\int_{\omega_h\Delta\tilde{\omega}_h}|D\varphi|^2.$$

Lastly we need to show that

$$\bar{c}\to c \text{ as } |\tau-\tau_0|\to 0.$$

To see this, first note that $u_h(x,h)\leq(\phi(x,h)+\tau_0)_+$. In particular

$$u_h(\cdot,h)\leq C|\tau-\tau_0| \qquad \text{on } \partial\tilde{w}_h-\partial w_h\subset\partial\{x:\phi(x,h)+\tau\geq 0\}$$

where C depends on the C^2-norm of ϕ. It follows that $u_h(\cdot,h)\big|_{\omega_h}\leq\bar{u}_h+C|\tau-\tau_0|$, and therefore $c\leq\bar{c}+O(\tau-\tau_0)$. Hence we conclude.

□

5 The continuum limit: Existence of weak sub– and super–solutions

In this section we show that in the limit $h\to 0$ with $\epsilon=h$ the limit infimum (resp. limit supremum) of the time discrete solutions is a weak super– (resp. sub–) solutions of

(P), in the sense that these limit solutions satisfy the barrier property at infinitesimal time scale: see Definition 5.2 and 5.3. To this end we carry over the information in Propositions 4.1 and 4.2 to the limits of u_h. Of course, if these coincide the results in this section would simplify. See Remark 5.6.

Let us go back to the time discrete solutions u_h. Define

$$\mathcal{G} := \{k2^{-n}, k, n \in \mathbb{N}\} \text{ and } h = h(n) = 2^{-n}, n \in \mathbb{N}.$$

Then u_h is defined on grid times $t \in \mathcal{G}$ by (3.2), with the choice of $\epsilon = h$. Due to the Dirichlet energy bound, along a subsequence

$$u_h(\cdot, t) \to u(\cdot, t) \qquad \text{weakly in } H^1(\mathbb{R}^N) \text{ for each } t \in \mathcal{G}. \tag{5.1}$$

We could then choose a common subsequence of $h(n)$ such that (5.1) holds along the same sequence for each time. We obtain a weak form of convergence in the continuum limit $h \to 0$ along a subsequence.

Unfortunately a stronger, point-wise convergence of u_h seem to be unobtainable without extra regularity property of u_h such as equicontinuity in time. Instead we consider the limit infimum and supremum:

$$u_*(x,t) := \lim_{r \to 0} \inf_{\{|x-y| \le r,\ |s-t| \le r,\ h \le r\}} u_h(y,s)$$

and

$$u^*(x,t) := \lim_{r \to 0} \sup_{\{|x-y| \le r,\ |s-t| \le r,\ h \le r\}} u_h(y,s).$$

Note, that we do not know that

$$\Omega(u_*) \ = \ \Omega(u) \ = \ \Omega(u^*).$$

This would lead to a full solution of problem (P). See Remark 5.6.

Next we define the"liminf" and "limsup" for the Lagrange multipliers λ.

Definition 5.1 *Suppose ω is a connected domain with finite BV–norm. Then we define*

$$\lambda^{in}(\omega) \ := \ \lim_{\delta \to 0} \lambda(\omega_\delta)$$
$$\lambda^{out}(\omega) \ := \ \lim_{\delta \to 0} \lambda(\omega^\delta).$$

for $\omega^\delta := \{x : d(x,\omega) \le \delta\}$ *and* $\omega_\delta := \{x : B_\delta(x) \subset \omega\}$.

Clearly $\lambda^{in} \ge \lambda^{out}$, as $\omega_\delta \subset \omega^\delta$. These two λ's do not have to coincide if the complement of ω has infinite number of complements. We will call the approximation from outside the *outer* solution, and approximation from inside the *inner* solution.

Let us now define a *weak sub-* and *super-solution.* First define

$$\lambda_t^{in}(u) := \sup\{\lambda^{in}(\omega) : \omega_i \text{ is a connected component of } \Omega_t(u)\}$$

and

$$\lambda_t^{out}(u) := \inf\{\lambda^{out}(\omega_i) : \omega_i \text{ is a connected component of } \Omega_t(u)\}.$$

Definition 5.2 (weak super-solution) *A lower semi-continuous function $u : I\!\!R^N \times [0,\infty) \to I\!\!R$ is a weak super-solution if u cannot cross, from above, a local smooth sub-solution. More precisely, u is a weak super-solution if the following holds:*
Suppose there exists a smooth function ϕ with $|D\phi| \neq 0$ in $B_r(x_0) \times [t_1, t_2]$. Further suppose that

$$-\Delta\phi(\cdot,t) < \lambda_t^{out}(u), \quad \frac{\phi_t}{|D\phi|} - (|D\phi|^2 - 1) < 0 \text{ in } B_r(x_0) \times [t_1,t_2]. \tag{5.2}$$

If $\phi \le u$ on the parabolic boundary of $B_r(x_0) \times [t_1, t_2]$, then $\phi \le u$ in $B_r(x_0) \times [t_1, t_2]$.

The notion of a subsolution is a bit weaker than that of supersolution, as we have to take into account the possibility that the wet region of the h-solution leave thin segments or isolated points in the limit, which are not traceable from the limit of u_h. We get around this (rather technical) difficulty by including a set Σ in the definition:

Definition 5.3 (weak sub-solution) *Let $u : I\!\!R^N \times [0,\infty) \to I\!\!R^+$ be upper semi-continuous, and let Σ be a closed subset of $I\!\!R^N \times [0,\infty)$ containing $\Omega(u)$. Then the pair (u,Σ) is a weak sub-solution if the following holds:*
Suppose there exists a smooth function ϕ with $|D\phi| \neq 0$ in $B_r(x_0) \times [t_1, t_2]$. Further suppose that

$$-\Delta\phi(\cdot,t) > \lambda_t^{in}(u), \quad \frac{\phi_t}{|D\phi|} - (|D\phi|^2 - 1) > 0 \text{ in } B_r(x_0) \times [t_1,t_2]. \tag{5.3}$$

If $u \le \phi$ and $\Sigma \subset \Omega(\phi)$ on the parabolic boundary of $B_r(x_0) \times [t_1, t_2]$, then $u \le \phi$ and $\Sigma \subset \Omega(\phi)$ in $B_r(x_0) \times [t_1, t_2]$.

We call u a *weak solution* of (P) if u^* is a weak super-solution and $(u_*, \Omega(u_*))$ is weak sub-solution. Note that smooth solutions of (P), if they exist, are weak solutions of (P) in our definition. Furthermore, the notion of weak solution defined in [9] coincides with ours, as long as the evolution of the droplet is continuous in time (with respect to Hausdorff distance) without topology changes.

We will show that u_*, is a weak super-solution and (u^*, Σ) is a weak sub-solution with Σ, where Σ is given as

$$\Sigma := \{(x\,,\,t) \,\big|\, \text{there exists a sequence } (x_h, t_h) \to (x,t) \text{ such that } x_h \in \Omega(u_h(\cdot, t_h))\}.$$

Note that Σ contains $\Omega(u^*)$. Σ is a closed set, including "traces" of supports of $u_h(\cdot,t)$ which may degenerate into zero set of u^* in the limit $h \to 0$. Let us denote
$\Sigma(s) := \Sigma \cap \{t = s\}$.

Proposition 5.4 *(a) Suppose $(x,t) \in \bar{\Omega}(u_*)$. Then there is $x_h \in \Omega_{t_h}(u_h)$ such that $(x_h, t_h) \to (x,t)$. Let w_* be the connected component of $\Omega(u_*)$ containing x, and let w_h be the corresponding connected component containing x_h. Then*

$$\limsup_{h\to 0} \lambda(w_h) \le \lambda^{in}(w_*).$$

(b) Suppose $(x,t) \in \Sigma$. There is $x_h \in \Omega_{t_h}(u_h)$ such that $(x_h, t_h) \to (x,t)$. Let w^* be the connected component of $\Sigma(t)$ containing x and let w_h be the corresponding connected component containing x_h. Then

$$\liminf_{h\to 0} \lambda(w_h) \ge \lambda^{out}(w^*). \tag{5.4}$$

Proof. To prove (a), note that for any δ, there exists h_0 such that $w_\delta := \{x : B_\delta(x) \subset w_*\}$ is contained in w_{h_0}. This is due to the following contradiction: Suppose $\omega_\delta \not\subset \omega_{h_0}$ for some $\delta > 0$. Then there exists a sequence of points x_h converging to a point $\bar{x}$ in ω_δ such that $u_h(t_h, x_h) = 0$. This is a contradiction to the fact $\omega_\delta \subset \Omega_t(u_*)$. Therefore $\omega_\delta \subset \omega_{h_0}$ and

$$\lambda^{in}(w_*) = \lim_{\delta\to 0} \lambda(w_\delta) \ge \limsup_{h\to 0} \lambda(w_h).$$

To prove (b), first note that for fixed δ we have that $u(\cdot, t_h)$ converges uniformly to zero outside of $w^\delta := \{x : d(x, w^*) \le \delta\}$. Therefore we can lower u_h to its essential part:

Consider $\tilde{u}_h := c_h\,(u_h - \epsilon_h)$ with c_h such that $\int \tilde{u}_h = 1$. Then by definition

$$\lambda(\Omega_{t_h}(\tilde{u}_h)) \;\leq\; \int |D\tilde{u}_h|^2 \;\leq\; c_h^2 \int |Du_h|^2 \;=\; c_h^2 \lambda(\omega_h).$$

Also $\Omega_{t_h}(\tilde{u}_h) \subset \omega^\delta$ and therefore $\lambda(\omega^\delta) \leq \lambda(\Omega_{t_h}(\tilde{u}_h))$. This gives (5.4) by the uniform convergence of u_h and $c_h \to 1$. □

Theorem 5.5 *(u^*, Σ) is a sub-solution, and u_* is a super-solution.*

Proof. The proof carries over the barrier properties of the time discrete solutions. Let us first show by contradiction that u_* is a super-solution. Suppose not. That is suppose there exists a smooth function ϕ satisfying (5.2) in $B_r(x_0) \times [t_1, t_2]$ such that u_* crosses ϕ from above: i.e. $u_* - \phi$ has a local strict minimum zero at (x_1, t_0) in $B_r(x_0) \times (t_1, t_0]$ with $t_0 \leq t_2$. For simplicity we may assume that $x_1 = x_0$. Suppose first that x_0 is an interior point of $\Omega_{t_0}(u_*)$. Since

$$-\Delta\phi \;<\; \lambda_t^{out}(u_*).$$

By Proposition 5.4(b) there exists $\delta > 0$ such that $-\Delta\phi \;<\; \lambda_h(\omega_i)$ for any component ω_i of $\Omega_\tau(u_h)$ intersecting $B_\delta(x_0)$ with $|\tau - t|, |h| \leq \delta$. This contradicts the maximum principle applied to ϕ and u_h.
Therefore $x_0 \in \Gamma_{t_0}(u_*)$. Choose n large enough that (5.2) still holds in $B_r(x_0) \times [t_1, t_2]$ with $\phi + \frac{1}{n}(t - t_1)$ instead of ϕ. By definition of u_*, there exists a sequence $t_h \in \mathcal{G}$, such that $u_h(\cdot, t_h)$ crosses $\psi := \phi + \frac{1}{n}(t - t_1)$ from above at x_h with $(x_h, t_h) \to (x_0, t_0)$. This violates the barrier property of discrete solutions, Proposition 4.1, as ψ satisfies (4.1) for some h and δ small enough.

Similarly we show by contradiction that (u^*, Σ) is a sub-solution. Suppose not. Then there exists a smooth function ϕ satisfying (5.3) in $B_r(x_0) \times [t_1, t_2]$ such that either u^* crosses ϕ from below or Σ crosses $\Omega(\phi)$ from inside.
First assume the former: that is, $u^* - \phi$ has a local strict maximum zero at (x_1, t_0) in $B_r(x_0) \times (t_1, t_0]$ with $t_0 \leq t_2$. For simplicity we may assume that $x_1 = x_0$. Suppose first x_0 is an interior point of $\Omega_{t_0}(u^*)$. Since

$$-\Delta\phi \;>\; \lambda_t^{in}(u_*).$$

By Proposition 5.4(a) there exists $\delta > 0$ such that $-\Delta\phi \;>\; \lambda_h(\omega_i)$ for any component ω_i of $\Omega_\tau(u_h)$, intersecting $B_\delta(x_0)$ with $|\tau - t|, |h| \leq \delta$. This contradicts the maximum

principle applied to ϕ and u_h.
Therefore we have $(x_0, t_0) \in \Gamma(u^*)$, but since $\Omega(u^*)$ is a subset of Σ this means that Σ has crossed ϕ even before $t = t_0$. Hence we may assume that $(x_0, t_0) \in \partial\Sigma$.
As before, choose n large enough that (5.3) still holds in $B_r(x_0) \times [t_1, t_2]$ with $\psi(x,t) := \phi(x,t) - \frac{1}{n}(t - t_1)$ instead of ϕ. By definition of u^* and Σ, there exists a sequence $t_h \in \mathcal{G}$, such that $u^h(\cdot, t_h)$ crosses ψ_+ from below at x_h with $(x_h, t_h) \to (x_0, t_0)$. This contradicts Proposition 4.2. $\square$

Remark 5.6 (Agreement of super– and sub–solution) *For free boundary problems which satisfy comparison principle (such as the mean-curvature flow), the sub-solution would stay below the super-solution, which would then yield that $u^* \leq u_*$. This in turn yields $u^* = u_*$ and in particular the uniform convergence of u_h to a weak solution of (P) readily follows. For us this line of argument cannot be applied since (P) does not satisfy a comparison principle. However, strong convergence still would hold if one could develop (a) a bit stronger notion of distance between sets or (b) some notion of equicontinuity between u_h. In general some regularity for each discrete solution u_h seems plausible, at least away from "isolated" (surface measure zero) singular points (see [16] for relevant work). Stronger regularity results should also hold for specific class of initial data, such as convex sets. Convex sets are expected to stay convex, and therefore simply connected, throughout the evolution: this is an open question for now.*

6 Further discussions

The investigation performed in this paper brings up several interesting questions, some of which are under investigation by the authors. We list some of these questions and comments.

◦ *Long time behavior and properties of stationary solutions*

Due to the gradient flow structure, as time goes to infinity the solution will converge to either local minimizer or a saddle point of the energy $E(\omega)$. This brings the energy landscape of $E(\omega)$ into the question. There seem to be some nontrivial saddle points: if we put two round, stationary droplets close together so that they touch each other at one point of their boundaries, then the droplets can either stay still or they can merge together and evolve: note that the thin neck generated by merging of the two droplets would be highly concave, therefore the neck would fatten fast. We expect that these two round droplets just before merging is in fact a saddle point in the energy landscape, and the non-uniqueness of the solutions indeed happens at such saddle points. It is not clear to the authors whether there is a natural selection principle in the event of non-uniqueness.

◦ *Putting constraints on the path of gradient flow*

As one way to amend the difficulties in the limit, we propose to put some regularity condition (such as bounded mean curvature) on the choice of the Caccioppoli sets over the time-discrete evolution. Such constraint would result in stronger convergences. The interesting point is that for this modified scheme we still expect the barrier properties to hold, but only for a selected class of barriers. For example in the case of bounded mean curvature as a constraint we would only be able to consider barriers with bounded C^2-norms and interface curvatures. Numerically constructed solutions seem to satisfy with the selective barrier properties.

◦ *Further geometric properties of solutions.*

The barrier property for discrete solutions is proven here using variational arguments with a perturbed alternative. One can also hope to show other geometric properties of solutions by variational arguments, such as preservation of convexity or star-shapedness over time. It seems also likely that variational argument yields certain free boundary regularity for each discrete solution u_h (see [16]), however it remains open whether one can obtain a uniform regularity of u_h in the limit $h \to 0$.

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