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MODELLING AND ANALYSIS OF DROPLET MOTION ON A PLANE

KAREL ŠVADLENKA[1] AND SEIRO OMATA[1]

Abstract. Slow motion of droplets on nonhomogeneous surfaces is modeled by a nonlocal parabolic free boundary equation. We show existence and Hölder continuity of a unique weak solution by a combination of smoothing and a variational method that can be directly applied to numerical computation.

Key words. partial differential equation of parabolic type, integral constraint, free boundary, discrete Morse flow, variational method

AMS subject classifications. 35K55, 35R35, 47J30

1. Introduction. Many applications require proper understanding of motion of liquid droplets on a surface. These include micro- and nano-fluidics, development of surfaces with special wetting properties, effective heat transfer, spraying pesticides on plant leaves or paint to surfaces, printing, etc. The possibility of changing the qualities of the surface using nanomachines has been reported recently. This method could regulate the motion of a drop with high accuracy.

In the paper [6] we started developing a model for motion of droplets on a surface which is treated to produce a gradient in its surface tension. The equilibrium contact angle θ of a droplet depends on the properties of the liquid and of the material on which the droplet is lying. It is described by Young's equation

$$\gamma_{SG} - \gamma_{SL} = \gamma_{LG} \cos\theta,$$

where γ_{SG} is the solid surface tension, γ_{LG} the liquid surface tension and γ_{SL} the solid/liquid interfacial surface tension. If we create a wettability gradient on the underlying surface, the drop stretches in the direction of greater wettability, which may result into translation of the drop.

Although many experiments and measurements of moving drops have been done, there is no well-established analytic model to describe the dynamical aspects of drop motion. Many papers have been devoted to analyzing the shape of steady drops on horizontal and inclined surfaces. Works dealing with the motion of droplets often make some kind of steady or quasisteady assumptions. The authors of [9] take a similar approach as [5] or [3] and develop a model for a drop that does not change its shape and moves steadily overcoming shear exerted by the solid surface. They consider a small droplet and rely on the lubrication approximation of de Gennes ([4]).

Taking into account the principles of surface tension and the feature of positive contact angle, another natural and reasonable design for the model of moving drop is to approximate the drop by a film, representing the surface of the drop. The film can be then filled with a fluid behaving in accordance with a model of fluid dynamics, and these two models can be coupled. This approach is similar to the group of methods

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based on a modification of Navier-Stokes equations, such as phase-field methods (see, e.g., [7] or [11]) but our model is substantially different. In [6] it was shown that if the motion is slow, then it can be modeled by a parabolic operator and the approximation of the drop by its surface is sufficient. In this way, we obtain a parabolic problem for the evolution of a scalar volume-preserving membrane with an obstacle and positive contact angle.

Here we focus on the analysis of such problems. We propose construction of approximate solutions by a variational method and show their convergence to a unique weak solution. Application of variational principles to constrained problems of this type is effective. Another method that was successful in abstract analysis of constrained evolutionary problems relies on the technique of subdifferentials and Yosida approximation. Although this framework is able to solve a large class of problems, it inherits some disadvantages which we try to overcome by introducing a different approach. The most substantial contribution of the new proof is that, contrary to subdifferential approach, it is reproducible in numerical computations (for an example of numerical results, see [6]). Another feature of our method is the absence of assumptions on convexity, which are in essence indispensable for the definition of subdifferentials. This fact is significant in regard of future consideration of sharp contact angles.

2. Model. In this section, we derive a model for a droplet moving due to the difference in contact angles. We approximate the drop by its surface and assume that the area density of the surface is constant and that the surface tension is homogeneous. We also consider only the cases when the contact angle θ is smaller than $90°$, as in Figure 2.1. Then surface tension, contact angle and volume preservation become the main aspects determining the shape of the moving drop.

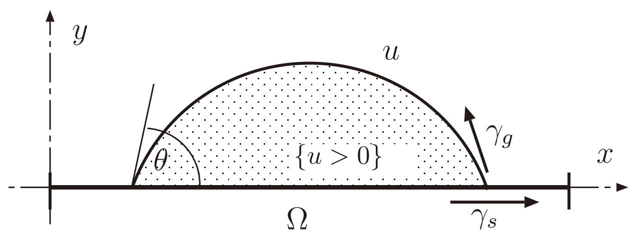

FIG. 2.1. *The setting and notation of the model.*

Since $\theta < 90°$, we can describe the surface as a scalar function $u : (0,T) \times \Omega \to \mathbb{R}$, where $(0,T)$ is the time interval and Ω is the domain where the motion is considered. The plane, on which the drop rests, corresponds to 0-level set of the function u. The domain $\Omega \subset \mathbb{R}^m$ is taken bounded but large enough so that the drop does not touch its boundary during the motion. The boundary of the set $\{u > 0\} \equiv \{(t,x) \in (0,T) \times \Omega : \, u(t,x) > 0\}$ will be called *free boundary*.

Let us use the symbol $\chi_{u>0}$ for the characteristic function of the set $\{u > 0\}$ and simplify the notation for surface tensions:

$$\gamma_g = \gamma_{LG}, \qquad \gamma_s = \gamma_{LS} - \gamma_{SG}.$$

The surface energy of a drop can be written in the following way:

$$E = \gamma_g \int_\Omega \left(\sqrt{1 + |\nabla u|^2} \right) \chi_{u>0} \, dx + \int_\Omega \gamma_s(x) \chi_{u>0} \, dx. \tag{2.1}$$

The drop assumes the shape which minimizes energy E under the volume constraint

$$\int_\Omega u \chi_{u>0} \, dx = V, \tag{2.2}$$

where $V > 0$ is the volume of the drop.

If γ_g and γ_s are constant and the drop is small so that it is not influenced by gravitation forces, it has the shape of a spherical cap (see [3]). Mathematically, this can be shown using Schwarz symmetrization and isoperimetric inequality in the framework of BV functions. In this case, we can derive the well-known Young's equation for the contact angle θ

$$\gamma_s = -\gamma_g \cos\theta \tag{2.3}$$

by explicitly minimizing functional (2.1) under condition (2.2). If we assume that the minimizer is smooth, we can also derive (2.3) for nonuniform distribution of γ_s (i.e., nonspherical drops).

Besides assuming $0 < \theta < \pi/2$, i.e., $0 < -\gamma_s < \gamma_g$, we consider hydrophilic surfaces, where the value of γ_s is close to $-\gamma_g$, which gives small gradients in the shape of the drop and makes possible the approximation

$$\sqrt{1 + |\nabla u|^2} \approx 1 + \frac{1}{2} |\nabla u|^2. \tag{2.4}$$

This linearization of the minimal surface operator is relevant only from the mathematical point of view but is not necessary as far as numerical computation is concerned.

Putting $\gamma := 1 + \gamma_s/\gamma_g$ and taking into account the nonnegativity of u, we can replace (2.1) with

$$\tilde{E} = \gamma_g \left[\frac{1}{2} \int_\Omega |\nabla u|^2 \, dx + \int_\Omega \gamma(x) \chi_{u>0} \, dx \right]. \tag{2.5}$$

Functionals of the form (2.5) are studied in [1], where it is shown that their minimizers without volume constraint are Lipschitz continuous.

In our model, the varying value of γ_s is the driving force of the droplet motion. A drop placed on a surface with nonuniform wettability tends to move or deform in the direction of smaller values of γ_s. This motion is prevented by the surface tension of the drop, which forces the drop into a ball. Volume preservation added to these aspects results in a deformation and possibly translation of the drop.

If the tension gradient is not extremely large, the movements are very slow and the shape is transforming little by little by pouring of the liquid towards the front edge. Therefore, the influence of inertial forces and friction can be assumed negligible. In such situation, it is acceptable to consider the motion as a result of vertical displacement of the film. This is inevitably the only available motion in a scalar model that we have adopted here. Nevertheless, the comparison of numerical and experimental results in [6] suggests that it is an adequate approximation.

The equation of motion is derived by standard Lagrangian approach. Using (2.5) as the potential energy in the Lagrangian for the drop, considering the kinetic energy proportional to u_t^2 and noting that the resistance force acting against the vertical motion of the film is proportional to the speed of the film, we get the following relation

$$\chi_{u>0}\beta u_{tt} + \alpha u_t = \gamma_g[\Delta u - \gamma\chi'_\varepsilon(u) + \chi_{u>0}\lambda].$$

Here, β is proportional to area density of the region constituting the membrane, α is a drag coefficient and λ is a Lagrange multiplier originating in the volume constraint. We have replaced the characteristic function in the second term of (2.5) by a function $\chi_\varepsilon \in C^2(\mathbb{R})$ satisfying

$$\chi_\varepsilon(s) = \begin{cases} 0, & s \le 0 \\ 1, & \varepsilon \le s \end{cases}$$

and $|\chi'_\varepsilon(s)| \le C/\varepsilon$ for $s \in (0,\varepsilon)$ (see Figure 2.2). The purpose of the smoothing is to avert the appearance of delta function in the equation.

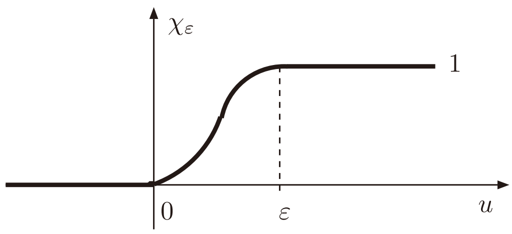

FIG. 2.2. *Smoothing of characteristic function.*

If we consider a long time-scale motion ($|\beta u_{tt}| << |\alpha u_t|$), it can be sufficiently expressed by the following parabolic equation

$$u_t = \Delta u - \gamma\chi'_\varepsilon(u) + \chi_{u>0}\lambda, \tag{2.6}$$

where we have put $\mu/\gamma_g = 1$ in order to simplify the subsequent formulas. The specific form of the time-dependent function λ can be derived by a volume-preserving variation of the Lagrangian:

$$\lambda = \frac{1}{V}\int_\Omega \left[uu_t + |\nabla u|^2 + \gamma u\chi'_\varepsilon(u)\right]\,dx. \tag{2.7}$$

This is a parabolic problem with free-boundary $\partial\{u > 0\}$ and a complicated term λ having the form of the integral of the unknown function. Multiplying equation (2.6) by u and integrating over Ω, we see that any solution of (2.6) preserves volume. Because of the nonlocal multiplier, the solution of this equation, as it is, seems very difficult. However, it is possible to solve the problem by the variational method called *discrete Morse flow*, which is presented in the following paragraphs. In this method we use the minimality property of a time-discretized functional, and insert the volume constraint, which gives rise to the nonlocal term, into the admissible function set. Thus, we can handle the multiplier without considering it explicitly.

3. Model equation and its properties. In the previous section, we have obtained a model equation for droplet motion. Imposing appropriate initial and boundary conditions, we have the following problem:

Find $u : (0,T) \times \Omega \to \mathbb{R}$ satisfying

$$u_t(t,x) = \Delta u(t,x) - \gamma(x)\chi'_\varepsilon(u(t,x)) + \chi_{u>0}\lambda(t) \quad \text{in } Q_T, \tag{3.1}$$

$$u(0,x) = u_0(x) \qquad \text{for } x \in \Omega, \tag{3.2}$$

$$u(t,x) = 0 \qquad \text{on } (0,T) \times \partial\Omega. \tag{3.3}$$

Here $Q_T = (0,T) \times \Omega$ with a bounded domain $\Omega \subset \mathbb{R}^m$ having a Lipschitz boundary $\partial\Omega$, and λ is given by (2.7).

Remark. *It is possible to add also a general "outer force" term $f(t,x,u)\chi_{u>0}$ to the right-hand side of model equation (3.1). However, this would only complicate the formulas, so we keep only the smoothed delta function representing the contact angle condition, in order to emphasize its features important for later deliberations on the sharp contact angle case ($\varepsilon = 0$). For example, gravity acting on a drop on a tilted plane with inclination angle ω would give the form $f(x,u) = -gu\cos\omega + gx\sin\omega$. This function satisfies assumptions necessary to carry out the proof in the subsequent section. In a coupled model considering also the motion of the fluid, this term would include the force exerted on the film by the fluid.*

In the present section, we mention some features of the model equation (3.1), especially the relation that holds on the free boundary when the smoothing parameter ε is taken to zero.

First, we shall formally discuss the maximum principle for our equation. Let us consider the set $Q_T \cap \{u < 0\}$. If u is smooth, then it is an open set. Moreover, from the definition of χ_ε we see that $u_t = \Delta u$ holds in this set. Since u is zero on its boundary and $u_0 \geq 0$, from the maximum principle we have that u must vanish inside $\{u \leq 0\}$. This means that the solution of (3.1)–(3.3) is either zero or positive satisfying $u_t = \Delta u - \gamma\chi'_\varepsilon(u) + \lambda$. We see that the characteristic function in front of the Lagrange multiplier realizes the obstacle and gives rise to a free boundary. Moreover, reasoning from the maximum principle, it appears that it will be convenient to set up the volume preservation condition in the form

$$\int_\Omega \chi_{u(t,x)>0} u(t,x)\, dx = V \qquad \forall t \in [0,T], \tag{3.4}$$

so that we can make use of the "cut-off at zero" argument.

Next, we shall formally compute the free boundary condition for the problem corresponding to (3.1)–(3.3) for $\varepsilon \to 0+$. The obtained identity is to be compared with Young's equation (2.3), since, besides the ε-smoothing, we have adopted a linearization of minimal surface operator.

Proposition 3.1. *Let us suppose there exists a classical solution u^ε to (3.1)–(3.3) and that for $\varepsilon \to 0+$ it converges in a sufficiently strong sense to a function v satisfying in $Q_T \cap \{v > 0\}$ the equation $v_t = \Delta v + \Lambda$, where $\Lambda = \frac{1}{V}\int_\Omega (vv_t + |\nabla v|^2)\, dx$, and the equation $v \equiv 0$ in $Q_T \cap \{v \leq 0\}$. We also assume that $\partial\{v > 0\}$ is a smooth m-dimensional hypersurface in $\Omega_T \cap \{t = \tau\}$ for all $\tau \in [0,T]$. Then $|\nabla v|^2 = 2\gamma$ holds on $\partial\{v > 0\}$ for $\partial\{v > 0\} \llcorner \mathcal{H}^{m+1}$-almost all $(t,x) \in \partial\{v > 0\}$.*

Proof. We select an arbitrary $\zeta \in C_0^\infty(Q_T)$ and multiply equation (3.1) by the function $\zeta u_k^\varepsilon \left(\equiv \zeta \frac{\partial u^\varepsilon}{\partial x_k}\right)$, $k = 1, ..., m$. Next, we integrate the resulting identity over Q_T and obtain (see [2])

$$\int_{Q_T} \zeta u_k^\varepsilon \left(\Delta u^\varepsilon - u_t^\varepsilon + \lambda\chi_{u^\varepsilon>0}\right) dz = \int_{Q_T} \gamma\zeta u_k^\varepsilon \chi'_\varepsilon\left(u^\varepsilon\right) dz. \tag{3.5}$$

The simplifying notation $z = (x_1, ..., x_m, t)$ is used here. Applying Green's formula, we derive an equation with only first order derivatives of u^ε and then take ε to zero. Noting that $[\chi_\varepsilon(u^\varepsilon)]_{x_k} = \chi'_\varepsilon(u^\varepsilon)\, u^\varepsilon_k$, and assuming that $\chi_\varepsilon(u^\varepsilon) \to \chi_{v>0}$ a.e., we have for the right-hand side of (3.5),

$$\int_{Q_T} \gamma\zeta u^\varepsilon_k \chi'_\varepsilon(u^\varepsilon)\, dz = -\int_{Q_T} (\gamma\zeta)_k \chi_\varepsilon(u^\varepsilon)\, dz \xrightarrow[\varepsilon\to 0]{} -\int_{Q_T\cap\{v>0\}} (\gamma\zeta)_k\, dz = -\int_{Q_T\cap\partial\{v>0\}} \gamma\zeta\nu_k\, dS. \quad (3.6)$$

The symbol ν_k stands for the k-th component of the outer normal $\nu = (\nu_1, \ldots, \nu_{m+1})$ to the set $\{v > 0\} \subset Q_T$, ν_{m+1} being the time-direction component.

As for the left-hand side of (3.5), we can proceed in the following way:

$$\begin{aligned}
&\int_{Q_T} \zeta u^\varepsilon_k \left(\Delta u^\varepsilon - u^\varepsilon_t + \lambda\chi_{u^\varepsilon>0}\right) dz \\
&= -\int_{Q_T} \left[\nabla(\zeta u^\varepsilon_k)\nabla u^\varepsilon + \zeta u^\varepsilon_k u^\varepsilon_t - \zeta u^\varepsilon_k\lambda\right]\chi_{u^\varepsilon>0}\, dz \\
&\quad= -\int_{Q_T} \left(u^\varepsilon_k\nabla\zeta\nabla u^\varepsilon - \frac{1}{2}|\nabla u^\varepsilon|^2\zeta_k + \zeta u^\varepsilon_k u^\varepsilon_t - \zeta u^\varepsilon_k\lambda\right)\chi_{u^\varepsilon>0}\, dz \\
&\quad\xrightarrow[\varepsilon\to 0]{} -\int_{Q_T} \left(v_k\nabla\zeta\nabla v - \frac{1}{2}|\nabla v|^2\zeta_k + \zeta v_k v_t - \zeta v_k\Lambda\right)\chi_{v>0}\, dz \\
&\quad= \int_{Q_T\cap\{v>0\}} \zeta v_k(\Delta v - v_t + \Lambda)\, dz - \int_{Q_T\cap\partial\{v>0\}} \left(\zeta v_k(\nabla v, 0)\cdot\nu - \frac{1}{2}|\nabla v|^2\zeta\nu_k\right) dS \\
&\quad= -\int_{Q_T\cap\partial\{v>0\}} \left(\zeta v_k(\nabla v, 0)\cdot\nu - \frac{1}{2}|\nabla v|^2\zeta\nu_k\right) dS.
\end{aligned}$$

Under the notation $Dv = (v_{x_1}, \cdots, v_{x_n}, v_t)$, the outer unit normal can be expressed as $\nu = -Dv/|Dv|$. Hence, on $\partial\{v > 0\}$ we get $v_k = -\nu_k|Dv|$ and

$$-\int_{Q_T\cap\partial\{v>0\}} \left(\zeta v_k(\nabla v, 0)\cdot\nu - \frac{1}{2}|\nabla v|^2\zeta\nu_k\right) dS = -\frac{1}{2}\int_{Q_T\cap\partial\{v>0\}} |\nabla v|^2\zeta\nu_k\, dS. \quad (3.7)$$

By (3.6) and (3.7), we conclude that

$$|\nabla v|^2 = 2\gamma \quad \text{on } \partial\{v > 0\}. \quad (3.8)$$

for almost all points $(t, x) \in \partial\{v > 0\}$. □

Let us study the relation between the free boundary condition (3.8), which we have just formally derived, and Young's equation (2.3). Using (2.3), we find

$$2\gamma = 2\left(1 + \frac{\gamma_s}{\gamma_g}\right) = 2(1 - \cos\theta) = \theta^2 + O(\theta^4), \qquad \theta \to 0.$$

On the other hand,

$$|\nabla v|^2 = \tan^2\theta = \theta^2 + O(\theta^4), \qquad \theta \to 0.$$

We see that the smoothing χ_ε of the characteristic function in (3.1) is reasonable and that by the approximation (2.4) we have introduced an error of order $O(\theta^3)$ in the contact angle.

4. Existence of weak solution. Here we show the main result concerning our problem – the existence of a weak solution to (3.1)–(3.3) that is nonnegative and satisfies the volume conservation identity (3.4). We assume that $\gamma \in L^\infty(\Omega)$ and $u_0 \in L^\infty(\Omega) \cap H_0^1(\Omega)$ are nonnegative. We also assume that u_0 is Hölder continuous and has volume V.

The main idea of the proof is to state and solve a minimization problem corresponding to a smoothing of the original problem. Specifically, we regularize the volume constraint (3.4) by smoothing the characteristic function. We show the existence and several important properties of the solution to the smooth problem using the discrete Morse flow variational technique. Since we also obtain the uniform convergence of approximate solutions with respect to the smoothing parameter δ, we shall finally be able to construct a weak solution to the original problem.

To begin with, we introduce the approximate problem parametrized by $\delta > 0$:

$$\begin{aligned} &u_t^\delta = \Delta u^\delta - \gamma\chi_\varepsilon'(u^\delta) + \left(\tilde\chi_\delta(u^\delta) + u^\delta\tilde\chi_\delta'(u^\delta)\right)\lambda^\delta \quad \text{in } Q_T, &(4.1)\\ &u^\delta(0,x) = u_0(x) \quad \text{in } \Omega,\\ &u^\delta(t,x) = 0 \quad \text{on } \partial\Omega, \end{aligned}$$

where

$$\lambda^\delta = \frac{\int_\Omega \left(u_t^\delta u^\delta + |\nabla u^\delta|^2 + \gamma\chi_\varepsilon'(u^\delta)u^\delta\right)\,dx}{V + \int_\Omega \tilde\chi_\delta'(u^\delta)(u^\delta)^2\,dx}, \tag{4.2}$$

and $\tilde\chi_\delta(u)$ is a smoothing of the characteristic function $\chi_{u>0}$ (see Figure 4.1):

$$\tilde\chi_\delta(u) = \begin{cases} 0, & u \le -\delta\\ 1, & u \ge 0,\end{cases}$$

interpolating in $(-\delta, 0)$ by a smooth increasing function so that

$$\tilde\chi_\delta'(u) \le C/\delta \quad \text{for } u \in (-\delta, 0).$$

Note that the denominator in (4.2) is positive.

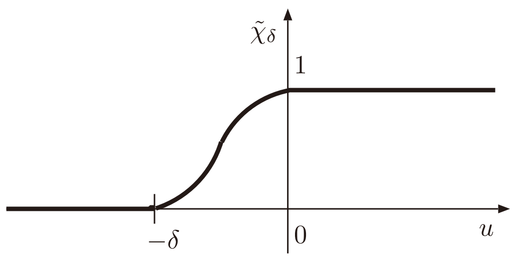

FIG. 4.1. *Smoothing of characteristic function.*

A weak solution is defined in the following way.

DEFINITION 4.1. *A function $u^\delta \in H^1(Q_T) \cap L^\infty(0,T;H_0^1(\Omega))$ is called a weak solution of (4.1), if it satisfies the initial condition and*

$$\begin{aligned} &\int_0^T\int_\Omega \left(u_t^\delta\varphi + \nabla u^\delta\nabla\varphi + \gamma\chi_\varepsilon'(u^\delta)\varphi\right)dx\,dt &(4.3)\\ &\quad= \int_0^T \lambda^\delta\int_\Omega \left(\tilde\chi_\delta(u^\delta) + u^\delta\tilde\chi_\delta'(u^\delta)\right)\varphi\,dx\,dt \quad \forall\varphi \in L^2(0,T;H_0^1(\Omega)), \end{aligned}$$

where λ^δ is given by (4.2).
We note that $\lambda^\delta \in L^2(0,T)$ and all the integrals in the above equation have sense for u^δ with the stated regularity.

To solve this problem, we make use of the mentioned variational method. The results are summarized in the following theorem.

THEOREM 4.2. *There exists a weak solution of the above approximate problem satisfying*

$$u^\delta \geq -\delta, \tag{4.4}$$

the perturbed volume constraint

$$\int_\Omega \tilde{\chi}_\delta(u^\delta) u^\delta \, dx = V \tag{4.5}$$

and the following estimate

$$\|u_t^\delta\|^2_{L^2(Q_T)} + \|\nabla u^\delta(t)\|^2_{L^2(\Omega)} + \int_\Omega \gamma \chi_\varepsilon(u^\delta)(t)\, dx \leq C(u_0) \tag{4.6}$$

for a.e. $t \in (0,T)$, where $C(u_0)$ does not depend on δ.

Moreover, the solutions are uniformly bounded in $[0,T] \times \bar{\Omega}$ and uniformly Hölder continuous on $\bar{Q}_T$ with respect to the parameter δ.

The rough structure of the proof, based on the result [10], is to use a minimizing method for a time-discretized functional in order to construct approximate solutions (see [8]), and to show that these approximations converge to a weak solution. We divide the time interval $(0,T)$ equidistantly into N subintervals of length $h = T/N$, $N \in \mathbb{N}$, and for each $h > 0$ we construct an approximate solution $u^{\delta,h}$ in the following manner.

First of all, put $u^{\delta,0} = u_0$, and for $n = 1, 2, \ldots, N$, find a minimizer $u^{\delta,n}$ of the functional

$$J_n^\delta(u) = \int_\Omega \Big(\frac{|u - u^{\delta,n-1}|^2}{2h} + \frac{1}{2}|\nabla u|^2 + \gamma \chi_\varepsilon(u) \Big)\, dx \tag{4.7}$$

in the admissible function set

$$\mathcal{K}_V^\delta = \Big\{ u \in H_0^1(\Omega);\ \int_\Omega \tilde{\chi}_\delta(u) u \, dx = V \Big\}.$$

This functional is called the discrete Morse flow corresponding to (4.1). We remark that both in (4.1) and in (4.7), the role of a penalty is played by the smoothed characteristic function modifying the volume constraint in the set $\mathcal{K}_V^\delta$. The maximum principle then yields the estimate (4.4).

As the next step, we interpolate the minimizers $u^{\delta,n}$, $n = 0, 1, 2, \ldots, N$ in time, i.e., we introduce the following functions (see Figure 4.2):

$$\bar{u}^{\delta,h}(t,x) = \begin{cases} u_0(x), & t = 0 \\ u^{\delta,n}(x), & t \in ((n-1)h, nh],\ n = 1, \ldots, N \end{cases} \tag{4.8}$$

$$u^{\delta,h}(t,x) = \begin{cases} u_0(x),\ t = 0 \\ \frac{t-(n-1)h}{h} u^{\delta,n}(x) + \frac{nh-t}{h} u^{\delta,n-1}(x),\ t \in ((n-1)h, nh]. \end{cases} \tag{4.9}$$

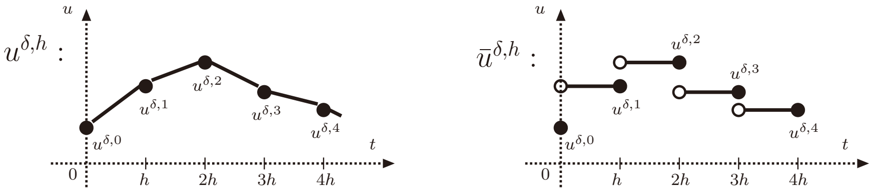

FIG. 4.2. *Time interpolation of minimizers.*

We prove Theorem 4.2 by sending h to zero. Above all, we have to show that there exists a minimizer of J_n^δ, that the functions $u^{\delta,h}$ are bounded in a certain norm and that they converge to a weak solution of the smooth problem (4.1). Here we omit the technical proof since it can be recovered from [10] by careful modification of the constraint.

Now we prove the main result - existence of weak solution to (3.1)–(3.3), the meaning of which is explained in the following Definition.

DEFINITION 4.3. *A function u belonging to the space $H^1(Q_T)\cap L^\infty(0,T;H_0^1(\Omega))$ is called a weak solution to (3.1), provided it satisfies the initial condition (3.2) and the identities*

$$\int_0^T\int_\Omega (u_t\varphi+\nabla u\nabla\varphi+\gamma\chi_\varepsilon'(u)\varphi)=\int_0^T\int_\Omega \lambda\varphi \quad \forall\varphi\in C_0^\infty(Q_T\cap\{u>0\}),$$
$$u\equiv 0 \qquad in \quad Q_T\setminus\{u>0\}, \tag{4.10}$$

with λ defined in (2.7).

THEOREM 4.4. *There exists a unique weak solution to the problem (3.1)–(3.3) that is Hölder continuous in $[0,T]\times\bar{\Omega}$.*

Proof. Recollecting (4.6) provides us with a subsequence of $\{u^\delta\}_{\delta>0}$ converging weakly in $H^1(Q_T)$:

$$\begin{aligned} u_t^\delta &\rightharpoonup u_t && \text{weakly in } L^2(Q_T),\\ \nabla u^\delta &\rightharpoonup \nabla u && \text{weakly}^* \text{ in } L^\infty(0,T;L^2(\Omega)),\\ u^\delta &\to u && \text{strongly in } L^2(Q_T). \end{aligned} \tag{4.11}$$

Moreover, in virtue of the uniform Hölder continuity and boundedness, we can use the Arzelà-Ascoli theorem to extract another subsequence converging uniformly on Q_T.

We fix an arbitrary function $\varphi\in C_0^\infty(Q_T\cap\{u>0\})$ and denote its support as S_φ. Then we have

$$u^\delta \rightrightarrows u \qquad \text{uniformly in } S_\varphi. \tag{4.12}$$

Our goal is to show (4.10) for this u and φ by passing to the limit as $\delta\to 0+$ in (4.3). First, we have by (4.11)

$$\int_0^T\int_\Omega \left(u_t^\delta\varphi+\nabla u^\delta\nabla\varphi\right)\,dx\,dt\to\int_0^T\int_\Omega (u_t\varphi+\nabla u\nabla\varphi)\,dx\,dt.$$

Since χ_ε' is continuous and bounded and $|\gamma\chi_\varepsilon'(u^\delta)\varphi|\le C\gamma\in L^1(\Omega)$, we obtain

$$\int_0^T\int_\Omega \gamma\chi_\varepsilon'(u^\delta)\varphi\,dx\,dt\to\int_0^T\int_\Omega \gamma\chi_\varepsilon'(u)\varphi\,dx\,dt.$$

Also, by the uniform convergence (4.12), we see that $u^\delta > 0$ on S_φ for δ small enough. Consequently, we have for small δ the key identity

$$\int_\Omega \left(\tilde{\chi}_\delta(u^\delta) + u^\delta \tilde{\chi}'_\delta(u^\delta)\right) \varphi \, dx = \int_\Omega \tilde{\chi}_\delta(u^\delta) \varphi \, dx = \int_\Omega \varphi \, dx.$$

The definition of support of test function φ becomes relevant here, leading us back to the characteristic function in (3.1). Finally, due to an estimate on approximate Lagrange multipliers, we have the uniform boundedness of λ^δ in $L^2(0,T)$. Thus, reselecting a subsequence, there is a function $\tilde{\lambda} \in L^2(0,T)$ such that

$$\lambda^\delta \rightharpoonup \tilde{\lambda} \qquad \text{weakly in } \; L^2(0,T).$$

We have arrived at the following identity:

$$\int_0^T \int_\Omega \left(u_t \varphi + \nabla u \nabla \varphi + \gamma \chi'_\varepsilon(u) \varphi\right) \, dx \, dt = \int_0^T \tilde{\lambda} \int_\Omega \varphi \, dx \, dt. \tag{4.13}$$

It remains to show that $\tilde{\lambda}$ corresponds to the form of λ from (2.7), that u is nonnegative and that it satisfies the volume condition (2.2). The nonnegativity of u is seen from (4.4) and the uniform convergence. Volume preservation is shown, for example, in the following way:

$$\begin{aligned}\Big| \int_\Omega u \chi_{u>0} \, dx - V \Big| &= \Big| \int_\Omega \left(u \chi_{u>0} - u^\delta \tilde{\chi}_\delta(u^\delta)\right) \, dx \Big| \\ &= \Big| \int_\Omega \left(u \tilde{\chi}_\delta(u) - u^\delta \tilde{\chi}_\delta(u^\delta)\right) \, dx \Big| \\ &\le C \int_\Omega |u - u^\delta| \, dx \to 0 \quad \text{for } \delta \to 0+ .\end{aligned}$$

Now, the form of $\tilde{\lambda}$ would be ensured if we could put

$$\varphi(t,x) = \begin{cases} u(t,x), & t \le t_0 \\ 0, & t > t_0 \end{cases} \tag{4.14}$$

in (4.13). We cannot do so directly because this function does not have compact support inside $\{u > 0\}$. We also cannot apply any approximation technique. Indeed, we only know that function u is a Hölder continuous H^1-function, which is not good enough information to get necessary regularity (Lipschitz continuity) of the boundary of $\{u > 0\}$. Thus, we cannot use approximations by functions from $C_0^\infty(\{u > 0\})$. Still, we notice that (4.14) is an admissible function in (4.3). Then we get

$$\int_0^{t_0} \int_\Omega \left(u_t^\delta u + \nabla u^\delta \nabla u + \gamma \chi'_\varepsilon(u^\delta) u\right) dx \, dt = \int_0^{t_0} \lambda^\delta \int_\Omega \left(\tilde{\chi}_\delta(u^\delta) + u^\delta \tilde{\chi}'_\delta(u^\delta)\right) u \, dx \, dt. \tag{4.15}$$

For the left-hand side terms of (4.15), the convergences from (4.11) are sufficient. In the remaining terms, we use the uniform convergence, boundedness of u^δ from below (see (4.4)), properties of the function $\tilde{\chi}_\delta$ and the following estimates:

$$\begin{aligned}\Big| \int_\Omega \tilde{\chi}_\delta(u^\delta) u \, dx - V \Big| &= \Big| \int_\Omega \left(\tilde{\chi}_\delta(u^\delta) u^\delta + \tilde{\chi}_\delta(u^\delta)(u - u^\delta)\right) dx - V \Big| \\ &= \Big| \int_\Omega \tilde{\chi}_\delta(u^\delta)(u - u^\delta) \, dx \Big| \\ &\le C \max_{Q_T} |u - u^\delta| \to 0 \quad \text{ as } \; \delta \to 0,\end{aligned}$$

$$|\int_\Omega u^\delta \tilde\chi_\delta'(u^\delta) u\, dx| = |\int_\Omega \big((u^\delta)^2 \tilde\chi_\delta'(u^\delta) + u^\delta \tilde\chi_\delta'(u^\delta)(u-u^\delta)\big)\, dx| \\ \le C\delta + C \max_{Q_T} |u-u^\delta| \to 0 \quad \text{as } \delta \to 0.$$

Hence, taking δ to zero in (4.15) yields

$$\int_0^{t_0} \tilde\lambda\, dt = \frac{1}{V}\int_0^{t_0}\int_\Omega \big(u_t u + |\nabla u|^2 + \gamma \chi_\varepsilon'(u) u\big)\, dx\, dt,$$

which immediately implies $\tilde\lambda(t) = \lambda(t)$ almost everywhere in $(0,T)$.

The uniqueness follows from the uniqueness of the solution obtained by the method of variational inequalities (see Remark below). □

Remark. *We show that the weak solution constructed above is the same as the solution obtained by the technique of variational inequality. More precisely, we prove that our solution satisfies the relation*

$$\int_0^T \int_\Omega \Big[(-u_t - \gamma\chi_\varepsilon'(u))(z-u) - \nabla u \nabla (z-u)\Big]\, dx\, dt \le 0 \qquad \forall z \in \mathcal{K}, \tag{4.16}$$

where

$$\mathcal{K} = \big\{u \in L^2(0,T; H_0^1(\Omega));\ u \ge 0,\ \int_\Omega u\, dx = V\big\}.$$

Since solution of (4.16) is unique (this can be seen taking two solutions $u, v \in \mathcal{K}$, setting $z = v$ in (4.16) and $z = u$ in the corresponding relation for v, adding the resulting inequalities and using Gronwall's lemma), we conclude that there is a unique weak solution in the sense of Definition 4.3, which is identical to the unique solution in the sense of Yosida approximation.

To start with, take any $z \in \mathcal{K} \cap C(0,T; H_0^1(\Omega))$ and define function $\bar z^h$ by

$$\bar z^h(t,x)|_{t \in (nh, nh+h)} = z^n(x) = z(nh, x), \qquad x \in \Omega.$$

Then for $\epsilon \in (0,1)$ the function $u^{\delta,n} + \epsilon(z^n - u^{\delta,n})$ is nonnegative and has volume V, thus is an admissible variation for the functional (4.7), yielding

$$\frac{1}{\epsilon}\big(J_n^\delta(u^{\delta,n}) - J_n^\delta(u^{\delta,n} + \epsilon(z^n - u^{\delta,n}))\big) \le 0.$$

Letting $\epsilon \to 0+$ gives

$$\int_0^T \int_\Omega \Big[\big(-u_t^{\delta,h} - \gamma\chi_\varepsilon'(\bar u^{\delta,h})\big)(\bar z^h - \bar u^{\delta,h}) - \nabla \bar u^{\delta,h}\nabla(\bar z^h - \bar u^{\delta,h})\Big]\, dx\, dt \le 0.$$

Using an analogy for (4.11) in the limit as $h \to 0+$, we find

$$\int_0^T \int_\Omega \Big[\big(-u_t^\delta - \gamma\chi_\varepsilon'(u^\delta)\big)(z - u^\delta) - \nabla u^\delta \nabla z\Big]\, dx\, dt + \liminf_{h\to 0}\int_0^T\int_\Omega |\nabla \bar u^{\delta,h}|^2\, dx\, dt \le 0.$$

Hence, by the lower semicontinuity of the Dirichlet integral, we obtain

$$\int_0^T \int_\Omega \Big[\big(-u_t^\delta - \gamma\chi_\varepsilon'(u^\delta)\big)(z - u^\delta) - \nabla u^\delta \nabla(z - u^\delta)\Big]\, dx\, dt \le 0.$$

Results (4.11) and the same reasoning as above finally give (4.16).

5. Conclusion. We have proved the existence, uniqueness and certain regularity of a weak solution to a parabolic free boundary problem with integral constraint. The equation can describe slow motion of drops on surfaces, where the contact angles are smoothed. The volume constraint results in a time-dependent outer force term having a nonlocal form depending on the solution. The problem was solved by the discrete Morse flow method, which is a variational method based on the minimization of a time-discretized functional. The constraints can then be included in the set of functions admissible for minimization. The possibility of direct application to numerical schemes and independence of convexity of the problem distinguishes the construction of approximate solutions in the present proof from the subdifferential technique using Yosida approximation. In the future, we aim at employing the independence of convexity to study constrained evolutionary equations with delta function terms, corresponding to sharp contact angles in the droplet model.

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