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On a volume-preserving free boundary problem

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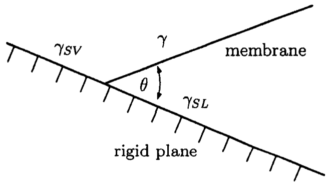
We are interested in the motion of a membrane that is in contact with a rigid plane. In this report, we state some important previous results, explain our new results and present several related open problems.



In many cases, the membrane is described by some partial differential equation (such as heat equation) and on the free boundary (points where the membrane touches the plane) a contact angle condition is prescribed which originates in the physical properties of the materials in contact (i.e., surface tensions $\gamma, \gamma_{SV}, \gamma_{SL}$). A typical example of such free boundary condition is Young's equation

$$\gamma \cos\theta = \gamma_{SV} - \gamma_{SL}.$$

A pioneering beautiful paper related to this phenomenon by Alt and Caffarelli (1981) [1] deals with the stationary problem

$$\Delta u = 0 \quad \text{in } \Omega \cap \{u > 0\}, \qquad |\nabla u| = Q,\ u = 0 \quad \text{on } \Omega \cap \partial\{u > 0\}.$$

The authors study the functional

$$\int_\Omega \left(|\nabla u|^2 + Q^2 \chi_{u>0}\right) dx,$$

where $\chi_{u>0}$ is characteristic function of the set $\{u > 0\} = \{x \in \Omega;\ u(x) > 0\}$, and show that it possesses minima which are Lipschitz continuous and have linear growth away from the free boundary. For such harmonic functions they find the representation formula $\Delta u = q_u \mathcal{H}^{n-1} \lfloor_{\partial\{u>0\}}$ and show that the minima are weak solutions, while the free boundary is a smooth surface except of a set of zero $(n-1)$-dimensional Hausdorff measure. Of course, the smoothness depends on the smoothness of the datum Q: for example, if Q is Hölder continuous then the function whose graph determines locally the shape of the free boundary has Hölder continuous first derivatives.

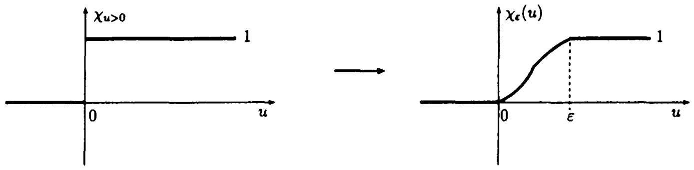
On the other hand, Caffarelli and Vázquez (1995) [2] studied the evolutionary problem

$$u_t - \Delta u = 0 \quad \text{in } \{u > 0\}, \qquad |\nabla u| = 1,\ u = 0 \quad \text{on } \partial\{u > 0\}$$

by a different technique. They regularize the problem by adding an absorption term in the following way

$$u_t^\varepsilon - \Delta u^\varepsilon = -\tfrac{1}{2}\chi_\varepsilon'(u^\varepsilon), \qquad u^\varepsilon \geq 0.$$

Here, χ_ε is an appropriate smoothing of the characteristic function in the interval $(0, \varepsilon)$:

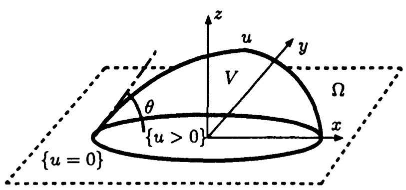


They show uniform estimates for the solution of the regularized equation (Lipschitz in space and Hölder in time) and use them to construct a weak solution of the original problem. The regularity of free boundary is also studied in case of shrinking support. The above results were extended and generalized by several researchers later on.

We are interested in the study of evolutionary problem with volume constraint

$$\int_\Omega u(t,x)\,dx = V \qquad \forall t,$$

which appears, for example, in the free boundary problem modelling the motion of bubbles or droplets on a surface (see [6]).



The full model equation is

$$\chi_{u>0}\beta u_{tt} + \mu u_t = \Delta u - \gamma\chi_\varepsilon'(u) + \chi_{u>0}\lambda_\varepsilon(u) \qquad \text{in } \Omega\times(0,T), \tag{1}$$

where u describes the shape of the bubble under the assumption that it can be represented as graph of scalar function. It is derived from the surface energy functional

$$\gamma_g\int_\Omega \sqrt{1+|\nabla u|^2}\chi_{u>0}\,dx + \int_\Omega \gamma_s\chi_{u>0}\,dx \approx \frac{\gamma_g}{2}\int_\Omega |\nabla u|^2\,dx + \int_\Omega \gamma_s\chi_\varepsilon(u)\,dx$$

by applying Hamilton's principle and taking into account the constraint and the presence of obstacle. The second time derivative term has a degenerating coefficient (see [17]) and λ_ε is a function of time only representing a Lagrange multiplier for the volume constraint.

If we minimize the unapproximated surface energy under volume constraint, we discover that the stationary contact angle θ satisfies $\gamma_s = -\gamma_g\cos\theta$, which is identical to Young's equation. However, if the shape of the membrane evolves in time, there is no generally accepted physical theory for the dynamic contact angle. The advantage of our model is the fact that the dynamic contact angle is not prescribed but is determined implicitly from other data of the model.

Based on the mathematical analysis described below, a numerical scheme for the computation of this equation has been developed and simulation of various phenomena was attempted (see, e.g., [6] [10] [16] [8]).

To start the mathematical analysis of the above model equation, we consider the following parabolic problem:

$$u_t - \Delta u = \lambda \quad \text{in } \{u>0\}, \qquad |\nabla u|^2 = 2\gamma \quad \text{on } \partial\{u>0\}$$

The regularized version is

$$u_t = \Delta u - \gamma\chi_\varepsilon'(u) + \chi_{u>0}\lambda_\varepsilon \qquad \text{in } (0,T)\times\Omega,$$

where

$$\lambda_\varepsilon = \int_\Omega \left[u_t u + |\nabla u|^2 + \gamma\chi_\varepsilon'(u)u\right]dx$$

is the nonlocal Lagrange multiplier coming from the volume constraint. Notice that the second derivative term in the original model has been neglected, which can be interpreted as considering relatively slow motion.

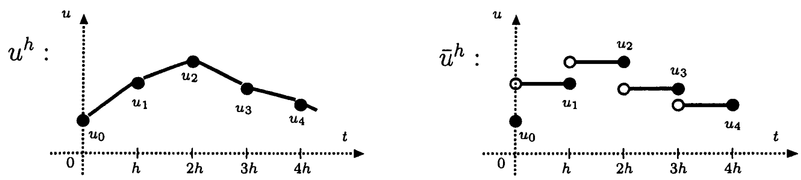
One can see by maximum principle that solutions to the regular problem are nonnegative because the right-hand side vanishes for negative values of u. This is the mathematical reason for multiplying the nonlocal term by characteristic function. The physical reason is that the outer force or source representing the volume constraint should not act on the region where the solution vanishes.

In the regularized problem the volume constraint gives rise to an obstacle-type problem with a nonlocal obstacle function depending on the solution. Accordingly, the sharp contact angle limit $\varepsilon \to 0$ is expected to have two factors influencing the behaviour on the free boundary: the stronger linear growth due to contact angle condition and the quadratic growth (curvature) originating in the volume constraint.

With the view of numerical approximation and because of the presence of the global constraint we analyse the regularized obstacle problem by a minimization method, where time variable is discretized and the functional

$$J_n(u) = \int_\Omega \left(\frac{|u-u_{n-1}|^2}{2h} + \frac{1}{2}|\nabla u|^2 + \gamma\chi_\varepsilon(u)\right)dx \tag{2}$$

is minimized. Here h is the time step and u_{n-1} refers to the minimizer on the previous time level. The computation starts from minimizing J_1, where u_0 is given as initial datum. This gives u_1 and minimizers u_n on the following time levels are computed inductively. Finally, minimizers are interpolated in time as in the following picture to obtain functions u^h and $\bar{u}^h$:



If we minimize J_n in H_0^1, it is easy to find from the first variation that the interpolated functions satisfy

$$u_t^h = \Delta\bar{u}^h - \gamma\chi_\varepsilon'(\bar{u}^h)$$

in the weak sense and are, therefore, candidates for approximate solutions. However, in the case of problems with volume constraint we have to restrain the space of functions admissible for minimization. This was done together with regularity analysis in the paper [11] for parabolic problems and in the paper [12] for hyperbolic problems.

Here we have an additional constraint represented by the obstacle and hence we define a special constrained space

$$\mathcal{K}^\delta = \left\{u \in H_0^1(\Omega)\,;\ \int_\Omega \chi_\delta(u)u\,dx = V\right\} \tag{3}$$

as the admissible space for minimization.

The characteristic function in the constraint of the admissible space is essential in order to satisfy the obstacle condition, while the regularization thereof is necessary to obtain an equality from the first variation. Indeed, the minimizers are shown to exist and be nonnegative. The weak solution is then constructed by deriving uniform estimates in h and δ and taking $h, \delta \to 0$ (see [13] for details).

It is to be noted that this minimization approach avoids direct treatment of the complicated nonlocal term λ_ε, naturally discards incorrect solutions mentioned in [2] and provides a theoretical background for numerical computation of this type of problems.

We show here two steps from the existence proof, namely the existence of minimizers and their nonnegativity. Since the functional (2) is nonnegative, there is a minimizing sequence $\{u^k\}$ such that $J_n(u^k) \downarrow \inf_{u\in\mathcal{K}^\delta} J_n(u)$. As this sequence is bounded in $H^1(\Omega)$, there is a subsequence converging weakly in $H^1(\Omega)$ and strongly in $L^2(\Omega)$ to some function $u_n \in H^1(\Omega)$. However, here we have to assume that domain Ω is bounded. From the weak lower semicontinuity of J_n in $H^1(\Omega)$ one can say that u_n is a minimizer, if it belongs to $\mathcal{K}^\delta$ defined in (3). Therefore, we compute

$$\begin{aligned} |\int_\Omega \chi_\delta(u)u\,dx - V| &= |\int_\Omega (\chi_\delta(u)u - \chi_\delta(u^k)u^k)\,dx| \\ &\le \int_\Omega |\frac{d}{du}(\chi_\delta(u)u)|_{u=\tilde{u}}|u-u^k|\,dx \to 0 \quad \text{as } k \to \infty. \end{aligned}$$

To show that minimizers are nonnegative a.e., let us assume that a minimizer u_n is negative on a set of positive measure and define a new function $\tilde{u}_n$ by $\tilde{u}_n = u_n\chi_{u_n>0}$. Then it is easy to check that $J_n(\tilde{u}_n) < J_n(u_n)$ which is in contradiction with minimality under the condition that $\tilde{u}_n$ belongs to $\mathcal{K}^\delta$. However, $\tilde{u}_n$ fulfills the constraint because the smoothing of characteristic function causes that only positive values of given function are taken into account and thus "cutting off" negative part as in the case of $\tilde{u}_n$ does not change the fact that the constraint is satisfied.

The analysis for the sharp contact angle limit $\varepsilon \to 0$ is yet to be done. Yamaura [15] constructed L^2 - generalized minimizing movement corresponding to the considered energy without taking into account the volume constraint. It is expected that a similar technique would basically work for the constrained problem. However, there is a problem closely related to the global constraint. Specifically, if we take $\Omega = \mathbb{R}^m$ in order to use Bernstein's technique to show uniform Lipschitz continuity which is indispensable for the existence proof, we are not able to proof the existence of minimizers as the above presented proof fails, i.e., the volume of the minimizing functions u^k may "leak out to infinity". On the other hand, if Ω is taken bounded, the application of Bernstein's method becomes difficult.

Since in the present model the contact angle cannot be larger than right angle, our future plan is to extend the theory from scalar functions to hypersurfaces. The goal is to rigorously derive the motion of a hypersurface according to a model equation with a given contact angle on the obstacle. To this end, we plan to consider the application of phase-field approximation, where the hypersurface is constructed as the limit of a layer between regions where a function u is identically equal to 0 and 1, for example. Specifically, to obtain the mean curvature flow, the following energy is considered:

$$\int_\Omega (\varepsilon^2|\nabla u|^2 + W(u))\,dx + \int_{\partial\Omega} \varepsilon\sigma(u)\,d\mathcal{H}^{n-1},$$

where ε is a small parameter corresponding to the width of the layer, W is a double-well potential with minima at 0 and 1 and σ is a function describing contact energy. In order to prove that the limit of the layer as $\varepsilon \to 0$ is a smooth hypersurface, the foremost task is to prepare a parabolic monotonicity formula holding up to the boundary. This might be possible if one consults the ideas regarding interior parabolicity formula derived in [4] and stationary boundary formula given in [14].

An obvious future task is to analyze the full hyperbolic model equation (1). Extracting a part of the features of the model equation we obtain slightly simpler problems. One of them is the equation

$$\chi_{u>0}u_{tt} + \alpha u_t = \Delta u$$

related in [17] to the vibration of a string with obstacle. Another similar problem

$$u_{tt} - \Delta u = 0 \quad \text{in } \{u > 0\}, \qquad |\nabla u|^2 - u_t^2 = Q^2 \quad \text{on } \partial\{u > 0\}$$

describes the peeling of a tape from a plane. The classical analysis of this problem is given in [9] and interesting numerical results were reported in [5]. Both problems were solved to some extent only in space dimension one, the same being true for the analysis of the model equation (1) in [3]. However, there is some doubt whether these results touch the core of the problems since in dimension one it is possible to use special tools such as Sobolev imbedding theorem or D'Alembert's formula.

Another challenging task is the analysis of contact problems arising, e.g., in the modelling of collision of elastic curves with an obstacle. One such example is mentioned in [7].

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