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Capillary surface discontinuities above re-entrant corners

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A capillary surface S is the (equilibrium) interface between two adjacent fluids that are also contacting rigid walls. Because the interface is in equilibrium one has information about the mean curvature of S and its contact angle γ with the bounding walls. The general problem in the mathematical theory of capillarity is to use this geometric information to deduce properties of S.

In this paper we study a particular configuration for which S is the interface between two fluids in a vertical capillary tube, in the presence of a downward pointing gravitational field. S is the graph a function u whose domain is the (horizontal) cross section Ω of the tube. The mean curvature of S is proportional to its height above a fixed reference plane, γ is a prescribed constant and may be taken between zero and $\pi/2$.

The particular question we study here is, are there domains Ω for which u is a bounded function but does not extend continuously to $\partial\Omega$? We find simple domains to show that the answer is yes and study the behavior of u in those domains.

In section 1 of this note we fix notation and briefly formulate the non-parametric capillary problem described in the second paragraph above.

In section 2 we review an important comparison principle that has been used (in the literature) to derive many of the results in capillarity. It allows one to deduce the approximate shape of a capillary surface by constructing comparison surfaces with mean curvature and contact angle close to those of the (unknown) solution surface. In the context of non-parametric problems the comparison principle leads to height estimates above and below for the function u. We describe an example from the literature where these height estimates have been used successfully. We indicate areas of possible future applications. In section 3 we construct the promised domains for which the bounded u does not extend continuously to the boundary. The point on the boundary at which u has a jump discontinuity will be the vertex of a re-entrant corner having any interior angle $\theta > \pi$. Using the comparison principle we study the behavior of u near this point.

Much of this paper uses material from the note, "On the behavior of a capillary surface at a re-entrant corner"[6] and from other sections of the Ph.D. dissertation, "Capillary surface behavior determined by the bounding cylinder's shape"[7], by this author.

Section 1: The non-parametric capillary problem

For a Lipschitz domain Ω in $\mathbf{R}^2$ a function $u \in C^2(\Omega) \cap C^1(\bar{\Omega})$ is a classical solution to the capillary problem in a gravitational field if

$$\operatorname{div} Tu = 2H(S_u) = \kappa u \quad \text{in } \Omega , \tag{1}$$

$$Tu = \frac{Du}{\sqrt{1+|Du|^2}}, \quad Du = \text{grad}\,u, \quad H(S_u) = \text{mean curvature of } S_u, \ \kappa > 0 ,$$

$$Tu\cdot n = \cos\gamma \quad \text{on } \partial\Omega, \tag{2}$$

$$0 \le \gamma \le \pi \ \text{prescribed}, \quad n = \text{exterior normal to } \partial\Omega .$$

Physically S_u describes the capillary surface formed when a vertical cylinder with horizontal cross section Ω is placed in an infinite reservoir of liquid having zero rest height. Then

$\kappa = \frac{\rho g}{\sigma}$ where ρ = density of liquid
g = (downward) acceleration of gravity
σ = surface tension between liquid and air

$\cos\gamma = \frac{\sigma_1}{\sigma}$ σ_1 = surface attraction between liquid and cylinder .

(More generally, by picking the reference height $u = 0$ appropriately, S_u can be the interface between any two different density fluids occupying a capillary tube. Then ρ is the density difference between the two fluids, σ_1 is the difference in surface attraction between the two fluids and the bounding cylinder, and σ is the surface tension between the two fluids).

Geometrically div Tu is twice the mean curvature of the surface S_u. In some sense this is the average amount the surface is curving: Writing the surface locally as a graph above its tangent plane at a point P, $\zeta = \phi(\eta)$, then one can verify that at P div Tu is the trace of the Hessian of ϕ. The correct choice of orthogonal coordinates η (called the principal directions) makes the Hessian a diagonal matrix. Then div Tu is the sum of the curvatures (second derivatives of ϕ) in these principal directions and $H(S_u)$ is the average.

Geometrically γ is the contact angle between the (downward normal to the) capillary surface S_u and the (exterior normal to the) bounding cylinder $\partial\Omega \times \mathbf{R}$ (see Figure 1). Thus if the cylinder is of uniform composition γ is constant. We consider that case here. By considering the function $-u$ if necessary (looking at the capillary tube upside down) we can assume

$$0 \le \gamma \le \pi/2 \ . \tag{3}$$

The most natural way to prove the existence of capillary surfaces is to solve the variational problem associated to (1), (2): u should minimize the energy

$$\tilde{E}(f) = \int_\Omega \left(\sigma\sqrt{1 + |Df|^2} + \frac{\rho g}{2} f^2\right) - \int_{\partial\Omega} \sigma_1 f$$

or equivalently

$$E(f) = \int_\Omega \sqrt{1 + |Df|^2} + \frac{\kappa}{2} f^2 - \int_{\partial\Omega} \nu f, \qquad \nu = \cos\gamma \tag{4}$$

over the appropriate space of functions. The three terms making up the energy functional are (in order) surface energy, potential energy from gravity, wetting energy. Emmer[4] and Finn-Gerhardt[5] have studied the existence of variational solutions to the capillary problem in Lipschitz domains Ω. (In particular, existence theorems are guaranteed for the particular piecewise smooth domains considered in section 3.) When it exists the function u is unique, real analytic in Ω and satisfies (1) classically. Wherever $\partial\Omega$ is smooth enough (C^4), u extends smoothly and satisfies the boundary condition (2) classically[9]. (In particular u can never be discontinuous at a point where $\partial\Omega$ is smooth.)

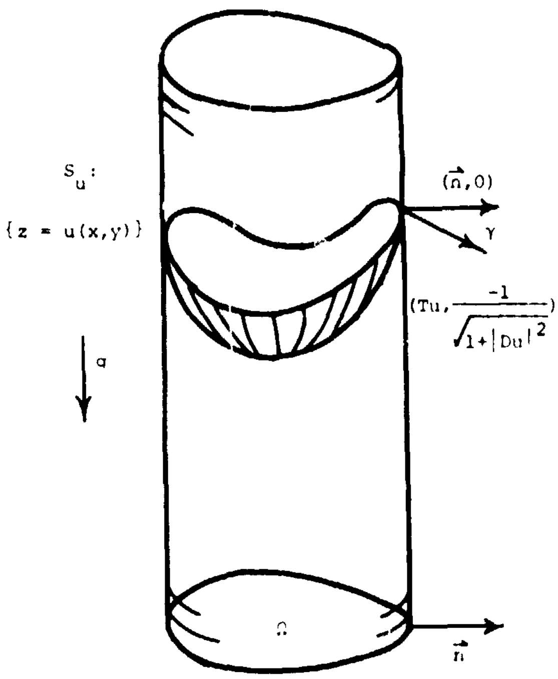

Figure 1: Configuration for the non-parametric capillary problem.

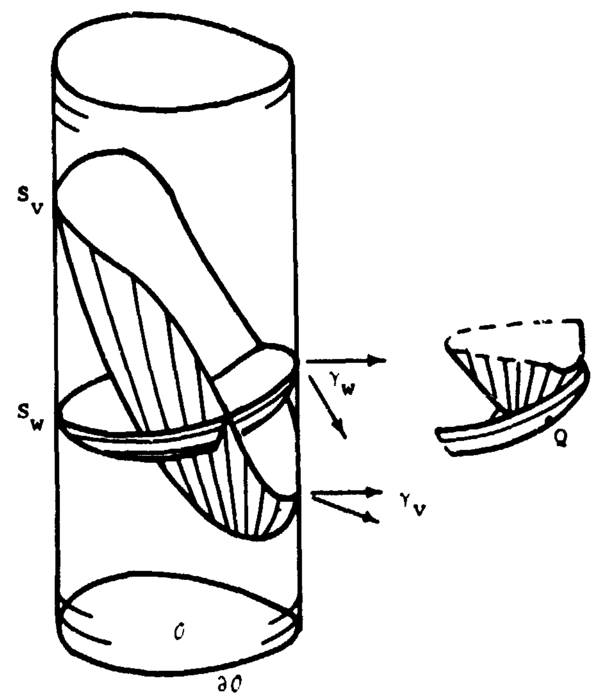

Figure 2: The comparison principle: If $\gamma_v < \gamma_w$ on $\partial\mathcal{O}$ (wherever $v < w$), then any last point of contact between S_v and S_w occurs inside $\mathcal{O} \times \mathbf{R}$. At such a point, $H(S_v) > H(S_w)$.

Section 2: The comparison principle

Let Ω be the domain being studied for the capillary problem. Let $\mathcal{O}$ be a (bounded) subdomain (possibly all of Ω). Let n be the exterior normal to $\partial\mathcal{O}$. For a function u let γ_u denote the contact angle of S_u with the subcylinder $\partial\mathcal{O} \times \mathbf{R}$. That is, $Tu\cdot n = \cos\gamma_u$. The comparison principle for non-parametric surfaces of related mean curvature and contact angle is:

Theorem 2.1: Let $v,w \in C^2(\mathcal{O})$ and suppose that

(i) wherever $v < w$ in $\mathcal{O}$, $\operatorname{div} Tv < \operatorname{div} Tw$

(ii) wherever $v < w$ on $\partial\mathcal{O}$, $Tv\cdot n \geq Tw\cdot n$ (i.e. $\gamma_v \leq \gamma_w$)

Then v is never actually less than w, $v \geq w$.

As applied to mean curvature and contact angle Theorem 2.1 is due to Concus and Finn[3]. It is a special case of a very general comparison principle for elliptic equations with suitable boundary conditions.

We roughly sketch the classical proof of this theorem, assuming that $\partial\mathcal{O}$ is smooth, that $v,w \in C^1(\bar{\mathcal{O}})$ and that (ii) is replaced by the stronger

$\overline{\text{(ii)}}$ wherever $v < w$ on $\partial\mathcal{O}$, $\gamma_v < \gamma_w$.

(See Figure 2.)

Suppose S_v does not lie entirely above S_w. Then lift S_v until it reaches a point Q of last contact with S_w. (Lifting S_v does not affect its mean curvature or contact angle with $\partial\mathcal{O} \times \mathbf{R}$). The condition $\overline{\text{(ii)}}$ implies that wherever $v < w$ on $\partial\mathcal{O}$, S_v rises more steeply than S_w to meet $\partial\mathcal{O} \times \mathbf{R}$. Hence Q cannot be a boundary point, on $\partial\mathcal{O} \times \mathbf{R}$, and must instead be contained in $\mathcal{O} \times \mathbf{R}$. Since Q is a point of last contact (the lifted) S_v and S_w are tangent there. But (the lifted) S_v contacts S_w at Q and never lies beneath it, so we must have $H(S_v) \geq H(S_w)$ there. This contradicts (i). Thus S_v did actually lie above S_w.

Filling in the details to the preceding proof one would see that it is only the ellipticity of the mean curvature operator that is used (for both the boundary and interior arguments).

There is another (less intuitive but still simple) proof that uses the divergence structure of the elliptic equation (1), (2). Using this proof and the fact that $|Tu| < 1$ it is possible to see that $\partial\mathcal{O}$ can be Lipschitz and that the boundary condition (ii) need only be attained in a certain weak sense. In particular the comparison principle will hold for the piecewise smooth domains considered in section 3 and for the solutions u to the capillary problems in these domains[3].

The specific form of Theorem 2.1 that we need for section 3 is:

Corollary 2.2: Let $\mathcal{O}$ be piecewise smooth. Let $u,v,w \in C^2(\mathcal{O})$ and suppose the contact angle for these three surfaces exists on the smooth parts of $\partial\mathcal{O}$. Suppose

$$\begin{array}{lll} \operatorname{div} Tv \leq \kappa v, & \operatorname{div} Tu = \kappa u, & \operatorname{div} Tw \geq \kappa w \quad \text{in } \mathcal{O} \\ \gamma_v \leq \gamma_u, & & \gamma_w \geq \gamma_u \quad \text{on } \partial\mathcal{O}\ . \end{array} \tag{5}$$

Then $v \geq u \geq w$ in $\bar{\mathcal{O}}$.

Proof: We show $v \geq u$: Condition (ii) of Theorem 2.1 is satisfied on all of $\partial\mathcal{O}$. Condition (i) is satisfied since $v < u$ implies $\operatorname{div} Tv \leq \kappa v < \kappa u \leq \operatorname{div} Tu$. Thus $v \geq u$.

Remark 2.3: Note that the comparison principle sounds backwards: If v has "less" mean curvature and "less" contact angle, S_v lies above S_u. If w has "more" mean curvature and "more" contact angle, S_w lies beneath S_u.

Remark 2.4: One of the most successful uses of the comparison principle has been to study the seemingly strange behavior of capillary surfaces above domains with corners, in the presence of gravity. This study was undertaken by Concus-Finn[3] who showed that above a corner with interior angle θ satisfying $\theta < \pi - 2\gamma$, u approaches infinity as the vertex is approached. In contrast they showed that for $\theta \geq \pi - 2\gamma$, u is bounded, uniformly as the corner is closed. In the unbounded case they actually constructed a comparison surface that describes u to within a constant. The methods we use in section 3 are very similar in spirit to theirs.

There are other instances in the literature where the non-parametric comparison principle yields interesting height estimates, but I feel the general comparison technique has not yet been fully utilized, as the following three remarks indicate:

Remark 2.5: Mean curvature and contact angle (i.e. capillarity) make sense in the more general parametric setting of surfaces. The proof of the comparison principle that I sketched roughly can also make sense in the parametric setting: If there are two surfaces S_1 and S_2 of "known" mean curvature (known in the sense that the mean curvature is determined by the perhaps unknown position of the surface), each making "known" contact angle with a fixed third surface S_3, then by considering appropriate families of transformations of S_1 relative to S_2 (not necessarily by rigid motions), one can conclude location bounds on possible parametric capillary surfaces.

Remark 2.6: There is a connection between comparison surfaces such as those in (5) and the energy functional (4). Roughly speaking if f is a candidate to minimize (4) and if one knows of supersolutions v or subsolutions w in the sense of (5) then one can assume without loss of generality that f lies beneath v and above w. This can be very useful in proving existence theorems, where it is often important to bound the minimizing sequence. For example, one can give direct proofs of the existence theorems for "admissible domains" in the sense of Finn-Gerhardt[5] using this observation and the direct variational techniques of Emmer[5]. For parametric variational problems the connection with the comparison principle has to do with the families of surfaces described in Remark 2.5. I am currently investigating this area and believe it will yield existence theorems for parametric capillary surfaces (of the type pictured in Figure 3) depending naturally on the geometry of the fixed bounding walls.

Remark 2.7: Relatively little numerical work has been done computing capillary surfaces. (There has been some[1].) The effective use of comparison surfaces can reduce the amount of computing time needed by giving a priori bounds above and below for the candidate functions (Remark 2.5). This can be especially useful in domains for which the capillary surface behaves in a singular fashion but for which good comparison surfaces can still be constructed, (for example the narrow wedges described in Remark 2.4 and the domains of section 3).

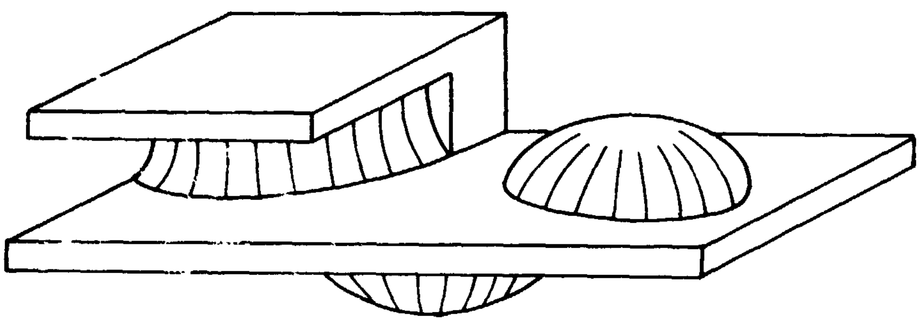

Figure 3: Some capillary surfaces.

Section 3: Re-entrant corner domains

Let θ and γ satisfy

$$\pi < \theta \leq 2\pi, \quad 0 < \gamma < \pi/2 . \tag{6}$$

We will construct a domain for which a bounded solution u to (1), (2) exists, but having a corner of interior angle θ at which there is a jump discontinuity in u. (The arguments can be modified to include the case $\gamma = 0$. If $\gamma = \pi/2$, $u \equiv 0$. All other cases reduce to one of these (3).)

Determine the domain scale by fixing $R > 0$ (Figure 4). Since $\theta > \pi$ we can pick θ_1 and θ_2 satisfying

$$\theta_1 > \pi - \gamma, \quad \pi/2 > \theta_2 > \gamma, \quad \theta_1 + \theta_2 = \theta . \tag{7}$$

For positive ε less than $R\sin\theta_2$, let Ω_ε be a bounded domain, of which the intersection with $B_{3R}(0)$ is shown in Figure 4, and which has C^4 boundary except at P_0 and P_1. $B_{3R}(0)$ is the disc of radius 3R centered at the origin.)

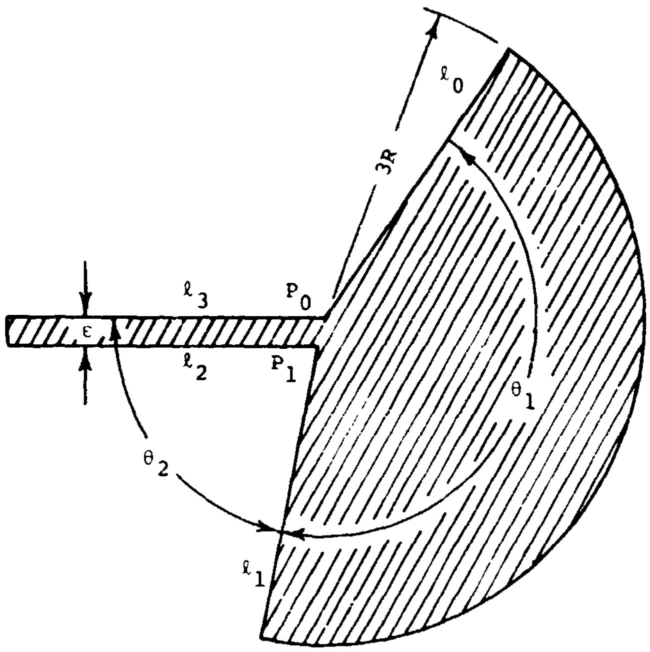

Figure 4: The intersection of Ω_ε with the disc of radius 3R.

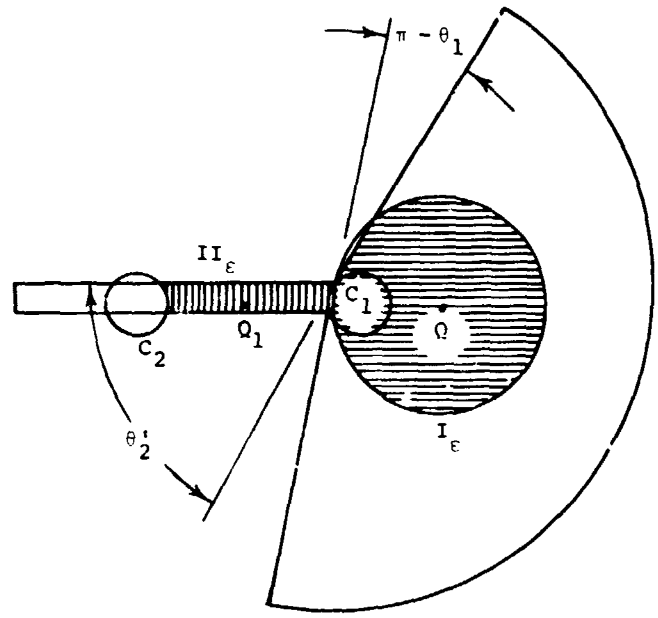

Figure 5: The subdomains I_ε and II_ε. $B_R(Q)$ is tangent to ℓ_1 at P_0. C_1 is the circle through P_0 and P_1 that hits ℓ_3 with angle θ_2'.

<u>Lemma 3.1</u>: There exists a unique solution to (1), (2) in any Ω_ε. It is bounded above, nonnegative, and extends smoothly to the smooth parts of $\partial\Omega_\varepsilon$.

<u>Proof</u>: The existence, regularity and boundedness follow from the references mentioned in section 1. The fact that $u > 0$ follows immediately from the comparison principle (Cor. 2.2), comparing u to $w \equiv 0$ on the entire domain Ω_ε.

We are interested in the behavior of u_ε near P_0, as ε approaches 0. We will show that u_ε stays uniformly bounded in one sector touching P_0 whereas in another it gets uniformly large. It follows that u_ε eventually has a jump discontinuity at P_0.

Let I_ε be the subdomain of Ω_ε shown in Figure 5. Then we have

<u>Lemma 3.2</u>: u_ε is uniformly bounded in I_ε, independently of ε.

<u>Proof</u>: We use the comparison principle, taking $\mathcal{O} = I_\varepsilon$. Our candidate for a supersolution is a function v whose graph is a lower hemisphere lying above $B_R(Q)$. Its contact angle with $B_R \cap \partial\Omega = B_R \cap \ell_0$ is exactly $\pi - \theta_1$. (If a plane slices a sphere the contact angle is the same along the entire circle of contact.) But by (7), $\pi - \theta_1 < \gamma$. Along $\partial B_R(Q) \cap \Omega$ the hemisphere is vertical, $\gamma_v = 0 < \gamma_u$ since u is smooth there. Thus v satisfies the supersolution boundary condition of Cor. 2.2. We must lift the hemisphere high enough to make

$$\operatorname{div} Tv \leq \kappa v \,. \tag{8}$$

But $\operatorname{div} Tv = 2H(S_v) = 2/R$, so (8) is satisfied if

$$v \geq 2/R\kappa \,.$$

This can be accomplished by placing the south pole at height $2/R\kappa$. Since the lower hemisphere varies in height by R, the comparison principle implies

$$u_\varepsilon \leq v \leq 2/R\kappa + R \quad \text{in } I_\varepsilon \,. \tag{9}$$

This estimate is independent of ε. (See Figure 6.) Q.E.D.

Now fix θ_2' with $\gamma < \theta_2' < \theta_2$ and let II_ε be the subregion of Ω_ε as described in Figure 5. Then we have

Lemma 3.3: u_ε approaches ∞ uniformly in II_ε as ε approaches zero.

Proof: We apply the comparison principle with $\mathcal{O} = II_\varepsilon$. Our candidate w for a subsolution is the "underside" of a torus. We take the unique (vertical) torus in $\mathbf{R}^3$ containing C_1 and C_2 (Figure 5). It is generated by rotating C_1 about an axis parallel to the y-axis and going through Q_1, the point midway between C_1 and C_2. Then in II_ε the "underside" $T = S_w$ of the torus is the graph of

$$w(x,y) = [(R - \sqrt{r^2 - (y - y_1)^2})^2 - (x - x_1)^2]^{1/2} ,$$

where $(x_1, y_1) = Q_1$. T contacts $\ell_3 \times R$ with contact angle $\theta_2' > \gamma$ and contacts $\ell_2 \times R$ with contact angle of at least θ_2'. It is vertical along C_1 and C_2 and has contact angle $\gamma_w = \pi > \gamma_u$ (since u is smooth along these arcs). Thus w satisfies the subsolution boundary condition of Cor. 2.2. In order to be a subsolution it must therefore be low enough to satisfy

$$\operatorname{div} Tw \geq \kappa w .$$

But the mean curvature of a torus can be calculated and satisfies

$$\operatorname{div} Tw \geq \frac{1}{r} - \frac{1}{R - r} . \tag{10}$$

So it suffices to satisfy $(\frac{1}{r} - \frac{1}{R - r}) \geq \kappa w$, i.e.

$$w \leq \frac{1}{\kappa} (\frac{1}{r} - \frac{1}{R - r}) . \tag{11}$$

This can be done by placing the highest part of S_w at the height (11). Since the total height of S_w varies by no more than R, we then have

$$w \geq \frac{1}{\kappa} (\frac{1}{r} - \frac{1}{R - r}) - R$$

and by the comparison principle,

$$u_\varepsilon \geq w \geq \frac{1}{\kappa} (\frac{1}{r} - \frac{1}{R - r}) - R \quad \text{in } II_\varepsilon . \tag{12}$$

But r is proportional to ε and R is fixed, so (12) implies that u_ε approaches infinity uniformly in II_ε as ε approaches zero.

Combining Lemmas 3.1-3.3 immediately yields the desired:

Theorem 3.4: For ε sufficiently small the solution u_ε to the capillary problem (1), (2) in Ω_ε cannot be extended continuously to the vertex of the re-entrant corner of angle θ.

One can study the behavior of u_ε near the vertex more carefully. Consider for example the particular case $\theta = 3/2\pi$, $\theta_1 = \pi$, $\theta_2 = \pi/2$. (This is the domain one gets by pushing two vertically held microscope slides close together in a bowl of water.) Since u_ε becomes vertical near P_0 the capillary surface must "look like" the picture in Figure 7: It has essentially no curvature in the vertical direction and its level sets are approximately circular arcs with curvature κz. In fact, one can construct comparison surfaces having exactly that form near P_0 (and then modified slightly near their high and low points to conform to the comparison principle). An easy calculation then implies that the jump in u at P_0 is given by

$$\limsup_{P \to P_0} u_\varepsilon(P) - \liminf_{P \to P_0} u_\varepsilon(P) = \frac{2\cos\gamma}{\varepsilon\kappa} + O(1) \tag{13}$$

as ε approaches zero. For distilled water and air κ is approximately 13 cm^{-2} and between water and glass the contact angle is near zero, so that one should be able to see a jump of about 1 cm. by taking

$$\varepsilon = 2/13 \text{ cm} .$$

This is quite narrow. Experimentally, better success will be obtained by using two fluids of approximately the same density (so that κ is considerably reduced). (Also, for a jump of only 1 cm. the $O(1)$ term in (13) could still play a destructive role.)

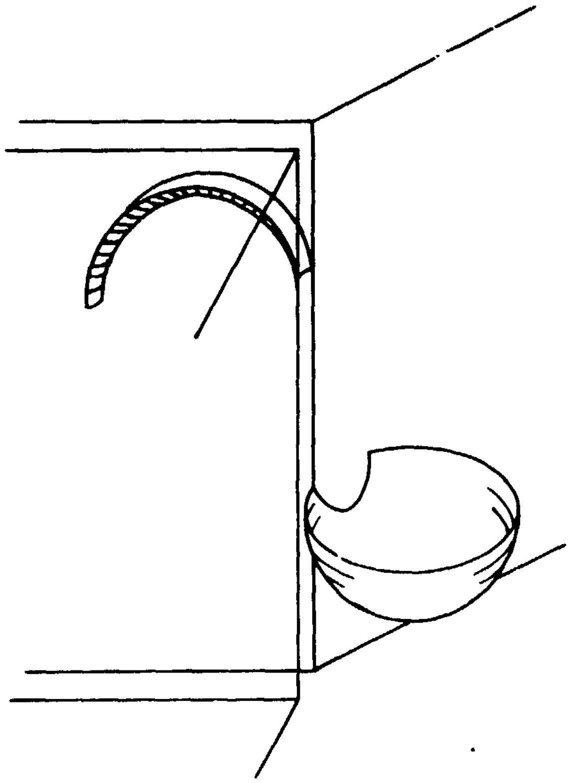

Figure 6: A lower hemisphere contacting $\partial\Omega_\varepsilon \times \mathbf{R}$ with angle less than γ. The "underside" of a torus with angle of contact greater than γ.

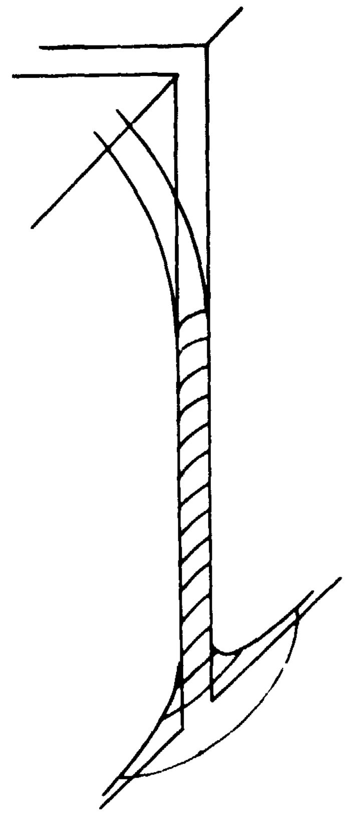

Figure 7: The asymptotic behavior of u_ε. (Here $\theta = \frac{3\pi}{2}$, $\theta_1 = \pi$, $\theta_2 = \pi/2$).

Remark 3.5: What happens in the complimentary case of convex corners? As remarked in section 2, if $\theta < \pi - 2\gamma$ u approaches infinity uniformly. Simon[8] has shown that in the case $\pi - 2\gamma < \theta < 2\pi$ u actually extends to be C^1 at the vertex[8]. Therefore it seems that the only way u can have a jump discontinuity is if there is a re-entrant corner. This is actually correct: u extends continuously to a point on the boundary of a Lipschitz domain if the boundary is locally C^1 or locally convex there[7].

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