Free Boundary Problems with Line Tension

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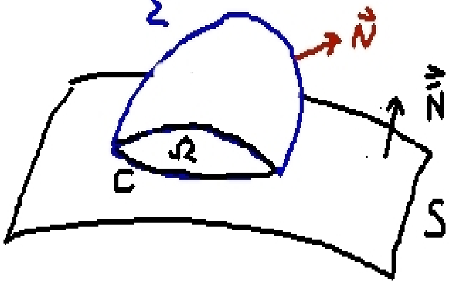
Three phase system e.g. liquid-solid-air.



We will assign an energy to each part of the boundary of the drop.

- $\Sigma \longrightarrow \text{Area of } \Sigma = \mathcal{A}[\Sigma] =$ *free surface energy*.
- $\Omega \longrightarrow \omega\text{Area }(\Omega) = \omega\mathcal{A}[\Omega], \quad \omega \in \mathbf{R}$ *wetting energy*.
- $C \longrightarrow \beta\text{Length}[C] = \beta\mathcal{L}[C], \ \beta \in \mathbf{R},$ *line tension*.

Total energy $= E = \mathcal{A}[\Sigma] + \omega\mathcal{A}[\Omega] + \beta\mathcal{L}[C]$.

Josiah Gibbs introduced the concept of line tension ($\approx$ 1878) as an excess energy assigned to the line common to the three phases.

The definition is analogous to the definition of surface tension with one important difference, line tension be either positive or negative.

Line tension only significantly affects the shape of the drop at a very small scale.

First variation

Admissible variations preserve volume and maintain $\partial\Sigma$ on the supporting surface S.

$$\mathbf{X}_\epsilon = \mathbf{X} + \delta\mathbf{X} + \mathcal{O}(\epsilon^2)\,, \quad \delta\mathbf{X}|_{\partial\Sigma} \cdot \bar{\mathbf{N}} \equiv 0\,.$$

$$\delta E = -\int_\Sigma 2H\psi\, d\Sigma + \oint_{\partial\Sigma} [\bar{\mathbf{N}} \cdot \mathbf{N} + \beta \bar{k}_g - \omega]\, \frac{d\mathbf{X}}{ds} \times \bar{\mathbf{N}} \cdot \delta\mathbf{X}\, ds\,,$$

where

$\bar{\mathbf{N}}$=normal to S.

$\mathbf{N}$ = unit normal to Σ

$\psi = \delta\mathbf{X} \cdot \mathbf{N}$

H = mean curvature of Σ

$\bar{k}_g$ = geodesic curvature of $\partial\Sigma$ in S.

Conditions for equilibrium

$H \equiv$ constant on Σ

$\bar{\mathbf{N}} \cdot \mathbf{N} = -\beta \bar{k}_g + \omega$, on $\partial\Sigma$.

For axially symmetric surfaces in a half space, the boundary condition reduces to

$$\nu \cdot (\pm E_3) = \omega + \frac{\beta}{r} \,,$$

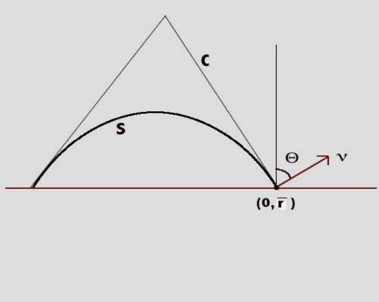
on each energy component.

Drops embedded in a slab having free boundary on the planes and with positive line tension are axially symmetric, so they are either spherical caps (sessile drops) or parts of Delaunay surfaces (Koiso-P 2012).

All sessile drops are in equilibrium for a one parameter family of functionals.
Delaunay bridges are in equilibrium for a two parameter family of energy functionals.

Drops with negative line tension are unstable. The sessile drops with negative line tension minimize the total energy in comparison to *axially symmetric surfaces* enclosing the same volume. (Widom)

This means that destabilizing variations cannot be axially symmetric. If these variations are resolved into Fourier series, their wavelengths may fall below a scale at which the energy model is valid.(Guzzardi)
Therefore drops with negative line tension might physically exist (as Gibbs predicted) in spite of their mathematical instability.



Theorem

(Koiso-P. 2012) Let $S \subset S^2(R)$ be a sessile drop with $\beta \geq 0$.

Then, S is stable if and only if

$$\beta \leq \frac{3V_C V}{\pi R\bar{r}(V_C - \mathrm{sgn}(\nu_3)V)} =: B\,. \qquad (1)$$

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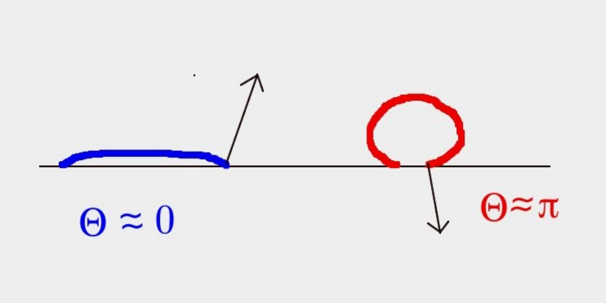
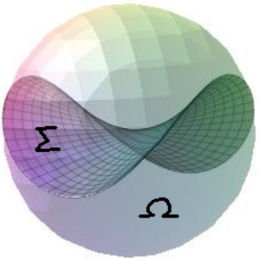


$$\mathcal{E} := \mathcal{A}[\Sigma] + \omega \cdot \mathcal{A}[\Omega] + \beta \cdot \mathcal{L}$$

$\Theta \approx 0$	$\Theta \approx \pi$
$\mathcal{A}[\Omega] >> \mathcal{L}$	$\mathcal{L} >> \mathcal{A}[\Omega]$
$\nu \cdot (-E_3) = \omega + \dfrac{\beta}{r} \approx -1$	$\nu \cdot (-E_3) = \omega + \dfrac{\beta}{r} \approx 1$
wetting transition	drying transition

Spherically confined drop



$$H \equiv \text{constant on } \Sigma$$

$$\mathbf{X} \cdot \mathbf{N} = -\beta \bar{k}_g + \omega \text{ , on } \partial\Sigma.$$

Partial examples, i.e. constant mean curvature surfaces having a boundary arc on the sphere where the boundary condition holds, can be produced using Bjorling's Formula. Let $\mathbf{C} : I \to S^2$ be curve which is real analytic in its arc length parametrization such that its geodesic curvature satisfies $|-\beta \bar{k}_g + \omega| < 1$ for constants ω, β. We also use $\bar{k}_g$ to denote the analytic extension of the geodesic curvature to a neighborhood of I in the complex plane. Then

$$\begin{aligned} \mathbf{X}(z = u + iv) \quad := \quad & \mathrm{Re}\biggl(\mathbf{C}(z) - i \int_{z_0}^{z} (\omega - \beta \bar{k}_g) \mathbf{C}(\zeta) \times \mathbf{C}'(\zeta) \\ & + \sqrt{1 - (\beta \bar{k}_g - \omega)^2} \mathbf{C}(\zeta)\, d\zeta \biggr) . \end{aligned}$$

Theorem

Let $X : (\Sigma, \partial\Sigma) \to (B^3, S^2)$ be a C^2 immersed equilibrium drop where Σ is the unit disc in $\mathbf{R}^2$. Then, if the surface is stable, $X(\Sigma)$ is a spherical cap or a flat disc.

We have not classified the the stable discs and caps. This is a straightforward and somewhat tedious task owing Fourier analysis. The result depends on the values of ω and τ.

We do not know if the interior or boundary regularity holds a priori.

Nitsche considered the free boundary problem with neutral wetting and line tension, ($\omega = \beta = 0$), and gave a beautiful complex analytic argument to show that the only equilibrium disc type solutions, stable or otherwise, are spherical caps and flat discs.

Ros and Souam extended this result to drops with wetting energy but no line tension ($\omega \neq 0$, $\beta = 0$).

Second variation $\Sigma \subset B^3$

$$\delta^2 E = -\int_\Sigma \psi L[\psi]\, d\Sigma + \oint_{\partial\Sigma} \psi B[\psi]\, ds\,. \qquad (2)$$

$$L = \Delta + (4H^2 - 2K)\,,$$

$$B[\psi] = \nabla\psi\cdot\mathbf{n} - \left(\frac{1}{\sin\alpha} - \cot\alpha\, d\mathbf{N}(\mathbf{n})\cdot\mathbf{n}\right)\psi - \frac{\beta}{\sin\alpha}\left(\left(\frac{\psi}{\sin\alpha}\right)_{ss} + \frac{\psi}{\sin\alpha}\right).$$

Here, $\mathbf{X}\cdot\mathbf{n} =: \sin\alpha = 0$. Wherever $\sin\alpha = 0$, $\psi/\sin\alpha$ must be replaced by $-\delta\mathbf{X}\cdot\mathbf{n}$

The second variation formula naturally extends to

$$\mathcal{K} := \{\psi \in H^1(\Sigma) \mid \tilde{\psi} := \psi / \sin\alpha \in H^1(\partial\Sigma)\} .$$

as

$$\begin{aligned} \delta^2 E &= \int_\Sigma |\nabla\psi|^2 - |d\mathbf{N}|^2 \psi^2 \, d\Sigma \\ &\quad + \oint_{\partial\Sigma} \beta[(\tilde{\psi}_s)^2 - \tilde{\psi}^2] - \psi^2 [\csc\alpha - \cot(\alpha) II(\mathbf{n}, \mathbf{n})] \, ds . \end{aligned}$$

An equilibrium surface will be called stable if $\delta^2 E \geq 0$ holds for all $\psi \in \mathcal{K}$ such that

$$\int_\Sigma \psi \, d\Sigma = 0 .$$

Diagonalizing the second variation leads to a spectral problem of the form

$$(L + \lambda)\psi = 0, \text{ on } \Sigma\,, B[\psi] = 0 \text{ on } \partial\Sigma\,.$$

The second condition is a type of Wentzell boundary condition, has been widely studied.

$$\mathbf{R}^3 \longrightarrow s0(3)\,, \quad \mathbf{c} \longrightarrow \ \mathbf{c} \times \cdot\,,$$

$$\psi_{\mathbf{c}} := \partial_\epsilon(\exp(\epsilon[\mathbf{c} \times \cdot])X))_{\epsilon=0} \cdot \mathbf{N} = \mathbf{c} \times \mathbf{X} \cdot \mathbf{N}$$

$$L[\psi_{\mathbf{c}}] = 0 \text{ on } \Sigma, \quad B[\psi_{\mathbf{c}}] \equiv 0 \text{ on } \partial\Sigma\,.$$

On $\partial\Sigma$, there holds

$$\begin{aligned} \psi_{\mathbf{c}} &= \mathbf{c} \times \mathbf{X} \cdot \mathbf{N} = -\mathbf{N} \times \mathbf{X} \cdot \mathbf{c} = -(\mathbf{X} \cdot \mathbf{n})\mathbf{N} \times \mathbf{n} \cdot \mathbf{c} \\ &= -(\mathbf{X} \cdot \mathbf{n})\mathbf{X}' \cdot \mathbf{c} \\ &= -(\mathbf{X} \cdot \mathbf{n}/|\mathbf{X}_\theta|)\mathbf{X}_\theta \cdot \mathbf{c} \end{aligned}$$

Lemma

If there exists an arc $\gamma \subset \partial\Sigma$ on which $\psi_{\mathbf{c}} \equiv 0$ holds for some vector $\mathbf{c} \neq \mathbf{0}$ holds, then $\psi_{\mathbf{c}} \equiv 0$ holds and the surface is axially symmetric.

If either $\mathbf{X}_\theta \cdot \mathbf{c} \equiv 0$ or $\mathbf{X}\cdot\mathbf{n} \equiv 0$ holds on an arc in $\partial\Sigma$, then the arc is circular and the boundary condition can be used to show that $\psi_{\mathbf{c}} \equiv 0 \equiv \partial_{\mathbf{n}}\psi_{\mathbf{c}}$ which implies that $\psi_{\mathbf{c}} \equiv 0$ on Σ and Σ is axially symmetric.

We will show that if we assume the surface is not axially symmetric, then there always exists a $\mathbf{c} \in (\mathbf{R}^3)^*$ such that the function $\psi_{\mathbf{c}}$ has, at least, four sign changes on $\partial\Sigma$.

$$\oint_{\partial\Sigma} \mathbf{X}_\theta \cdot \mathbf{c}\, d\theta = \oint_{\partial\Sigma} (\mathbf{X} \cdot \mathbf{c})_\theta\, d\theta = 0$$

Define:

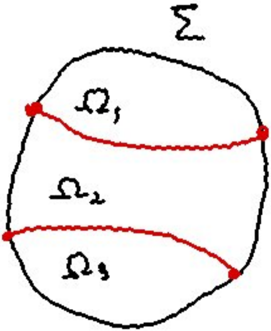
$$\oint_{\partial\Sigma} \mathbf{X}_\theta e^{i\theta}\, d\theta =: \mathbf{A} + i\mathbf{B} \in \mathbf{C}^3 \,.$$

Thus, there exists $\mathbf{c} \in \mathbf{R}^3$, $\mathbf{c} \neq \mathbf{0}$ with $0 = \mathbf{c} \cdot \mathbf{A} = \mathbf{c} \cdot \mathbf{B}$. It then follows that for this $\mathbf{c}$ the function $\mathbf{X}_\theta \cdot \mathbf{c}$ can be represented as a Fourier series of the form

$$\mathbf{X}_\theta \cdot \mathbf{c} = \sum_{j \geq 2} (a_j \cos(j\theta) + b_j \sin(j\theta)) \,.$$

This function can be interpreted as the boundary values of the real part of the complex analytic function

$$F(z) := \sum_{j \geq 2} (a_j - i b_j) z^j = z^2 (\text{analytic function}) \,.$$



$U = \Omega_1 \cup \Omega_2, \ V = \Sigma \setminus U$

Define $\mathcal{F}$ to be the set of all functions f on $\bar{U}$ satisfying the following conditions:

- f is piecewise C^1 on $\bar{U}$,
- $f/\mathbf{X}\cdot\mathbf{n}$ is piecewise C^1 on $\partial\Sigma$
- $f\equiv 0$ on $\partial U\setminus\partial\Sigma$.

Note that $\psi_c\chi_U\in\mathcal{F}$. Also, since $(\mathbf{X}\cdot\mathbf{N})^2+(\mathbf{X}\cdot\mathbf{n})^2\equiv 1$ on $\partial\Sigma$, $\mathcal{F}$ contains all functions vanishing identically on V which are of the form $v(1-(\mathbf{X}\cdot\mathbf{N})^2)$ near $\partial U\cap\partial\Sigma$, where v is smooth function. In particular, this includes $C_c^\infty(U)$. Define

$$\begin{aligned}\mu_1 \;=\; & \inf_{\mathcal{F}}\Big(\int_U |\nabla f|^2-(4H^2-2K)f^2\,d\Sigma \\ & -\int_{\partial\Sigma\cap\partial U}\big(\frac{1}{\sin\alpha}-\cot\alpha\,d\mathbf{N}(\mathbf{n})\cdot\mathbf{n}\big)f^2\,ds \\ & +\beta\int_{\partial\Sigma\cap\partial U}\hat{f}_s^2-\hat{f}^2\,ds\Big)\Big/\int_U f^2\,d\Sigma\,.\end{aligned}$$

By using the function $\psi_{\mathbf{c}}|_U$, we get that $\mu_1\leq 0$ holds.

If $\mu_1 = 0$, then

$$\psi^* := \begin{cases} \psi_{\mathbf{c}}, \ p \in \Omega_1 \\ 0, \ p \in \Sigma \setminus \Omega_1 \end{cases},$$

realizes the infimum μ_1. Taking the first variation of the functional, we get that ψ^* is a weak solution of $L = 0$ in Σ. This contradicts elliptic regularity and unique continuation property, so $\mu_1 < 0$ must hold.

Let $f \in \mathcal{F}$ which makes the quotient negative and let

$$\psi_2 := \begin{cases} \psi_{\mathbf{c}}, \ p \in \Omega_3 \\ 0, \ p \in U \end{cases}.$$

There is a superposition $\phi := f + a\psi_2$ with

$$\int_\Sigma \phi \, d\Sigma = 0$$

making the quotient negative.

Let w solve $\Delta^2 w = 0$ in Σ with $w \equiv 0$ on $\partial\Sigma$ and $\partial_{\mathbf{n}} w = -\phi/\mathbf{X} \cdot \mathbf{n}$ on $\partial\Sigma$. Define the variation

$$\delta \mathbf{X} = \nabla w + \phi \mathbf{N} \, ,$$

then on $\partial\Sigma$

$$\mathbf{X} \cdot \delta \mathbf{X} = \mathbf{X} \cdot \mathbf{n} \left(\frac{-\phi}{\mathbf{X} \cdot \mathbf{n}} \right) + \phi = 0 \, .$$

THANK YOU !