Equilibrium shapes for anisotropic surface energies

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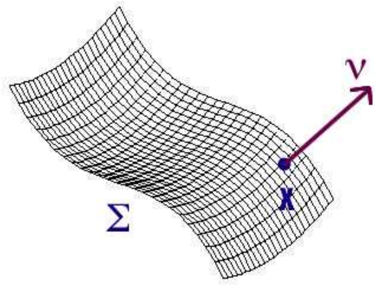
An anisotropic surface energy assigns to a surface a value which depends on the direction of the surface at each point. e.g.

$$\mathcal{F} = \int_\Sigma \gamma(\nu)\, d\Sigma \,,$$

.



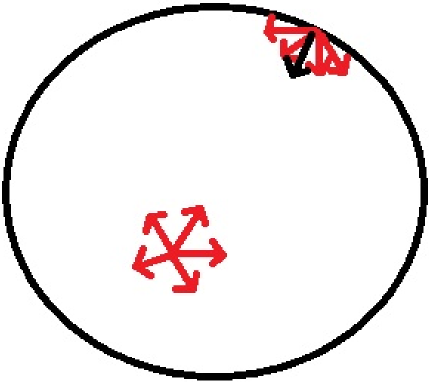
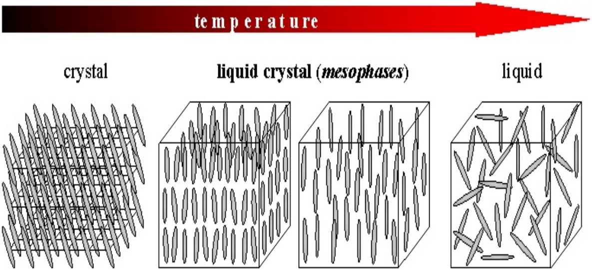


Figure: Small liquid drop

thermotropic liquid crystals



• 3-D lattice	• 1- (2-)D lattice	• no lattice	• no lattice
• orientation	• orientation	• orientation	• no orientation
• solid	• fluid	• fluid	• fluid
↳ ***anisotropic***	↳ ***anisotropic***	↳ ***anisotropic***	↳ ***isotropic***

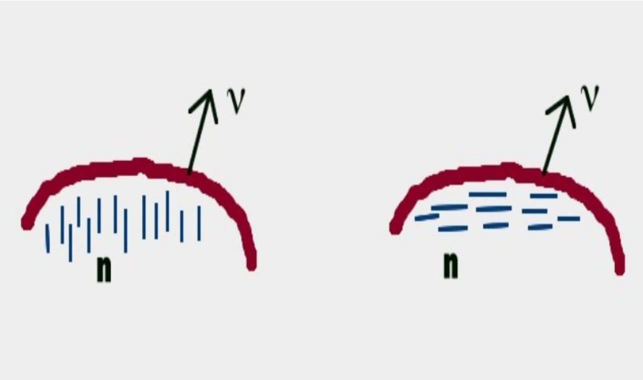


Figure: NLC with homogeneously aligned director field

$$\gamma = 1 + a(\nu \cdot n)^2 \ , \quad a > 0$$

$$\mathcal{F} = \int_\Sigma \gamma(\nu) \, d\Sigma \, .$$

First variation

$$\text{Gibbs free energy} = \mathcal{F} = \int_\Sigma \gamma(\nu)\, d\Sigma$$

Variation: $X_\epsilon = X + \epsilon(\delta X) + \ldots$

First variation

$$\delta\mathcal{F} = -\int_\Sigma \Lambda\, \delta X \cdot \nu\, d\Sigma + \text{boundary terms}$$

Λ = anisotropic mean curvature.

$$\delta\,\text{Volume} = \int_\Sigma \delta X \cdot \nu\, d\Sigma\,,$$

therefore $\Lambda \equiv$ constant characterizes critical points of $\mathcal{F}$ subject to a volume constraint.

Calculation of the anisotropic mean curvature :

Homogeneously extend the energy density:

$$\tilde{\gamma}(Y) := |Y|\gamma(\frac{Y}{|Y|})$$

Cahn-Hoffman field:

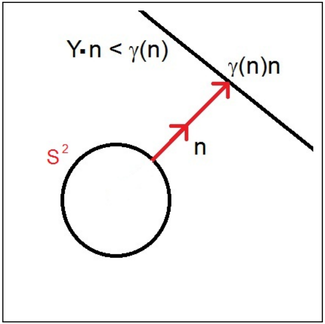
$$\xi(\nu(p)) := \nabla\tilde{\gamma}(\nu(p)) \, .$$

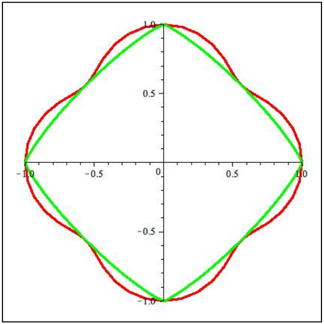
Anisotropic mean curvature:

$$\Lambda_p = -\mathrm{Div}\xi_{\nu(p)} \, .$$

Wulff Construction

$$\text{Wulff shape} = W = \partial \bigcap_{n \in S^2} \{Y \cdot n \leq \gamma(n)\}$$





We will assume a *convexity condition:*

W is a smooth, convex surface.($K_W > 0$)

Wulff's Theorem

(Dinghas, Liebmann, Herring, Chandrasekhar, Taylor, Brothers-Morgan, Fonseca..)

The Wulff shape W is the unique minimizer of the free energy $\mathcal{F}$ among all closed surfaces enclosing the same volume as W.

This is a generalization of the isoperimetric property of spheres

In particular, W has constant anisotropic mean curvature $\Lambda\,(=-2)$.

Generalized Barbosa-doCarmo Theorem (P.1997). *The only closed, stable surfaces with constant anisotropic mean curvature are rescalings of the Wulff shape*.

Generalized Alexandroff Theorem (Ge, He, Li, Ma .2009) *The only embedded closed surfaces with $\Lambda \equiv$constant are rescalings of the Wulff shape.*

Generalized Hopf Theorem (Koiso, P, 2009). *The only immersed topological spheres with $\Lambda \equiv$constant are rescalings of the Wulff shape.*

Variation of the anisotropic mean curvature

$$X_\epsilon = X + \epsilon(\delta X) + \dots.$$

$$\delta X = \psi\nu + T$$

$\delta\Lambda = J[\psi] + \nabla\Lambda \cdot T$ where

$$J[\psi] = \mathrm{Div}_\Sigma[(D^2\gamma + \gamma I)\nabla\psi] + \langle (D^2\gamma + \gamma I) \cdot d\nu, d\nu\rangle\psi\ ,$$

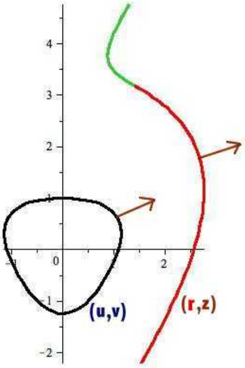
Because of the convexity condition, the operator J is elliptic for any sufficiently smooth surface. This implies that the equation for constant, or more generally prescribed, anisotropic mean curvature has a Maximum Principle.

Examples of surfaces with constant anisotropic mean curvature.

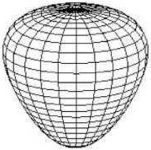
Axially symmetric surfaces with constant anisotropic mean curvature will be called anisotropic Delaunay surfaces. From Noether's Theorem:

$$(*)\ 2ur + \Lambda r^2 = c\,, \quad z = \int_0^v r_u\, dv\,. \quad c = \text{'flux parameter'}.$$

(r, z) = generating curve of Σ, (u, v) = generating curve of W

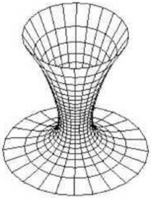


Wulff shape



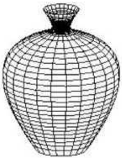
$\Lambda=-2,\ c=0$

anisotropic catenoid



$\Lambda=0,\ c<0$

anisotropic unduloid

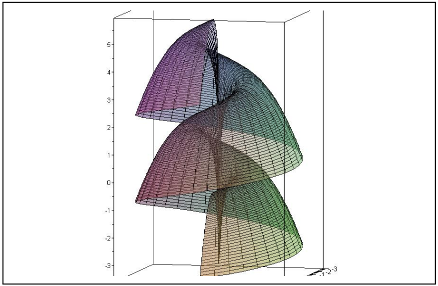


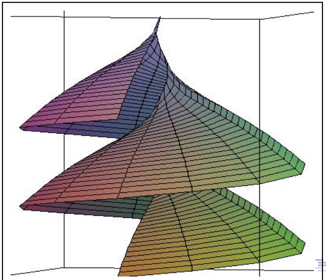
$\Lambda<0, c>0$

anisotropic nodoid

$\Lambda<0,\ c<0$

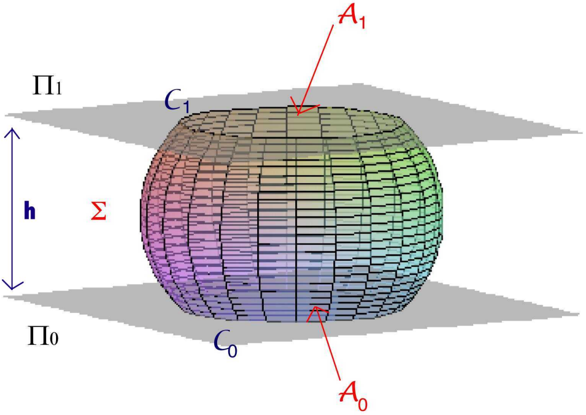
This construction can be generalized to produce helicoidal surfaces with constant anisotropic mean curvature. (Joint work with Chad Kuhns)





Free boundary problem

Fixed volume of material trapped between two horizontal planes.



Consider the volume as the body of a physical drop. We will assign an energy to each part of the boundary of the drop.

- $\Sigma \longrightarrow \mathcal{F}[\Sigma] = \int_\Sigma \gamma(\nu)\, d\Sigma$.

- $\mathcal{A}_i \longrightarrow \omega_i \cdot \text{Area}\,(\mathcal{A}_i)$ where ω_i are constants. This is called the *wetting energy*. $\omega_i > 0$ is called lyophobic wetting, $\omega_i < 0$ is called lyophilic wetting.

- $C_i \longrightarrow \tau_i \mathcal{L}[C_i]$ where τ_i are constants and $\mathcal{L}$ is a one dimensional anisotropic energy. This term is called the *line tension*.

The total energy is:

$$\mathcal{E} := \mathcal{F} + \omega \cdot \mathcal{A} + \tau \cdot \mathcal{L}\,, \;\; \omega, \tau \in \mathbf{R}^2 \,.$$

Here: $\omega \cdot \mathcal{A} = \omega_0 \mathcal{A}_0 + \omega_1 \mathcal{A}_1$, $\tau \cdot \mathcal{L} = \tau_0 \mathcal{L}_0 + \tau_1 \mathcal{L}_1$.

First assume $\gamma = \gamma(\nu_3)$, (or equivalently W is axially symmetric), and $\mathcal{L}[C_i] =$Length$[C_i]$. The equilibrium conditions for the free boundary problem are:

$$\delta\mathcal{E} = 0 \iff \begin{array}{l} \Lambda \equiv \text{constant on } \Sigma \\ \xi \cdot E_3 = (-1)^{i+1}(\omega_i + \tau_i \kappa) \text{ on } C_i \,, \; i = 0, 1 \,. \end{array}$$

Using the Maximum Principle, one obtains:

If $\tau_i \leq 0$ holds, all equilibrium surfaces are parts of anisotropic Delaunay surfaces.
Conversely, any part of an anisotropic Delaunay surface between two horizontal planes is in equilibrium for a two parameter continuum of energy functionals $\mathcal{E}$.

Basic problem: If the volume V, the plane separation h and the constants $\omega = (\omega_0, \omega_1)$, $\tau = (\tau_0, \tau_1)$ are specified, can we determine the equilibrium surface?

There are examples of equilibrium unduloids having the same volumes.

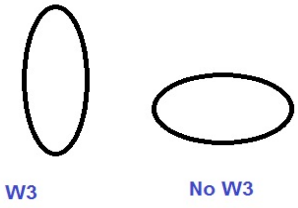
We will see that of we require that the equilibrium surfaces are stable, then in some cases we can predict the surface that will form.

Let W be the Wulff shape for the functional. We will be assumed the following conditions on W:

(W1) W is a uniformly convex surface of revolution with vertical rotation axis.

(W2) W is symmetric with respect to reflection through the horizontal plane $z = 0$.

(W3) The generating curve of W has non-decreasing curvature (with respect to the inward pointing normal) as a function of arc length on $\{z \geq 0\}$ as one moves in an upward direction.



Theorem

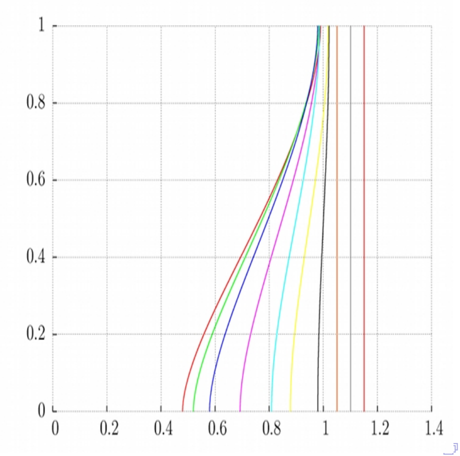
Assume $\omega = \tau = (0,0)$. If Σ is an equilibrium surface with free boundary on two horizontal planes for the functional $\mathcal{F}$ and with the Wulff shape for the functional satisfying the conditions (W1) through (W3) stated above, then Σ is stable if and only if the surface is either homothetic to a half of the Wulff shape or a cylinder which is perpendicular to the boundary planes which satisfies

$$\frac{\mu_1(0)}{\mu_2(0)}\, h^2 \leq (\pi R)^2 \, .$$

μ_i are the principal curvatures of W along its equator.

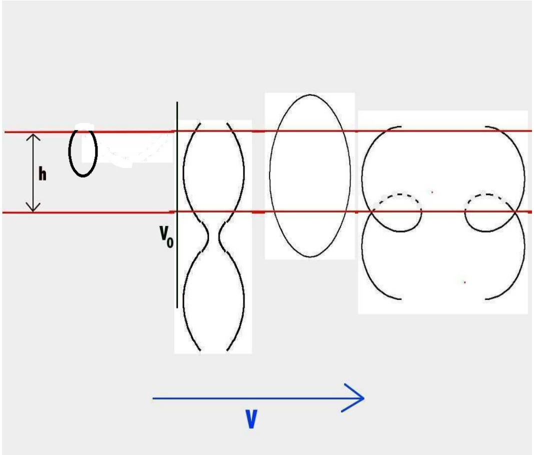
Experiments for this configuration of LC's were done by Charles Rosenblatt

Without the curvature condition (W3), anisotropic unduloids may form for some small values of the volume. Below are results of simulation using $\gamma = 1 - 0.45\nu_3^2$. (joint work with Josu Arroyo)

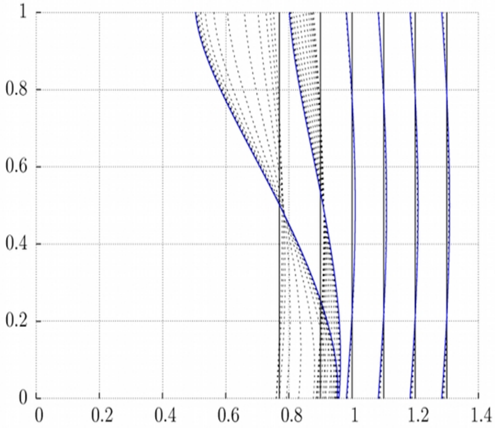


Lyophobic wetting

In the case $\omega_0 = \omega_1 > 0$ and the curvature condition(W3) holds, we have the following:



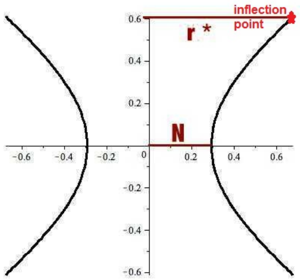
Lyophobic wetting-without (W3)



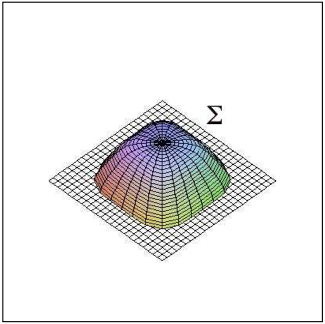
Lyophilic wetting $\omega_0 = \omega_1 < 0$, $\tau = 0$

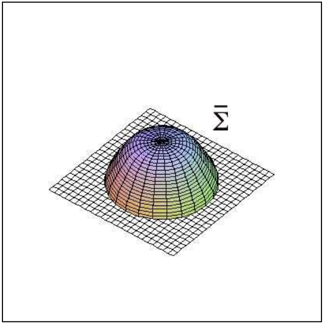
An anisotropic unduloid (with lyophilic wetting) is stable if it is ‘close to being a cylinder".

If the neck size N satisfies $\sqrt{3}N \geq r^*$, where r^* is the radius of the circle at an inflection point, then for any T, with $0 \leq T \leq -\omega$, the part of the unduloid with $T \leq v \leq -T$ is stable.



A sessile drop Σ is an equilibrium surface with one boundary component which is part of a rescaling of W, i. e. $\Sigma \subset RW$.



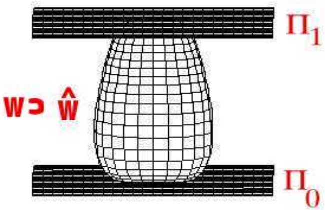


Negative line tension

- Liquid sessile drops with negative line tension are stable for rotationally symmetric variations. (Widom).
- Liquid sessile drops with negative line tension are always unstable.(Widom)

Guzardi et. al. [1] explains that instability need not rule out physical existence of liquid sessile drops since the wavelengths of destabilizing variations may fall below the scale where the surface energy model is valid.

$\tau_i < 0$



Theorem

Assume that $\omega = (\omega_0, \omega_1)$ *and* $\tau = (\tau_0, \tau_1)$*, with* $\tau_i < 0$ *are chosen so that* $\hat{W}$ *is in equilibrium. Then,* $\hat{W}$ *is the absolute minimizer of the energy*

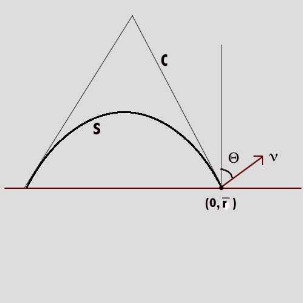
$$\mathcal{E} = \mathcal{F} + \omega \cdot \mathcal{A} + \tau \cdot \mathcal{L} \, ,$$

among all <u>*axially symmetric surfaces*</u> *enclosing the same volume and having free boundary on the two planes.*

However, if $\tau_i < 0$ holds for some $i = 0, 1$, then any equilibrium surface, including $\hat{W}$ is unstable.

When the line tension is non positive, the only equilibrium surfaces are anisotropic Delaunay surfaces. This follows from the Maximum Principle.

If $\tau_i \geq 0$ holds, Schwarz symmetrization implies that any energy minimizer is an anisotropic Delaunay surface.



Theorem

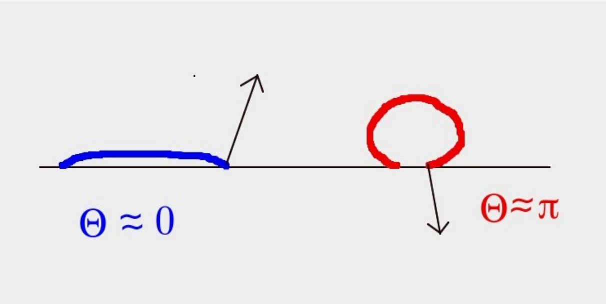
Let W be a rotationally symmetric Wulff shape which is symmetric with respect to the plane $z = 0$ and let $S \subset RW$ be a sessile drop with $\tau \geq 0$.

Then, S is stable if and only if

$$\tau \leq \frac{3V_C V}{\pi R\bar{r}(V_C - \mathrm{sgn}(\nu_3)V)} \,. \tag{1}$$

.

Loss of stability in limiting cases



$$\mathcal{E} := \mathcal{F} + \omega \cdot \mathcal{A} + \tau \cdot \mathcal{L}$$

	$\Theta \approx 0$	$\Theta \approx \pi$
	$\mathcal{A} >> \mathcal{L}$	$\mathcal{L} >> \mathcal{A}$
∂ condition :	$\omega + \frac{\tau}{r} \approx -1$	$\omega + \frac{\tau}{r} \approx 1$
	wetting transition	drying transition

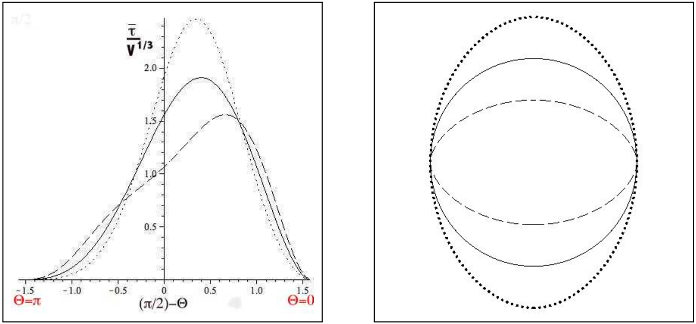


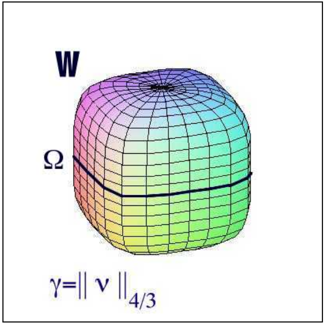
Figure: Plot of $\bar{\tau}/\mathrm{vol}^{1/3}$ for Wulff shapes with energy density $\gamma = 1 + e\nu_3^2$. dotted $\leftrightarrow$ $e = 0.4$, solid $\leftrightarrow$ $e = 0$, dashed $\leftrightarrow$ $e = -0.4$. The Wulff shapes are shown on the right.

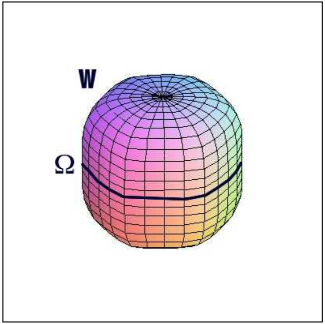
More general functionals

We now consider a functional with Wulff shape W of *product form*:

$$\xi(\sigma, \tau) = (u(\sigma)[\alpha(t), \beta(t)], v(\sigma)) \quad 0 \leq \sigma \leq \bar{\sigma}\,, 0 \leq t \leq \bar{t}\,.$$

It is assumed that (u, v) and (α, β) are smooth, convex, closed curves. The curve parameterized by (α, β) will be denoted by Ω.





The anisotropic line tension given by the one dimensional anisotropic energy whose Wulff shape is the curve Ω given by (α, β). To do this we define:

$$\mathcal{L}_\Omega[C] = \int_C \Gamma[N]\, dL\,,$$

Here N is the unit normal to the curve C.
With this definition and appropriate constants (ω_i, τ_i), the parts of the Wulff shape between horizontal planes are still in equilibrium when the line tension is included in the total energy:

$$\mathcal{E} := \mathcal{F} + \omega \cdot \mathcal{A} + \tau \cdot \mathcal{L}_\Omega\,, \;\; \omega, \tau \in \mathbf{R}^2\,.$$

Here: $\omega \cdot \mathcal{A} = \omega_0 \mathcal{A}_0 + \omega_1 \mathcal{A}_1$, etc.

Equilibrium conditions

Define $\tilde{\kappa} = \kappa_C / \kappa_\Omega$ anisotropic curvature of C_i,

$$\delta \mathcal{L}_\Omega := \int_C \tilde{\kappa} \, \delta C \cdot N \, ds$$

Critical points of $\mathcal{E}$ are characterized by:

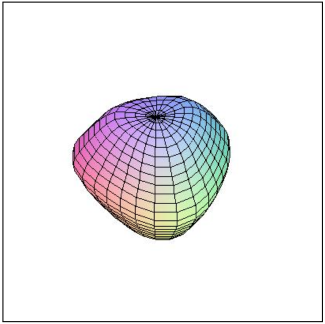
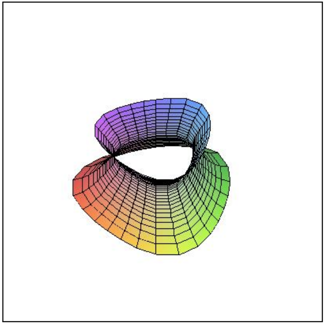
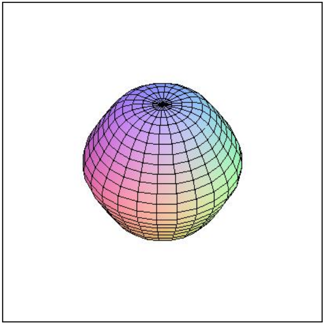
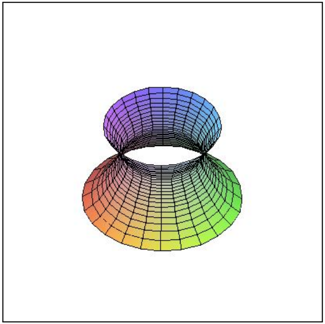
$$(*) \quad \Lambda \equiv \text{contant} \, , \; in \; \Sigma \, ,$$

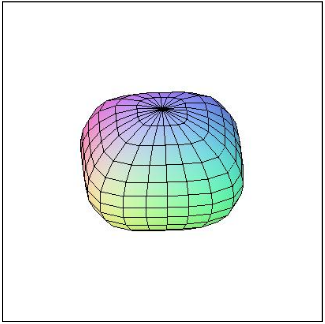
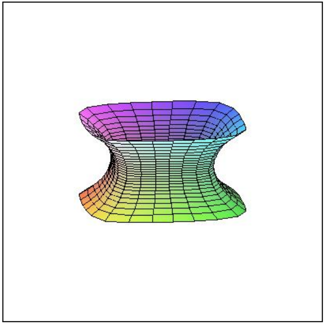
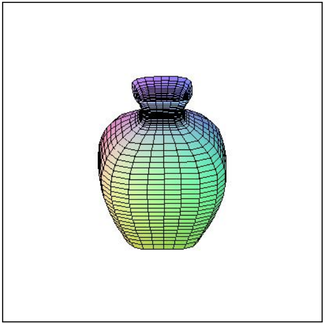
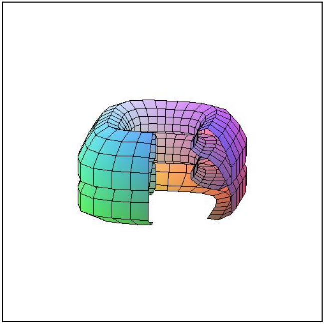
$$(**) \qquad E_3 + (-1)^i (\omega_i + \tau_i \tilde{\kappa}) \equiv 0 \qquad \text{on} \quad C_i, \; i = 0, 1$$

The construction of anisotropic Delaunay surfaces generalizes easily to this case:

$$\xi = \left(u(\sigma) \begin{pmatrix} \cos(\tau) \\ sin(\tau) \end{pmatrix}, v(\sigma) \right) \longrightarrow \left(u(\sigma) \begin{pmatrix} \alpha(\tau) \\ \beta(\tau) \end{pmatrix}, v(\sigma) \right)$$

$$X = \left(r(s) \begin{pmatrix} \cos(\tau) \\ sin(\tau) \end{pmatrix}, z(s) \right) \longrightarrow \left(r(s) \begin{pmatrix} \alpha(\tau) \\ \beta(\tau) \end{pmatrix}, z(s) \right)$$

For a Delaunay surface, the equilibrium boundary condition becomes

$$\xi \cdot E_3 + (-1)^i(\omega_i + \tau_i/r_i) = 0 \ , \ \text{on } C_i \ .$$

where r_i are the 'radii' of the boundary curves. Note that there is a whole continuum of pairs (ω_i, τ_i), with

$$(\sharp) \qquad \omega_i + \tau_i/r_i =: \omega_i^* \ .$$

for which the surface is in equilibrium.

Note that if we cut *any* Delaunay surface by two horizontal planes, we can always define

$$\omega_i^* := \xi|_{C_i} \cdot E_3 \ ,$$

then surface $\hat{\Sigma}$ is an equilibrium for $\mathcal{E} = \mathcal{F} + \omega \cdot \mathcal{A} + \tau \cdot \mathcal{L}_\Omega$ whenever (ω_i, τ_i) satisfy ($\sharp$).

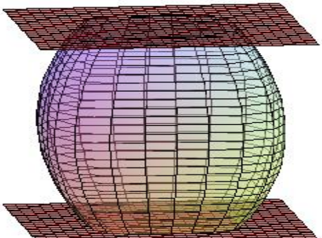
Theorem

Assume that $\omega = (\omega_0, \omega_1)$ *and* $\tau = (\tau_0, \tau_1)$*, with* $\tau_i < 0$ *are chosen so that* $\hat{W}$ *is in equilibrium. Then,* $\hat{W}$ *is the absolute minimizer of the energy*

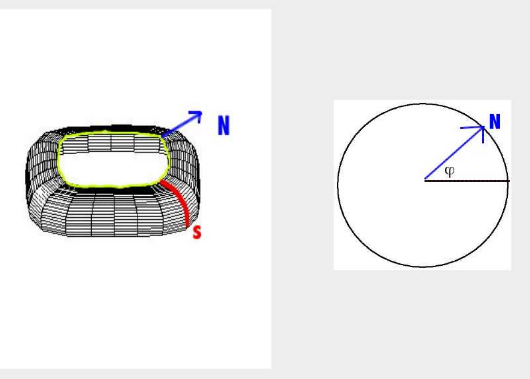
$$\mathcal{E} = \mathcal{F} + \omega \cdot \mathcal{A} + \tau \cdot \mathcal{L}_\Omega \,,$$

among all symmetric surfaces enclosing the same volume and having free boundary on the two planes.

(Here, symmetric surface means a surface whose cross sections are all homothetic to Ω.)



$\tau < 0$



$$\delta X \cdot \nu \, d\Sigma = f(s) \sin(M\varphi) \, ds d\phi \, ,$$

$$\text{For instability}: \quad M \approx A_1 + \frac{A_2}{\sqrt{s}} \, ,$$

where A_1, A_2 depend on the local geometry.

Schwarz symmetrization

Let S be an embedded surface . Define the 'symmetrized' surface $\tilde{S}$ by replacing each cross section $z =$ constant of S by the curve homothetic to Ω which encloses the same area. Then the volume within the surface is preserved and the free energy plus wetting energy is diminished:

$$(\mathcal{F} + \omega \cdot \mathcal{A})[\tilde{S}] \leq (\mathcal{F} + \omega \cdot \mathcal{A})[S] \, .$$

In addition, if $\tau_i \geq 0$ holds, then

$$(\mathcal{F} + \omega \cdot \mathcal{A} + \tau \cdot \mathcal{L})[\tilde{S}] \leq (\mathcal{F} + \omega \cdot \mathcal{A} + \tau \cdot \mathcal{L})[S] \, .$$

Let Σ be an equilibrium Delaunay surface and assume that $\tau_i \geq 0$, $i = 0, 1$ holds. Then, Σ is stable if and only if it is stable with respect to symmetric variations.

Let $X(s,t) = (r(s)\alpha(t), r(s)\beta(t), z(s))$ be an immersion of a capillary surface for an anisotropic energy with Wulff shape $\xi(\sigma,t) = (u(\sigma)\alpha(t), u(\sigma)\beta(t), v(\sigma))$. Let

$$\bar{X}(s,t) = (r(s)\cos(t), r(s)\sin(t), z(s)),$$

$$\bar{\xi}(\sigma,t) = (u(\sigma)\cos(t), u(\sigma)\sin(t), v(\sigma))\,.$$

Then Σ is stable with respect to symmetric variations, if and only if $\bar{\Sigma}$ is stable with respect to symmetric variations for the free energy with Wulff shape $\bar{W}$ given by $\bar{\xi}$.

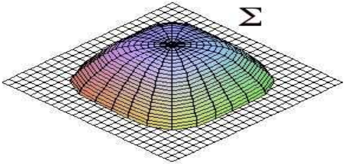
Non negative line tension

- For functionals with Wulff shape of product form, any energy minimizing surface is an anisotropic Delaunay surface. This follows from Schwarz symmetrization.

Theorem

Assume $\tau \geq 0$ holds. Let Σ be a sessile drop which is a subset of a rescaling of a Wulff shape of product form: $S \subset RW$. Assume that $0 \leq \tau$ holds. Then S is stable if and only if

$$\tau \leq \left(\frac{\pi}{\mathrm{area}(\Omega)}\right) \frac{3 V_C \bar{V}}{\pi R \underline{r} (V_C - \sigma(\nu_3) \bar{V})}\,, \tag{2}$$



Thank You!

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Second variation

If Σ is an equilibrium surface,

$$\delta^2\mathcal{E} = -\int_\Sigma \psi J[\psi]\, d\Sigma + \oint_{\partial\Sigma} \psi B_\tau[\psi]\, dL\,,$$

where

$$\psi := \delta X \cdot \nu \qquad \cot\phi := \nu_3/n_3$$

$$J[\psi] = \delta\Lambda = \mathrm{Div}_\Sigma[(D^2\gamma + \gamma I)\nabla\psi] + \langle (D^2\gamma + \gamma I)\cdot d\nu, d\nu\rangle\psi\ ,$$

The boundary operator B_τ is defined as follows:

$$B[\psi] = -\delta\xi\cdot n = A(\nabla\psi + \frac{\nu_3}{n_3}\psi d\nu(n))\cdot n\,.$$

$A := (D^2\gamma + \gamma I)_\nu$. Then

$$B_\tau[\psi] = B[\psi] - \frac{\tau}{n_3}\Big[\big(\frac{1}{\kappa_\Omega}(\frac{\psi}{n_3})_L\big)_L + \frac{\kappa^2}{\kappa_\Omega n_3}\psi\Big]\,.$$

An equilibrium surface is called *stable* if $\delta^2\mathcal{E} \geq 0$ holds for all ψ such that

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

holds. Consider the spectral problem:

$$(*) \quad J[\psi] + \lambda\psi = 0 \,, \qquad B_\tau[\psi] = 0 \,, \qquad \text{on} \quad \partial\Sigma \,.$$

Proposition

Assume that $\lambda_1 < 0 \leq \lambda_2$ holds. If there exists a solution of

$$(*) \;\; J[\phi] = 1 \,, \text{in} \;\; \Sigma, \qquad B_\tau[\phi] = 0 \;\; \text{on} \; \partial\Sigma \,.$$

Then, the surface is stable if and only

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

holds.
If no solution of (*) exists, the surface is unstable.

Anisotropic Delaunay surfaces

The orientation of an anisotropic Delaunay surface may be chosen so that $\Lambda \leq 0$ holds and then the anisotropic Delaunay surfaces fall into six cases as follows:

- (I-1) $\Lambda = 0$ and $c = 0$: *horizontal plane*.
- (I-2) $\Lambda = 0$ and $c \neq 0$: *anisotropic catenoid*.
- (II-1) $\Lambda < 0$ and $c = 0$: *Wulff shape (up to vertical translation and homothety)*.
- (II-2) $\Lambda < 0$ and $c = (c_0^2|\Lambda|)^{-1}$: *cylinder of radius* $(c_0|\Lambda|)^{-1}$.
- (II-3) $\Lambda < 0$ and $(c_0^2|\Lambda|)^{-1} > c > 0$: *anisotropic unduloid*.
- (II-4) $\Lambda < 0$ and $c < 0$: *anisotropic nodoid*.