Delaunay-like compact equilibria in the liquid drop model

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The liquid drop model. Gamow 1928

For an open, bounded region $\Omega \subset \mathbb{R}^3$, consider the *energy*

$$\mathcal{E}(\Omega) = \mathrm{Per}(\Omega) + \frac{1}{2}\int_\Omega \int_\Omega \frac{dxdy}{|x-y|},$$

where $\mathrm{Per}(\Omega)$ denotes the perimeter of Ω which in the smooth case corresponds to the area of its boundary, $\mathcal{A}(\partial\Omega)$.

In Gamow's $\mathcal{E}(\Omega)$ represents the energy of a *nucleus*, namely a collection of *nucleons* (protons and neutrons) uniformly distributed (constant density) in the region Ω, in this way its volume $|\Omega|$ is proportional to the total number of nucleons.

$$\mathcal{E}(\Omega) = \mathrm{Per}(\Omega) + \frac{1}{2}\int_\Omega\int_\Omega \frac{dxdy}{|x-y|},$$

In the energy the term $\mathrm{Per}(\Omega)$ corresponds to surface tension holding the nucleons together.

$\frac{1}{2}\int_\Omega\int_\Omega \frac{dxdy}{|x-y|}$ represents the Coulomb repulsion among the nucleons.

The ground state of a nucleus with a given mass m is a solution to the variational problem

$$\inf\{\mathcal{E}(\Omega) : |\Omega| = m\}.$$

It is known that ground states (minimizers) Ω exists for sufficiently small mass m while they do not exist for large m.

Bohr-Wheeler (1939): To compute the minimal energy required for nuclear fission, look at **critical points** of $\mathcal{E}(\Omega)$.

The problem consists in finding Ω with vanishing first variation with respect to normal perturbations of the boundary that preserve the volume m.

In the smooth case, this corresponds to finding a region Ω with $|\Omega| = m$, such that for some Lagrange multiplier λ we have

$$H_{\partial\Omega}(x) + \int_{\Omega} \frac{dy}{|x-y|} = \lambda \quad \text{for all} \quad x \in \partial\Omega \qquad (P)$$

$H_{\partial\Omega}(x)$ designates the *mean curvature* of the surface $\partial\Omega$ at x.

Derivation of problem (P).

We compute the first variation of the energy

$$\mathcal{E}(\Omega) = \mathrm{Per}(\Omega) + \frac{1}{2}\int_\Omega\int_\Omega \frac{dxdy}{|x-y|},$$

along normal domain perturbations of Ω. Let $\Sigma = \partial\Omega$ and $\nu(y)$ be a smooth unit normal vector field to Σ and consider a smooth small function $h : \Sigma \to \mathbb{R}$. Define

$$\Sigma_h = \{y + h(y)\nu(y) \ : \ y \in \Sigma\}$$

and let Ω_h the volume enclosed by Σ_h.

Critical point of the energy subject to volume constraint

$$\delta_h \mathcal{E}(\Omega_h)_{|h=0} = \lambda \delta_h |\Omega_h|_{|h=0}$$

We have

$$\frac{1}{2}\int_{\Omega_h}\int_{\Omega_h}\frac{dxdy}{|x-y|}-\frac{1}{2}\int_{\Omega}\int_{\Omega}\frac{dxdy}{|x-y|}$$
$$=\frac{1}{2}\int_{\Omega_h\setminus\Omega}\int_{\Omega}\frac{dxdy}{|x-y|}+\frac{1}{2}\int_{\Omega}\int_{\Omega_h\setminus\Omega}\frac{dxdy}{|x-y|}$$
$$\approx\int_{\Sigma}h(x)d\sigma(x)\int_{\Omega}\frac{dy}{|x-y|}$$

and

$$|\Omega_h|=\int_{\Omega_h}dx=\int_{\Omega}dx+\int_{\Omega_h\setminus\Omega}dx$$
$$\approx|\Omega|+\int_{\Sigma}h(x)d\sigma(x).$$

Consider now $\mathrm{Per}(\Omega_h) = \mathcal{A}(\Sigma_h)$.

Let $y = y(\omega),\ \omega \in S$ be a parametrization of a smooth surface Σ, and $\nu(\omega)$ the outer unit normal vector field. Consider the normal graph

$$\Sigma_h = \{y_h(\omega) = y(\omega) + h(\omega)\nu(\omega)\ :\ \omega \in S\}$$

for some smooth small function $h : S \to \mathbb{R}$.

Then its area is given by the formula

$$\mathcal{A}(\Sigma_h) = \int_S \sqrt{\det g(h)}\, d\omega, \quad g(h) = Y_h^T Y_h, \quad Y_h = D_\omega y_h.$$

Setting $B = D_\omega \nu$, it can easily be shown that

$$g(h) = g(0)(I + hA)^2 \left(I + O(h^2)\right), \quad A = (Y^T Y)^{-1} Y^T B,$$

and then

$$\sqrt{\det g(h)} = \sqrt{\det g(0)} \left(1 + h \,\mathrm{trace}\,(A) + h^2 \det A\right) (1 + O(h^2)).$$

Hence, for the area of the normal perturbation Σ_h and its first variation in h we get the expressions

$$\mathcal{A}(\Sigma_h) = \mathcal{A}(\Sigma) + \int_S \sqrt{\det g(0)} \,\mathrm{trace}\,(A)\, h d\omega + O(h^2)$$

$$\delta_h \mathcal{A}(\Sigma)[h] = \int_\Sigma H_\Sigma \, h, \quad H_\Sigma = \mathrm{trace}\,(A)$$

A standard expression for H_Σ can be computed as follows. For $z \in \mathbb{R}$, we expand

$$\sqrt{\det g(z)} = \sqrt{\det g(0)}\,\left(1 + z\,\mathrm{trace}\,(A) + z^2 \det A\right)(1 + O(z^2)).$$

Differentiating both sides in z we get

$$H_\Sigma = \mathrm{trace}\,(A) = \frac{d}{dz} \log \sqrt{\det g(z)}_{|z=0}.$$

Here

$$A = (Y^T Y)^{-1} Y^T B, \quad B = D_\omega \nu$$

Thus at a constraint critical point

$$\delta_h \mathcal{E}(\Omega_h)_{|h=0} = \lambda \delta_h |\Omega_h|_{|h=0}$$

satisfies

$$\int_\Sigma H_\Sigma(y)\, h(y) d\sigma(y) + \int_\Sigma h(y) d\sigma(y) \int_\Omega \frac{dx}{|x-y|} = \lambda \int_\Sigma h(y) d\sigma(y)$$

and since h is arbitrary this is equivalent to (P)

$$H_{\partial\Omega}(x) + \int_\Omega \frac{dy}{|x-y|} = \lambda \quad \text{for all} \quad x \in \partial\Omega \qquad (P)$$

Comparison with critical points of Perimeter subject to volume constraint:

$$\delta_h \mathrm{Per}(\Omega_h)_{|h=0} = \lambda\, \delta_h |\Omega_h|_{|h=0}$$

$\Sigma = \partial\Omega$ corresponds to surfaces with constant mean curvature (CMC):

$$H_\Sigma(x) = \lambda \quad \forall x \in \Sigma$$

Alexandrov: If Σ is a bounded and embedded CMC surface then $\Sigma = \partial B$ where B is a ball.

Our problem

$$\mathcal{E}(\Omega) = \mathrm{Per}(\Omega) + D(\Omega), \quad D(\Omega) = \frac{1}{2}\int_\Omega\int_\Omega \frac{dxdy}{|x-y|},$$

and

$$H_{\partial\Omega}(x) + \int_\Omega \frac{dy}{|x-y|} = \lambda \quad \text{for all} \quad x \in \partial\Omega \qquad (P)$$

Balls B with volume m are always solutions to (P), since they are critical for both, Perimeter and Coulomb interaction D.

- Classical isoperimetric inequality (De Giorgi, 1958).

$$|B| = m \quad \Rightarrow \quad \mathrm{Per}(B) = \inf\{\mathrm{Per}(\Omega) \,:\, |\Omega| = m\}.$$

thus $H_{\partial B}(y) = \lambda$.

- Riesz, 1930

$$|B| = m \quad \Rightarrow \quad D(B) = \sup\{D(\Omega) \,:\, |\Omega| = m\}.$$

thus $\int_B \frac{dx}{|x-y|} = \lambda$.

Hence, balls always solve (P)

$$H_{\partial B}(x) + \int_B \frac{dy}{|x-y|} = \lambda \quad \text{for all} \quad x \in \partial B.$$

Since the two terms of the energy describe opposite effects, the problem of finding *nontrivial* critical points is delicate.

Setting $\Omega = m^{\frac{1}{3}} E$, so that $|E| = 1$,

$$\mathcal{E}(\Omega) = m^{\frac{2}{3}} \left(\mathrm{Per}(E) + \, m \, D(E)\right)$$

This suggests that for any mass $m > 0$ sufficiently small, there is a global minimizer while for m large there are no global minimizers.

Consider the number $m_* > 0$ given by

$$m_* = 5\frac{2^{1/3} - 1}{1 - 2^{-2/3}} \approx 3.51$$

This is precisely the value of mass for which the energy of one ball and that of two balls with half that mass located at an infinite distance become equal.

$$\mathcal{E}\left(\left(\frac{m_*}{|B_1|}\right)^{\frac{1}{3}} B_1\right) = 2\mathcal{E}\left(\left(\frac{m_*}{2|B_1|}\right)^{\frac{1}{3}} B_1\right)$$

In fact

$$\mathcal{E}\left(\left(\frac{m}{|B_1|}\right)^{\frac{1}{3}} B_1\right) > 2\mathcal{E}\left(\left(\frac{m}{2|B_1|}\right)^{\frac{1}{3}} B_1\right) \quad \Leftrightarrow \quad m > m_*$$

Conjecture Choksi-Peletier (2011):

if $m < m_*$ then the infimum is attained precisely when Ω is a ball

if $m > m_*$ the infimum is not attained.

Known facts.

There exists a number m_1, $0 < m_1 < m_*$ such that for $m < m_1$ balls are minimizers. Knupfer-Muratov (2014), Julin (2014), Bonacini-Cristoferi (2014).

If $0 < m \leq 1$, balls are minimizers. Chodosh-Ruohoniemi (2024)

If $0 < m \leq m_*$, there exists a minimizer. Frank-Nam (2021)

No minimizer exists for large m Lu-Otto (2013)

If $m > 8$, no minimizer exists. Frank-Killip-Nam (2016).

For general Riesz potential: Knupfer-Muratov (2015); Lu-Otto (2014); Figalli -Fusco, Maggi - Millot - Morini (2015)

$$0 \underbrace{\longrightarrow}_{\text{balls minimize}} m_1 \underbrace{\longrightarrow}_{\exists \text{ minimizer}} m_* \underbrace{\longrightarrow}_{\text{balls no min}} 8 \underbrace{\longrightarrow}_{\nexists \text{ minimizer}} 10 \underbrace{\longrightarrow}_{\text{balls not stable}}$$

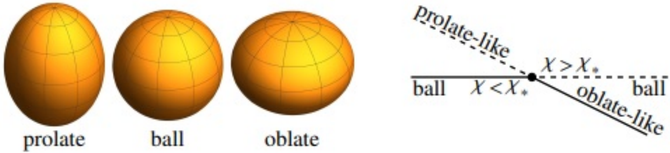
Question: Solutions to Problem (P) with large mass, not necessarily minimizers?

Recall that for CMC surface, the only compact and embedded is the sphere.

Known facts

Balls are stable (i.e. have a positive semi-definite second variation when restricted to variations of mean zero) if and only if $m \leq 10$

Frank (2019): bifurcation branch from $m = 10$



[Picture from Xu-Du 2023. χ_* corresponds to 10]

Bohr-Wheeler bifurcation branch [Picture from Xu-Du 2023]

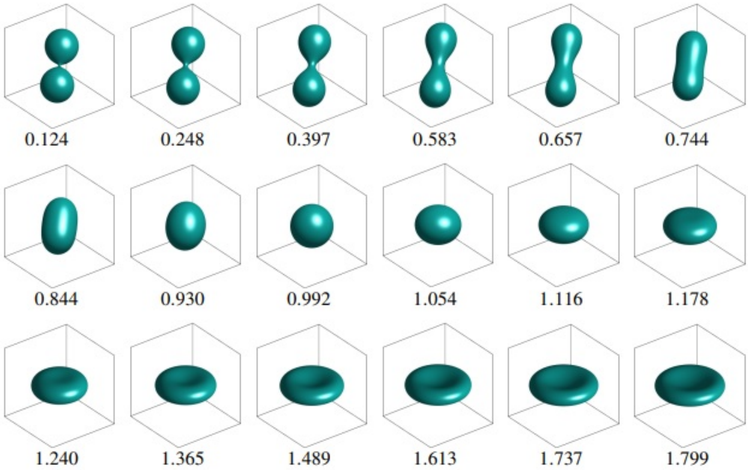


Figure 2: Computed Bohr–Wheeler bifurcation branch. Below each shape is $\widetilde{X}$.

Ren-Wei (2011): for all mass m sufficiently large, there exists an axially symmetric torus-like solution to Problem (P)

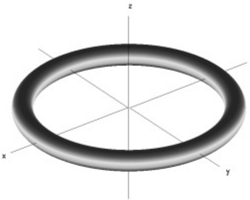


FIG. 1. A toroidal tube like solution.

with

$$R \sim m|\log m|^{\frac{2}{3}}, \quad r \sim |\log m|^{-\frac{1}{3}}, \quad \text{as} \quad m \to \infty$$

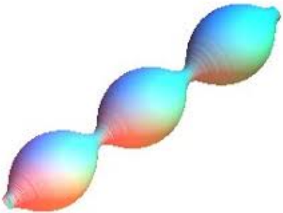
Solution is unstable. Stable under natural axi-symmetric perturbations

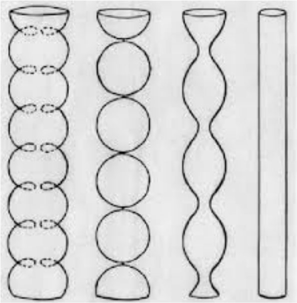
Choksi-Muratov-Topaloglu, Notices AMS (2017)

Concerning CMC surfaces, there are many non-compact solutions. Basic examples:

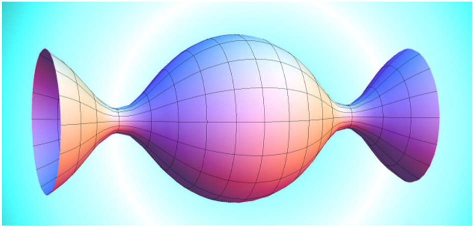
Delaunay surfaces (1841)

A family $\Sigma = \Sigma_a$ of periodic surfaces of revolution with constant mean curvature $= 2$





$a \in (0, \frac{1}{2})$ is the neck size
$a = \frac{1}{2}$: Cylinder
$a = 0$: Infinite array of tangent spheres



Denote $x = (\bar{x}, x_3) \in \mathbb{R}^3$

$$\Sigma = \{x \in \mathbb{R}^3 \;:\; |\bar{x}| = f(x_3)\}, \quad f : \mathbb{R} \to \mathbb{R}_+$$

f periodic of period $T = T_a$, $f(x_3) = f(-x_3)$.

Hence

$$\Sigma = \bigcup_{k=-\infty}^{\infty} \Sigma_k, \quad \Sigma_k = \{x \in \Sigma \,:\, -\frac{T}{2} + kT \le x_3 < \frac{T}{2} + kT\}.$$

Fix a number n and consider the truncated Delaunay,

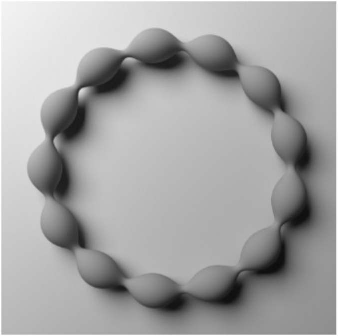
$$\Sigma^n = \bigcup_{k=0}^{n-1} \Sigma_k, \quad \Sigma_h^n = \{x + h(x)\nu(x) \,:\, x \in \Sigma^n\}$$

where $\nu(x)$ is the unit normal vector to Σ at $x \in \Sigma$, and $h : \Sigma \to \mathbb{R}$ is a small smooth function, even in x_1, T-periodic and even in x_3.

Let

$$2\pi R = nT.$$

We translate Σ_h^n to the point $R\mathbf{e}_2$ and rotate it in the plane (x_2, x_3)



In formulas:

$$\tilde{\Sigma}_n^n = X\left(\Sigma_h^n\right), \quad X\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_1 \\ (R + x_2)\cos\frac{x_3}{R} \\ (R + x_2)\sin\frac{x_3}{R} \end{pmatrix}$$

The 3-dimensional regions enclosed

$$\Omega_h^n = \{(r\bar{x}, x_3) \,:\, (\bar{x}, x_3) \in \Sigma_h^n,\ r \in [0,1]\}, \quad \tilde{\Omega}_h^n = X\left(\Omega_h^n\right)$$

with

$$|\tilde{\Omega}_h^n| \sim |\Omega_h^n| \sim n\, V_a \quad \text{as } n \to \infty$$

for $\frac{3\pi}{4} \leq V_a \leq \frac{\pi^2}{2}$.

Theorem del Pino-Musso-Zuñiga (2024).
For any $m > 0$ sufficiently large, there exists a smooth domain Ω with $|\Omega| = m$ of the form $\Omega = \gamma^{\frac{1}{3}}\,\tilde{\Omega}_h^n$ for a number $\gamma \approx \frac{c}{\log n}$ so that

$$|\Omega| = m \approx \frac{n}{\log n} V_a, \quad \|h\|_\infty \approx \frac{1}{\log n}$$

as $n \to \infty$, such that for some constant λ,

$$H_{\partial\Omega}(x) + N_\Omega(x) = \lambda \quad \text{for all } x \in \partial\Omega$$

where

$$N_\Omega(x) = \int_\Omega \frac{dy}{|x-y|}$$

Sketch of the Proof of the theorem.

For a number $\gamma > 0$ we consider the scaling $\tilde{\Omega} = \gamma^{-\frac{1}{3}}\Omega$, so that $|\Omega| = \gamma\,|\tilde{\Omega}|$. Then Ω solves Problem (P) if and only if $\tilde{\Omega}$ satisfies

$$H_{\partial\tilde{\Omega}}(x) + \gamma\, N_{\tilde{\Omega}}(x) = \lambda, \quad \text{for all } x \in \partial\tilde{\Omega} \qquad (P*)$$

for some constant λ.

We look for a region $\tilde{\Omega}$ close to a *twisted Delaunay* $\tilde{\Omega}^n$ with a large n, so that $|\tilde{\Omega}| \approx nV_a$ where $a > 0$ is a chosen fixed neck size.

For $a \in (0, \frac{1}{2})$, consider the Delaunay surface parametrized by

$$(f(x_3)\cos\theta, f(x_3)\sin\theta, x_3), \quad \theta \in [0, 2\pi),\ x_3 \in (-\frac{T}{2}, \frac{T}{2}).$$

Let

$$I_a = \int_0^{\frac{T}{2}} \frac{f}{(1+(f')^2)^{\frac{5}{2}}}[ff''(2-(f')^2) + (1+3(f')^2)(1+(f')^2)]ds$$

We have that $I_a > 0$ for $0 < a < a_*$ for some a_* small and $\frac{1}{4} < a < \frac{1}{2}$.

Main Proposition.

Let $a \in (0, \frac{1}{2})$ such that $I_a > 0$. For all sufficiently large n, there exists a number

$$0 < \gamma \sim \frac{1}{\ln n}$$

and a function h with $\|h\| \lesssim (\log n)^{-1}$ such that

$$H_{\tilde{\Sigma}_h^n}(x) + \gamma\, N_{\tilde{\Omega}_h^n}(x) = \lambda, \quad \text{for all } x \in \tilde{\Sigma}_h^n \equiv \partial\tilde{\Omega}_h^n.$$

Then $\Omega = \gamma^{\frac{1}{3}}\, \tilde{\Omega}_h^n$ solves Problem (P) with

$$|\Omega| = m = \gamma\, |\tilde{\Omega}_h^n| \approx \frac{n}{\log n}\, V_a$$

The proof is based on a Lyapunov-Schmidt reduction-type argument.

At a point $\tilde{y} = X(y) \in \tilde{\Sigma}^n$, $y = (f(x_3) \cos\theta, f(x_3) \sin\theta, x_3)$, we can show that

$$\begin{aligned} H_{\tilde{\Sigma}^n}(\tilde{y}) + \gamma\, N_{\tilde{\Omega}^n}(\tilde{y}) = 2 - \gamma\, \frac{2V_a}{T} \log n - \gamma\, \hat{g}(x_3) \\ + \frac{2\pi}{n\,T} \sin\theta \left(\tilde{g}(x_3) - \gamma \log n\, \frac{V_a}{T}\, g(x_3) \right) \\ + \text{smaller terms} \end{aligned}$$

with $\hat{g}$, $\tilde{g}, g$ T-periodic.

We perturb Σ^n with h in the normal direction as $\Sigma^n_h = \Sigma^n + h\nu$. To keep at main order the volume of the region, we work with perturbations h such that

$$\int_{\Sigma^n} h = 0.$$

The problem becomes

$$
\begin{aligned}
J_{\Sigma^n}[h] = {} & 2 - \gamma \, \frac{2 V_a}{T} \log n - \gamma \, \hat{g}(x_3) \\
& + \frac{2\pi}{n\, T} \, \sin\theta \left(\tilde{g}(x_3) \; - \gamma \log n \, \frac{V_a}{T} \, g(x_3) \right) \\
& + O(\frac{1}{n \log n}) + C \\
& + \gamma \ell_1[h] + n^{-1} \ell_1[h, Dh.D^2 h] + q[h, Dh.D^2 h]
\end{aligned}
$$

where $J_{\Sigma^n}[h]$ is the Jacobi operator of the surface Σ^n:

$$
J_{\Sigma^n}[h] = \frac{1}{\sqrt{\det g}} D_j \left(g^{ij} \, \sqrt{\det g} \, D_i h \right) + |A|^2 h.
$$

Conclusion

So far we have proved: For $a \in (0, \frac{a}{2})$ with $I_a > 0$ and all integer n sufficiently large, there exists a bounded, smooth domain Ω such that

$$|\Omega| \approx \frac{n}{\log n} V_a, \quad H_{\partial\Omega}(y) + N_{\Omega}(y) = \lambda$$

for all $y \in \partial\Omega$.

An elementary continuation argument on the explicit constant $a \to V_a$ gives the existence of a solution Ω with $|\Omega| = m$ to

$$H_{\partial\Omega}(y) + N_{\Omega}(y) = \lambda$$

for any m large enough.

Thanks for your attention