Droplet breakup in the liquid drop model with background potential

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- The perimeter $\mathrm{Per}(\Omega)$ is minimized by balls.

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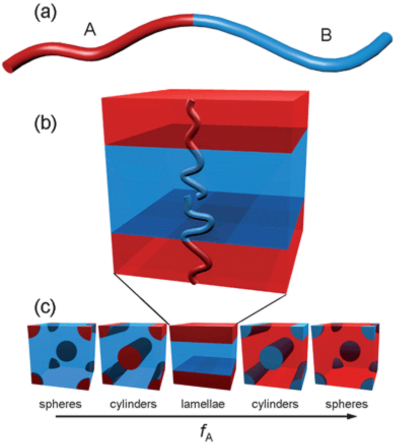
- Nature seems to agree: observed nuclei are spherical.

Diblock copolymers

Different physics, but similar variational structure.

- Polymer strands composed of two monomers *A*, *B* glued together.
- Monomers of the same type attract; of opposite type repel.



f_A denotes the volume fraction of A-type monomers.

- Diffuse-interface energy (Ohta-Kawasaki) model, $u: \ \Omega \subset \mathbb{R}^3 \to \mathbb{R}$ phase function,

$$\mathcal{K}_{\epsilon,\gamma}(u) = \int_\Omega \left[\frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}W(u)\right] dx + \gamma\|u-m\|^2_{H^{-1}}, \qquad m = \frac{1}{|\Omega|}\int_\Omega u\,dx.$$

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Extensive literature: Acerbi-Fusco-Morini, Alberti-Choksi-Otto, Bonacini-Cristoferi, Choksi-Glasner, Choksi-Peletier, Choksi-Ren, Choksi-Sternberg, Frank-Killip-Nam, Frank-Nam-Van den Bosch, Goldman-Muratov-Serfaty, Knüpfer-Muratov, Knüpfer-Muratov-Novaga, Lu-Otto, Muratov, Ren, Ren-Wei, Shirokoff-Choksi-Nave, Sternberg-Topaloglu,...

Minimizers of Gamow's model

Define

$$e_0(m) = \inf\left\{ E_0(\Omega) = \mathrm{Per}(\Omega) + \int_\Omega \int_\Omega \frac{dx\,dy}{|x-y|} \,:\, |\Omega| = m \right\}.$$

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- Locally minimizing solutions and non-min critical points by Ren-Wei, Julin-Pisante.

A generalization

The nonlocal term need not be the Newtonian potential; Riesz potentials may be substituted.

$$E_0^s(\Omega) = \mathrm{Per}(\Omega) + \int_\Omega \int_\Omega \frac{dx\,dy}{|x-y|^s}, \qquad |\Omega| = M,$$

for $\Omega \subset \mathbb{R}^d$ with $0 < s < d$. Call $e_0^s(M)$ the infimum value of E_0^s under the constraint $|\Omega| = M$.

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An important improvement for small s:

Theorem (Bonacini–Cristoferi 2014)

There exists $\bar{s} = \bar{s}(d)$ such that for all $0 < s < \bar{s}$ if $e_0^s(M)$ is attained, then Ω is a ball.

In other words, for sufficiently small s the critical values $m_{c1} = m_{c2} = m_{c3}$ coincide.

Background potentials

Lu-Otto, Frank-Nam-Van den Bosch (2016) add an attractive background potential to Gamow's model,

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- Idea: for large M, nuclear attraction of V is screened by Ω, compactness is lost at infinity.

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- Sharp-interface toy model of the Thomas–Fermi–Dirac–von Weizsäcker (TFDW) energy ("Ionization conjecture")
- Question: does the attractive potential $V(x) = Z/|x|$ enhance binding (existence of a min)?
- Answer: not much, but it gives a parameter to play with!
- Nonexistence of a min if $M > Z + C_2 \max\{Z^{2/3}, 1\}$, for constant $C_2 > 0$;
- Minimizer is a ball if $M \leq Z + C_1$, for constant $C_1 > 0$.
- Idea: for large M, nuclear attraction of V is screened by Ω, compactness is lost at infinity.

Questions: if $V(x)$ is of longer range than Coulomb, will it confine the minimizers, and give compactness? And if so, what will minimizers look like?

Long-range potentials

$$E_V(\Omega) = \operatorname{Per}\Omega + \int_\Omega \int_\Omega \frac{1}{|x-y|}\, dx\, dy - \int_\Omega V(x) dx.$$

with $V(x)$ longer range than $1/|x|$ (“super-Newtonian”,)

(H1) $V \geqslant 0$, and $V \in L^1_{loc}(\mathbb{R}^3)$.

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Theorem (Alama-B-Choksi-Topaloglu)

Under hypotheses (H1)–(H3), for **any** $M > 0$, E_V *attains its minimum among* $\Omega \subset \mathbb{R}^3$ *(Caccioppoli) with* $|\Omega| = M$.

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The proof uses concentration-compactness methods to ensure that mass does not escape to infinity.

More about that later...

Extension to TFDW

Thomas-Fermi-Dirac-von Weizsäcker (TFDW):

$$\mathcal{E}_V(u) := \int_{\mathbb{R}^3} \left(|\nabla u|^2 + |u|^{10/3} - |u|^{8/3} - V(x)|u|^2 \right) dx + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u(x)|^2 |u(y)|^2}{|x-y|} \, dxdy,$$

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Theorem (ABCT)

If V satisfies the long-range conditions (H1)–(H3), then $\mathcal{E}_V$ attains its minimizer for all masses $M > 0$.

Another generalization: Riesz potential interactions

For the more general Gamov-type model, with the Coulomb interaction replaced by a more general Riesz potential:

$$E_V^s(\Omega) = \mathrm{Per}(\Omega) + \int_\Omega \int_\Omega \frac{dx\,dy}{|x-y|^s} - \int_\Omega V(x)\,dx,$$

with $0 < s < d$.

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- The question remains (in all cases,) what do minimizers look like?
- To try to answer this, we study the concentration-compactness structure of minimizing sequences...

The basic splitting lemma

We use the following fundamental results for sequences of sets of finite perimeter: Assume $\Omega_n \subset \mathbb{R}^d$ are sets with volume $|\Omega_n| = M > 0$ and bounded perimeter $\mathrm{Per}(\Omega_n) \leq C$, for all n.

- Local compactness: There exists a subsequence, a set $U \subset \mathbb{R}^d$ of finite perimeter, and translations $x_n \in \mathbb{R}^d$ such that

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- Splitting: There exists disjoint decomposition $\Omega_n - x_n = U_n \cup V_n$, with

$$U_n \to U \quad \text{globally, and} \quad V_n \to \emptyset \quad \text{locally,}$$

so that

$$\mathrm{Per}(\Omega_n) = \mathrm{Per}(U_n) + \mathrm{Per}(V_n) + o(1), \qquad \mathcal{D}(\Omega_n) = \mathcal{D}(U_n) + \mathcal{D}(V_n) + o(1),$$

where $\mathcal{D}(\Omega) = \displaystyle\int_\Omega \int_\Omega \frac{dx\,dy}{|x-y|}$.

(Frank–Lieb 2016)

Concentration compactness structure

$$E_V(\Omega) = \operatorname{Per}\Omega + \int_\Omega \int_\Omega \frac{1}{|x-y|}\,dx\,dy - \int_\Omega V(x)\,dx, \qquad |\Omega| = M$$

Concentration Theorem (Alama-B-Choksi-Topaloglu)

Let $0 \le V \in L^1_{loc}$, $\lim_{|x|\to\infty} V(x) = 0$, and let Ω_n be a minimizing sequence for E_V. Then either:

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We may use this theorem with V of **long range** to prove existence of minimizers for all $M > 0$.

Remarks on the concentration theorem

Define: $\mathcal{M}_0 := \Big\{ m > 0 \colon e_0(m) \text{ admits a minimizer} \Big\}$.

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Corollary (A-B-C-T)

Let $0 \le V \in L^1_{loc}$, $\lim_{|x|\to\infty} V(x) = 0$. Then, every minimizing sequence for E_V, has a subsequence which converges to a generalized minimizer.

So the Concentration Theorem characterizes (up to subsequences) all possible minimizing sequences of E_V, including the Gamow functional E_0.

Exploring the structure of minimizers

To understand the geometry of minimizers, we consider a 1-parameter family of long-range potentials,

$$V(x) = V_Z(x) = \frac{Z}{|x|^p}, \quad 0 < p < 1,$$

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- If $Z \to 0^+$, we recover Gamow in the limit, and nonexistence for $M > m_{c3}$ large.
- For large M, we have dichotomy (splitting) of the minimizers as $Z \to 0$, so we expect that minimizers of E_Z will be disconnected for small $Z > 0$…

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- Minimize over $t > 0$, get $t = t_n = Z_n^{-\frac{1}{1-p}}$, the optimal scale of the pattern;

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- We may determine the scale and geometry of the multi-droplets via their interaction energy.
- Ansatz: (upper bound construction)
  - Take a generalized minimizer for E_Z: S_0 minimizes $e_Z(m^0)$, and $S_1, \ldots, S_N$ minimize $e_0(m^i)$.
  - Fix $t > 0$ and vectors $\{y_i\}_{i=1,\ldots,N}$ with $y_0 = 0$.
  - Define $\Omega_t = S_0 \cup \bigcup_{i=1}^{N} (S_i + t\, y_i)$.
- We calculate $E_{Z_n}(\Omega_t)$:

$$E_{Z_n}(\Omega_t) \simeq e_Z(m^0) + \sum_{i=1}^{N} e_0(m^i) - Z_n \int_{S_0} |x|^{-p}\, dx + t^{-1} \sum_{\substack{i,j=0 \\ i \neq j}}^{N} \frac{m^i\, m^j}{|y_i - y_j|} - t^{-p} Z_n \sum_{i=1}^{N} \frac{m^i}{|y_i|^p}$$

- Minimize over $t > 0$, get $t = t_n = Z_n^{-\frac{1}{1-p}}$, the optimal scale of the pattern;
- $E_{Z_n}(\Omega_{t_n}) \simeq e_Z(m^0) + \sum_{i=1}^{N} e_0(m^i) - Z_n \int_{S_0} |x|^{-p}\, dx + Z_n^{\frac{p}{1-p}} F_{\underline{m}}(y_1, \ldots, y_N) + o(Z_n^{\frac{p}{1-p}})$,

with $F_{\underline{m}}(y_1, \ldots, y_N) = \sum_{\substack{i,j=0 \\ i \neq j}}^{N} \frac{m^i\, m^j}{|y_i - y_j|} - \sum_{i=1}^{N} \frac{m^i}{|y_i|^p}$.

Main Theorem (Alama-B-Choksi-Topaloglu)

Theorem

Let $M \notin \mathcal{M}_0$, *and* $\Omega_n := \Omega_{Z_n}$, $Z_n \to 0$. *Then, there is a subsequence along which:*

$$\left|\Omega_n \bigtriangleup \left[S_0 + \bigcup_{i=1}^{N}(S_i + x_n^i)\right]\right| \longrightarrow 0$$

$$e_Z(m^0) = E_Z(S_0), \quad e_0(m^i) = E_0(S_i), \;\; i = 1, \ldots, N;$$

$$\left(\partial\Omega_n - x_n^i\right) \longrightarrow \partial S_i \quad \text{in } C^{1,\alpha}$$

$$\begin{cases} Z_n^{\frac{1}{1-p}} x_n^i \longrightarrow y_i \text{ as } n \to \infty, \;\; i = 1, \ldots, N, \\ \quad \text{where } (0, y_1, \ldots, y_N) \text{ minimize } F_{\underline{m}}. \end{cases}$$

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Remark: $F_{\underline{m}}$ attains its min for any choice of masses $\underline{m}$.

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- We conjecture that the masses are always equal.