From the liquid drop model for nuclei to the ionization conjecture for atoms

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The liquid drop model

Gamow (1928) suggested to describe the collection of protons and neutrons inside an atomic nucleus as an **incompressible, uniformly charged fluid**.
Mathematically, in this model a nucleus is a (measurable) set $\Omega \subset \mathbb{R}^3$. In suitable units, its measure $|\Omega| = A$ is the number of nucleons and its energy is

$$\mathcal{E}[\Omega] = \operatorname{Per}\Omega + \frac{1}{2}\iint_{\Omega\times\Omega} \frac{dx\,dy}{|x-y|} \,.$$

(Here $\operatorname{Per}\Omega$ equals the **surface area** for sufficiently regular Ω.)

This model allows to describe qualitatively (and, with some refinements and fitting parameters, also quantitatively) the **binding energy per nucleon** and the phenomenon of **fission**. It is also used in **astrophysics** to describe exotic phases of nuclear matter.

Assumptions. (1) Existence of **nuclear matter** with a **constant density**
(2) The model describes, perturbatively relative to the energy of nuclear matter, the finite size of a nucleus and the Coulomb repulsion between its protons

Questions for mathematical physicists

The liquid drop model has only recently attracted the attention of mathematical physicists (cf. review article in the **Notices of the AMS** by **Choksi–Muratov–Topaloglu** in December 2017). Several fundamental questions have not been addressed so far.

• Can one **derive** the liquid drop model from a **microscopic model** of a nucleus? A zeroth step is to understand nuclear matter and its constant density.

• Can one describe **dynamically** the process of **nuclear fission** in the liquid drop model? The equation is somewhat reminiscent of the mean-curvature flow, but with an additional long-range part (which is responsible for fission) and Hamiltonian instead of dissipative.

• Can one prove the existence of **nuclear pasta phases** for a system of many nuclei interacting with a uniform background of electrons? These are **periodic structures of different dimensionalities** suggested to occur in the crust of neutron stars.

Today: Ground state properties

The minimization problem

$$E(A) := \inf \{\mathcal{E}[\Omega] : \ |\Omega| = A\} \,, \qquad \mathcal{E}[\Omega] = \operatorname{Per}\Omega + \frac{1}{2}\iint_{\Omega\times\Omega} \frac{dx\,dy}{|x-y|}$$

Competition between **attractive short-range** and **repulsive long-range forces**:

- The term $\operatorname{Per}\Omega$ wants Ω to a ball
- The term $\frac{1}{2}\iint_{\Omega\times\Omega}\frac{dx\,dy}{|x-y|}$ wants to spread Ω apart

Let $A_* = 5(2-2^{2/3})/(2^{2/3}-1) \approx 3.518$. At $A=A^*$, the energy of a ball of volume A equals the energy of two infinitely far apart balls of volume $A/2$ each.

Conjecture ('No compromise'). (1) For $A \leq A_*$, every minimizer for $E(A)$ is a ball. (2) For $A > A_*$ there is no minimizer for $E(A)$.

What is known: (1) There is an $A_1 > 0$ such that all minimizers for $A < A_1$ are balls (**Knüpfer–Muratov, Julin**). This uses recent developments concerning 'stable' versions of the **isoperimetric inequality**. The value A_1 is via compactness.
(2) There is an $A_2 < \infty$ such that there is no minimizer for $A > A_2$ (**Knüpfer–Muratov, Lu–Otto**). The proof uses ideas from **geometric measure theory**. The value A_2 is, in principle, explicit, but certainly way too large.

A non-existence result for a large number of nucleons

$$E(A) := \inf\{\mathcal{E}[\Omega] : \ |\Omega| = A\}\ , \qquad \mathcal{E}[\Omega] = \operatorname{Per}\Omega + \frac{1}{2}\iint_{\Omega\times\Omega} \frac{dx\,dy}{|x-y|}$$

Here is a quantitative non-existence result.

Theorem 1 (F., Killip, Nam (2016))**.** *If $A > 8$, then $E(A)$ has no minimizer.*

It is an **open problem** for further decrease the non-existence threshold. Recall the conjecture is $A_* \approx 3.518$.

The value $A = 8$ is already in the **physically relevant regime**. Indeed, it is known that balls are stable against local perturbations up to $A = 10$. Thus, the theorem establishes a region of A-values, where balls are locally stable but not minimizers. This can be thought as a region of '**radioactive nuclei**'.

Proof of the theorem

Let Ω be a **minimizer** for $E(A)$. We show that $A = |\Omega| \leq 8$. For $\nu \in \mathbb{S}^2$ and $\ell \in \mathbb{R}$ let

$$\Omega^+_{\nu,\ell} := \{x \in \Omega : \ x\cdot\nu > \ell\} \qquad \text{and} \qquad \Omega^-_{\nu,\ell} := \{x \in \Omega : \ x\cdot\nu < \ell\}\,.$$

By **minimality** of Ω, for any $L > 0$

$$\mathcal{E}\left[\left(\Omega^+_{\nu,\ell} + L\nu\right) \cup \Omega^-_{\nu,\ell}\right] \geq \mathcal{E}[\Omega]\,.$$

As $L \to \infty$, the left side tends to $\mathcal{E}[\Omega^+_{\nu,\ell}] + \mathcal{E}[\Omega^-_{\nu,\ell}]$. Rewriting the obtained inequality,

$$2\mathcal{H}^2(\Omega \cap \{x\cdot\nu = \ell\}) \geq \iint_{\Omega^+_{\nu,\ell}\times\Omega^-_{\nu,\ell}} \frac{dx\,dy}{|x-y|} = \iint_{\Omega\times\Omega} \frac{\mathbb{1}_{\{\nu\cdot x<\ell<\nu\cdot y\}}}{|x-y|}\,dx\,dy\,.$$

Integrating with respect to $\ell \in \mathbb{R}$, we obtain

$$2|\Omega| \geq \iint_{\Omega\times\Omega} \frac{(\nu\cdot(y-x))_+}{|x-y|}\,dx\,dy\,.$$

Averaging with respect to $\nu \in \mathbb{S}^2$, using $(4\pi)^{-1}\int_{\mathbb{S}^2}(\nu\cdot a)_+\,d\nu = |a|/4$, we obtain

$$2|\Omega| \geq \frac{1}{4}\iint_{\Omega\times\Omega} \frac{|x-y|}{|x-y|}\,dx\,dy = \frac{1}{4}|\Omega|^2\,, \qquad \text{that is, } |\Omega| \leq 8\,. \qquad \square$$

The ionization problem

And now for something completely different...

Atoms: The relevant particles are electrons, the nucleus is a point

Question: How many electrons can a nucleus of charge Z bind? Again, we want to say that for $N \geq N_c$ a certain minimization problem has no minimizer.

This is a **major open problem** for the many-body Coulomb Schrödinger operator,

$$\sum_{n=1}^{N} \left(-\Delta_n - \frac{Z}{|x_n|} \right) + \sum_{1 \leq n < m \leq N} \frac{1}{|x_n - x_m|} \qquad \text{in } L^2_{\mathrm{anti-symm}}(\mathbb{R}^{3N})$$

Ionization conjecture. $N_c \leq Z + 1$

Brief history. (1) **Ruskai**, **Sigal** (1982): $N_c < \infty$
(2) **Lieb** (1984): $N_c < 2Z + 1$ (improved by **Nam** (2012))
(3) **Lieb–Sigal–Simon–Thirring** (1988): $N_c \leq Z(1 + o(1))$
(4) **Fefferman–Seco** (1990): $N_c \leq Z + CZ^{5/7}$.

We have nothing new to report on this problem ☹

The ionization problem in approximate theories

There are **simpler** models for an atom. How about the ionization problem there?

In (one of) the most complicated one of these, namely **Hartree–Fock theory**, the bound $N_c \leq Z + C$ is shown in a fundamental work of **Solovej** (2003).
Moreover, **Solovej** lays out a general path, based on a **universality property** of **Thomas–Fermi theory**. He uses a **multi-scale analysis**, based on the following ingredients:

- **Sommerfeld asymptotics** for solutions of a Thomas–Fermi-like equation
- **Concergence** to a Thomas–Fermi-like model problem
- **A-priori bound** on the number of 'outside electrons'.

Here: Focus on the last item, namely a-priori bounds.
Usually, a-priori bounds on the number of outside electrons are proved using the **Benguria–Lieb strategy** of multiplying the Euler–Lagrange equation by $|x|$. For **Solovej**'s proof it is not important if a factor is lost, but it is important that the bound holds on all scales.

Problem: In some models the **Benguria–Lieb strategy** does not work.

A TOY PROBLEM

As a mathematical toy model, **Lu–Otto** consider an atom as a uniformly charged, incompressible fluid, similarly as a nucleus in the liquid drop model.

$$\mathcal{E}_Z[\Omega] := \operatorname{Per}\Omega - Z\int_\Omega \frac{dx}{|x|} + \frac{1}{2}\iint_{\Omega\times\Omega} \frac{dx\,dy}{|x-y|}$$

$$E_Z(N) := \inf\{\mathcal{E}_Z[\Omega] :\ |\Omega| = N\}$$

The same argument as before shows that there is no minimizer if $N > 2Z + 8$. For large Z this can be improved.

Theorem 2 (F., Nam, v.d.Bosch (2018)). *If $N > Z + CZ^{1/3}$, then $E_Z(N)$ has no minimizer.*

Remarks. (1) This improves a result of **Lu–Otto**, who required $N > Z + CZ^{2/3}$.
(2) In this model the bound $CZ^{1/3}$ on the excess charge might be optimal.
(3) We improve the previous argument by capturing a **screening effect**. Namely, if Ω is a minimizer, then, for any $R > 0$,

$$|\Omega \cap \{|x| > R\}| \leq 2\left(Z - \sup_{|x|=R} |x| \int_{\Omega\cap\{|x|<R\}} \frac{dy}{|x-y|}\right) + \text{ error terms}$$

This follows as in the liquid drop model, by a somewhat more involved cutting argument.

The Thomas–Fermi–Dirac–von Weizsäcker model

For some constants $c_1, c_2, c_3, c_4 > 0$ consider

$$\mathcal{E}_Z[\rho] := \int_{\mathbb{R}^3} \left(c_1 \rho^{5/3} - \frac{Z}{|x|}\rho - c_2 \rho^{4/3} + c_3 |\nabla \sqrt{\rho}|^2 \right) dx + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(x)\,\rho(y)}{|x-y|}\, dx\, dy$$

$$E_Z(N) := \inf \left\{ \mathcal{E}_Z[\rho] :\ \rho \geq 0\,,\ \int_{\mathbb{R}^3} \rho\, dx = N \right\}.$$

Theorem 3 (F., Nam, v.d.Bosch (2018))**.** *If $N > Z + C$, then $E_Z(N)$ has no minimizer.*

Remarks. (1) This settles a problem posed by **Lieb** in 1981. Not even $N_c < \infty$ was known. Previous methods do not work.
(2) Our proof uses **Solovej**'s strategy, together with an a-priori bound of the form

$$\int_{|x|>R} \rho\, dx \leq C \left(Z - \sup_{|x|=R} |x| \int_{|y|<R} \frac{\rho(y)}{|x-y|}\, dy \right) + \text{error terms}$$

(3) Our proof also works for **Müller theory** (a density matrix theory), and perhaps even for completely different problems...

Conclusion

• We have seen the **liquid drop model** which, despite its simplicity, shows a rich mathematical structure.

• Many interesting questions in this model remain open.

• Techniques that were useful in the study of the liquid drop model have allowed us to prove the **ionization conjecture** in Thomas–Fermi–Dirac–von Weizsäcker theory.

THANK YOU FOR YOUR ATTENTION!