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

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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

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

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

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

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

Competition between \textbf{attractive short-range} and \textbf{repulsive long-range forces}:

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

Let \( A_* = 5\left(2 - 2^{2/3}\right)/(2^{2/3} - 1) \approx 3.518 \). 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.

\textbf{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 \( E(A) \).

\textbf{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 \textbf{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 \textbf{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

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

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 $\Omega$ 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

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

By minimality of $\Omega$, 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

$$2|\Omega| \geq \frac{1}{4} \iint_{\Omega \times \Omega} \frac{|x - y|}{|x - y|} \, dx \, dy = \frac{1}{4} |\Omega|^2,$$

that is, $|\Omega| \leq 8$. \qed
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,

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

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
- Congercence 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.

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

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

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 \( \Omega \) 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...
We have seen the \textbf{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 \textit{ionization conjecture} in Thomas–Fermi–Dirac–von Weizsäcker theory.
THANK YOU FOR YOUR ATTENTION!