Consider the following functional:

$$\mathcal{E}(\rho) = \int_{\mathbb{R}^3} \rho^{5/3}(x) \, dx - \int_{\mathbb{R}^3} V(x) \rho(x) \, dx + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho(x) \rho(y)}{|x-y|} \, dx \, dy$$

where $V(x)$ is a given function [an important example of such $V$ is a Coulomb potential $V(x) = \sum_{i=1}^{k} \frac{m_i}{|x-a_i|}$, $m_i > 0, a_i \in \mathbb{R}^3$ fixed] and $\rho(x)$ is a non-negative function on $\mathbb{R}^3$.

The following problem arises in quantum mechanics:

\[(1) \min_{\rho \in K} \mathcal{E}(\rho),\]

where $K$ denotes the convex set

$$K = \{ \rho \in L^1(\mathbb{R}^3), \rho \geq 0 \text{ a.e. } \int \rho(x) \, dx = I \}$$

and $I > 0$ is given.

When $V(x) = \sum_{i=1}^{k} \frac{m_i}{|x-a_i|}$ we are in presence of a system which consists of $k$ positive nuclei placed at points $a_i$ in space, with positive charge $m_i$. They are surrounded by a "cloud of electrons" with a probability density $\rho(x)$ to be determined.

Problem (1) is a convex minimization problem; however it does not possess always a solution.

For example if $V \equiv 0$ a.e. and $V(x) \equiv 0$ as $|x| \to \infty$ one can show that Problem (1) has never a solution (no matter what $I$ is). To prove this fact, one checks that $\inf_{\rho \in K} \mathcal{E}(\rho) = 0$ by showing that $\mathcal{E}(\rho_n) \to 0$

where $\rho_n(x) = \frac{1}{\text{meas}(B_n)}$ when $x \in B_n$, $\rho_n(x) = 0$ when $x \not\in B_n$ and
B_n(x) = \{x \in \mathbb{R}^3 \mid |x| < n\}.

The first existence result for Problem (1) has been proved by Lieb and Simon [6]:

**Theorem 1** Assume \( V(x) = \sum_{i=1}^{k} \frac{m_i}{|x-a_i|} \) and set \( I_0 = \sum_{i=1}^{k} m_i \).

Then:

(a) If \( 0 < I < I_0 \), Problem (1) has a unique solution

(b) If \( I > I_0 \), Problem (1) has no solution.

In addition if \( I < I_0 \) the solution of Problem (1) has a compact support.

Theorem 1 has been extended by Benilan and myself [1]. We replace in (1), \( \rho^{5/3} \) by a general convex function \( j(\rho) \) where \( j: [0, \infty) \rightarrow [0, \infty) \) is a \( C^1 \) convex function such that \( j(0) = j'(0) = 0 \). We also consider the case where \( V(x) \) is a general function - not just a Coulomb potential.

Our technique is the following:

- Derive the Euler equation corresponding to (1) (this is a variational inequality)
- Transform the Euler equation into a nonlinear partial differential equation.
- Solve that nonlinear partial differential equation.

The Euler equation corresponding to Problem (1) is the following (at least formally):

Find \( \rho \in K \) and find a constant \( \lambda \) such that

\[
(2) \begin{cases}
    j'(\rho) - V + B\rho = -\lambda & \text{on the set } [\rho > 0] \\
    -V + B\rho \geq -\lambda & \text{on the set } [\rho = 0]
\end{cases}
\]

where \( (B\rho)(x) = \int \frac{\rho(y)}{|x-y|} \, dy = (-\Delta)^{-1} \rho \)

(assuming \( 4\pi = 1! \)).

The constant \( \lambda \) which appears in (2) is a Lagrange multiplier which is naturally associated with the constraint \( \int \rho = I \) in (1).
Our next result states what is the exact relationship between Problems (1) and (2).

**Proposition 2**  Assume \( \rho \) is a solution of (1), then \( \rho \) is always a solution of (2). Conversely if \( \rho \) is a solution of (2), and if the following holds:\(^{(1)}\):

(3) there is a constant \( C \) such that \( j^*(\nu-C) \epsilon L^1 \)

Then \( \rho \) is a solution of (1).

**Remarks:**
1) Proposition 2 asserts that Problem (2) has "more often" a solution that Problem (1).

It is therefore natural to study first Problem (2).

2) Suppose \( j(r) = r^p \) and \( V(x) = \sum_{i=1}^{k} \frac{m_i}{|x-a_i|^p} \), then (3) holds provided \( p > \frac{3}{2} \). When \( p = \frac{3}{2} \) Problem (1) has no solution; in fact \( \inf_{K} \epsilon = -\infty \).

However Problem (2) has a solution.

Our main result concerning Problem (2) is the following

**Theorem 3**

Assume

(4) \( V > 0 \) on some set of positive measure,
(5) \( V \in \mathcal{B}(L^1) \) (i.e. \( \Delta V \in L^1 \) and \( V(x) \to 0 \) as \( |x| \to \infty \), in a weak sense).

Then there is some \( 0 < I_0 < \infty \) such that

(a) If \( I < I_0 \), Problem (2) has a unique solution
(b) If \( I > I_0 \), Problem (2) has no solution.

In addition:

(c) If \( I < I_0 \) and \( V(x) \to 0 \) as \( |x| \to \infty \), or if \( I \leq I_0 \) and \( |x| V(x) \to 0 \) as \( |x| \to \infty \) then the solution of (2) has compact support.

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\(^{(1)}\) \( j^* \) denotes the conjugate function of \( j \), i.e.

\[ j^*(r) = \sup_{s \geq 0} \{ rs - j(s) \} \]
(7) Assume \( j(r) = r^p \) near \( r = 0 \) with \( p > 4/3 \), then \( -\int_0^r (\Delta V) \leq I_0 \leq \int_0^r (-\Delta V)^+ \).

In particular \( I_0 = -\int \Delta V \) when \( -\Delta V > 0 \).

(8) Assume \( j(r) = r^p \) near \( r = \infty \) with \( p > 4/3 \) and replace assumption (5) by the more general assumption \( V \in B(M) \) - where \( M \) denotes the set of bounded measures on \( \mathbb{R}^3 \). Then all the above conclusions still hold.

For the proof of Theorem 3 we refer to [1]. We shall make a number of remarks about Theorem 3.

Remarks

1) When \( p = \frac{5}{3} \) and \( V(x) = \sum \frac{m_i}{|x - a_i|} \), then \( V = B(\sum m_i \delta(x - a_i)) \); we may then apply (8) and derive the Theorem of Lieb and Simon.

2) Under the assumption (6) the set \([\rho > 0]\) is bounded; we are therefore in the presence of a free boundary, namely the boundary of the cloud of electrons \([\rho > 0]\). Caffarelli and Friedman [5] have obtained some results about the regularity of the free boundary when \( V(x) = \sum_{i=1}^k \frac{m_i}{|x - a_i|} \) and \( \frac{3}{2} < p < 2 \).

It is also natural to ask questions about the geometry of the set \([\rho > 0]\). For example under what conditions on \( V \) is \([\rho > 0]\) connected? In general, estimate the number of connected components of the set \([\rho > 0]\). This seems to be an open problem.

3) As \( I + I_0 \), the set \([\rho > 0]\) increases and in general, at the limit becomes all of \( \mathbb{R}^3 \). We have obtained a sharp estimate for the size of \([\rho > 0]\) in terms of \( (I_0 - I) \), (see [1]).

4) An essential ingredient in the proof of Theorem 3 is the following transformation which turns Problem (2) into a nonlinear p.d.e.

Set \( u = V - B\rho \). Then \( u \) satisfies \( -\Delta u + \gamma(u - \lambda) = -\Delta V \) where \( \gamma(t) = 0 \) if \( t < 0 \) and \( \gamma \) is the reciprocal function of \( j' \) if \( t \geq 0 \). Therefore Problem (2) is equivalent to the following:
Find a function \( u \) and a constant \( \lambda > 0 \) such that

\[
\begin{cases}
-\Delta u + \gamma (u - \lambda) = -\Delta V \\
u(x) \to 0 \quad \text{as} \quad |x| \to \infty \\
\gamma (u - \lambda) dx = 1
\end{cases}
\]  
(9)

Once Problem (9) has been solved, then \( \rho = \gamma (u - \lambda) \) provides a solution of (2). The following Lemma play a useful role in solving (9).

**Lemma 1** [2] Assume \( \beta : \mathbb{R} \to \mathbb{R} \) is any continuous non decreasing function such that \( \beta(0) = 0 \). Let \( f \in L^1 \). Then there exists a unique solution \( u \) of the equation

\[
\begin{cases}
-\Delta u + \beta(u) = f \\
u(x) \to 0 \quad \text{as} \quad |x| \to \infty
\end{cases}
\]

with the property that \( \beta(u) \in L^1 \).

**Lemma 2** [1]. Assume \( \beta : \mathbb{R} \to \mathbb{R} \) is a continuous non decreasing function such that \( \beta(0) = 0 \) and

\[
\beta \left( \pm \frac{1}{|x|} \right) \in L^1 (|x| < 1)
\]

(10)

Assume \( f \in M \). Then there exists a unique solution \( u \) of the equation

\[
\begin{cases}
-\Delta u + \beta(u) = f \\
u(x) \to 0 \quad \text{as} \quad |x| \to \infty,
\end{cases}
\]

(11)

with the property that \( \beta(u) \in L^1 \).

**Remark about Lemma 2**

Note the difference between Lemma 1 and Lemma 2. In Lemma 1, \( \beta \) could be arbitrary provided \( f \in L^1 \). In Lemma 2 we assume that \( \beta(u) \) has a "slow" growth as \( |u| \to \infty \) (this is expressed by assumption (10)) and we may then handle the case where \( f \) is a bounded measure.

If we remove assumption (10), then (11) need not have a solution.

For example the equation

\[
-\Delta u + u^3 = \delta
\]

(12)
δ denotes the Dirac mass at 0) has no solution (even in a local sense near 0).

The fact that (12) has no solution is a consequence of the following

**Theorem 4** [4]. Assume \( u \in L^3_{\text{loc}}(0 < |x| < 1) \) satisfies \(-\Delta u + u^3 = 0\) in \( \mathcal{D}'(0 < |x| < 1) \).

Then in fact \( u \) is smooth on \( |x| < 1 \) (including at 0) and satisfies

\[ -\Delta u + u^3 = 0 \quad \text{in} \quad \mathcal{D}'(|x| < 1). \]

In other words, the solutions of \(-\Delta u + u^3 = 0\) cannot have any kind of isolated singularities. A similar result holds for

\[ (13) \quad -\Delta u + |u|^{q-1} u = 0 \]

if \( q > 3 \).

When \( 1 < q < 3 \), there are solutions of (13) with isolated singularities; in fact isolated singularities of (13) have been fully classified by L. Veron [7] using some of the results of [3].

**REFERENCES**


