A FREE BOUNDARY PROBLEM IN QUANTUM MECHANICS: THOMAS - FERMI EQUATION

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Consider the following functional:

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

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) $\quad \min_{\rho\in K} \mathcal{E}(\rho)$,

where K denotes the convex set

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

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 $V\leq 0$ a.e. and $V(x)\to 0$ as $|x|\to\infty$ one can show that Problem (1) has <u>never</u> a solution (no matter what I is). [To prove this fact, one checks that $\operatorname{Inf}_{\rho\in K}\mathcal{E}(\rho)=0$ by showing that $\mathcal{E}(\rho_n)\to 0$ where $\rho_n(x)=\frac{I}{\text{meas}(B_n)}$ when $x\in B_n$, $\rho_n(x)=0$ when $x\notin B_n$ 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]:

<u>Theorem 1</u> 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 $0<I\leqslant I_0$, Problem (1) has a unique solution

(b) If $I>I_0$, Problem (1) has <u>no</u> 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 $j:[0,\infty)\to[0,\infty)$ 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 λ such that

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

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

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

The constant λ 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).

<u>Proposition 2</u> Assume ρ is a solution of (1), then ρ is always a solution of (2). Conversely if ρ is a solution of (2), and if the following holds[1]:

(3) there is a constant C such that $j^*(V-C)\in L^1$

Then ρ is a solution of (1).

<u>Remarks</u>:

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 $V(x) = \sum_{i=1}^{k} \frac{m_i}{|x-a_i|}$, then (3) holds provided $p>\frac{3}{2}$. When $p=\frac{3}{2}$ Problem (1) has <u>no</u> solution; in fact $\operatorname{Inf}_K \mathcal{E}=-\infty$

However Problem (2) has a solution.

Our main result concerning Problem (2) is the following

<u>Theorem 3</u>

Assume

(4) $V>0$ on some set of positive measure,

(5) $V\in B(L^1)$ (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 $I\leqslant I_0$, Problem (2) has a unique solution

(b) If $I>I_0$, Problem (2) has no solution.

In addition:

(6) If $I<I_0$ and $V(x)\to 0$ as $|x|\to\infty$, or if $I\leqslant I_0$ 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.

$j^*(r)= \sup_{s\geqslant 0} \{rs-j(s)\}$.

(7) Assume $j(r)=r^p$ near $r=0$ with $p\geq 4/3$, then $-\int(\Delta V)\leq I_0\leq\int(-\Delta V)^+$.
In particular $I_0=-\int\Delta V$ when $-\Delta V\geq 0$.

(8) Assume $j(r)=r^p$ near $r=\infty$ with $p>4/3$ and replace assumption (5) by the more general assumption $V\in B(\mathfrak{M})$ - where $\mathfrak{M}$ 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 $V(x) = \Sigma \frac{m_i}{|x-a_i|}$, then $V=B(\sum_{i=1}^{k} m_i\delta(x-a_i))$; 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 $I\to I_0$, 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 $t\leq 0$ and γ 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 $\lambda \geq 0$ such that

$$(9)\quad \begin{cases} -\Delta u + \gamma(u-\lambda) = -\Delta V \\ u(x) \to 0 \quad \text{as} \quad |x| \to \infty \\ \int \gamma(u-\lambda)\,dx = I \end{cases}$$

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).

<u>Lemma 1</u> [2] Assume $\beta: \mathbb{R} \to \mathbb{R}$ is <u>any</u> 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 $\beta(u) \in L^1$.

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

$$(10)\qquad \beta\left(\pm \frac{1}{|x|}\right) \in L^1(|x|<1)$$

Assume $f \in \mathfrak{M}$. Then there exists a unique solution u of the equation

$$(11)\qquad \begin{cases} -\Delta u + \beta(u) = f \\ u(x) \to 0 \quad \text{as} \quad |x| \to \infty, \end{cases}$$

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

<u>Remark about Lemma 2</u>

Note the difference between Lemma 1 and Lemma 2. In Lemma 1, β 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 <u>not</u> have a solution. For example the equation

$$(12)\qquad -\Delta u + u^3 = \delta$$

(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 $u \in L^3_{loc}(0<|x|<1)$ 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 $-\Delta u+u^3=0$ can not have any kind of isolated singularities. A similar result holds for

$$(13) \qquad -\Delta u + |u|^{q-1}u = 0$$

if $q \geq 3$.

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].

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