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Nonlinear equations of the Thomas-Fermi type.

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We shall report on various recent works by E. Lieb - B. Simon [7], Ph. Benilan - H. Brezis [2], H. Brezis - E. Lieb [5], H. Brezis - L. Veron [6], L. Veron [8], R. Benguria - H. Brezis - E. Lieb [1] related to the Thomas - Fermi equation. For a function $\rho(x) : \mathbb{R}^3 \longrightarrow [0,\infty)$ we define the functional

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

where $V(x)$ is a given measurable function. Let

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

where $I > 0$ is fixed.

The Thomas -Fermi (T.F.) problem is the following:

(1) $\displaystyle \operatorname*{Min}_{\rho \in K} \mathcal{E}(\rho)$

The unknown $\rho(x)$ to be determined represents a probability density of Fermions. Of special interest in quantum mechanics is the particular case where $V(x)$ is a Coulomb potential,

$$V(x) = \sum_{i=1}^{k} \frac{m_i}{|x - a_i|} \qquad (m_i > 0\ ,\ a_i \in \mathbb{R}^3)\ ;$$

here, the system consists of k positive nuclei of charge m_i, placed at the points a_i in space and surrounded by a cloud of Fermions with density ρ.

We first recall an important result due to Lieb - Simon [7]:

Theorem 1 Assume

$$V(x) = \sum_{i=1}^{k} \frac{m_i}{|x - a_i|} \quad \text{and set} \quad I_0 = \sum_{i=1}^{k} m_i .$$

Then

(a) If $0 < I \leq I_0$, problem (1) has a unique solution.

(b) If $I > I_0$, problem (1) has no solution.

(c) If $I < I_0$, the solution of (1) has compact support.

In what follows we consider Problem (1) with a more general functional $\mathcal{E}$; namely

$$\mathcal{E}(\rho) = \int j(\rho(x))dx - \int V(x)\,\rho(x)dx + \frac{1}{2}\iint \frac{\rho(x)\,\rho(y)}{|x-y|}\,dxdy$$

where $j(\rho)$ is a C^1 convex function such that $j(0) = j'(0) = 0$ and $V(x)$ is an arbitrary function — not just a Coulomb potential. The Euler "equation" corresponding to (1) is the following :

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

where λ is a constant — the Lagrange multiplier arising from the constraint $\int \rho = I$ — and $B\rho = \frac{1}{|x|} * \rho$.

Problem (2) consists of finding a constant λ and a function ρ for which (2) holds. In [2] (see also [4]) one shows that if ρ is a solution of (1) then ρ is a solution of (2) [under no restrictions]. Conversely if ρ is a solution of (2) and if

(3) $j^*(V - C) \in L^1(\mathbb{R}^3)$ for some constant C,

then ρ is a solution of (1). Here $j^*(t) = \sup_{s \geq 0} \{ts - j(s)\}$ denotes the conjugate convex function of j. Observe that if $j(\rho) = \rho^p$, and $V(x)$ is a Coulomb potential, then (3) holds only when $p > \frac{3}{2}$. In fact when $p \leq \frac{3}{2}$, then $\inf_K \mathcal{E} = -\infty$; assumption (3) is imposed essentially in order to guarantee that $\inf_K \mathcal{E} > -\infty$.

Our main results — which extends Theorem 1 — is the following.

Theorem 2 Assume

(4) $V \in \frac{1}{|x|} * L^1$ (i.e. $\Delta V \in L^1$ and $V(x) \to 0$ at infinity in some "weak" sense).

(5) $V > 0$ on a set of positive measure.

Then :

(A) There exists a critical value I_0 , $0 < I_0 < \infty$, depending on j and V such that

(a) If $0 < I \leq I_0$, Problem (2) has a unique solution.

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

(B) Assume $I < I_0$, and $V(x) \to 0$ as $|x| \to \infty$ in the usual sense [or $I = I_0$ and $|x| V(x) \to 0$ as $|x| \to \infty$] then the solution ρ of (2) has compact support.

(C) Assume

(6) $j(\rho) \sim \rho^p$ for $\rho \sim 0$ with $p \geq 4/3$,

then
$$\int -\Delta V \leq I_0 \leq \int (-\Delta V)^+.$$

In particular
$$I_0 = \int -\Delta V \quad \text{if} \quad -\Delta V \geq 0.$$

(D) Instead of (4), assume now the weaker condition

($\tilde{4}$) $V \in \frac{1}{|x|} * \mathcal{M}$ ($\mathcal{M}$ = space of bounded measures on $\mathbb{R}^3$).

Suppose also that

(7) $j(\rho) \sim \rho^p$ for $\rho \sim \infty$ with $p > 4/3$.

Then (A), (B), (C) still hold.

Remarks

1) Note that if $V(x)$ is a Coulomb potential, then ($\tilde{4}$) holds, but (4) does not hold.

2) As we shall see later if $j(\rho) \sim \rho^p$ for $\rho \sim \infty$ with $p \leq 4/3$, and V is a Coulomb potential, then (2) has no solution.

Sketch of the proof of Theorem 2

First, observe that in (2) we must have $\lambda \geq 0$. Indeed we have $j'(\rho) - V_+ B_\rho \geq -\lambda$ on $\mathbb{R}^3$; as $|x| \to \infty$, $\rho \to 0$, $V \to 0$, $B_\rho \to 0$ (in a weak sense) and thus $\lambda \geq 0$. We introduce now as new unknown the function

$$u = V - B_\rho$$

so that $-\Delta u = -\Delta V - \rho$ (more precisely $-\Delta B_\rho = 4\pi\rho$, but we shall ignore 4π!). Thus (2) becomes

$$j'(\rho) = u - \lambda \quad \text{on } [\rho > 0]$$

$$j'(\rho) \geq u - \lambda \quad \text{on } [\rho = 0]$$

i.e. $\rho = \gamma(u - \lambda)$ with

$$\gamma(t) = \begin{cases} 0 & \text{for } t \leq 0 \\ (j')^{-1}(t) & \text{for } t \geq 0 \end{cases}$$

[$(j')^{-1}$ denotes the reciprocal function of the function j'].

Finally (2) is equivalent to finding a constant $\lambda \geq 0$ and a function u such that

$$(\tilde{2}) \begin{cases} -\Delta u + \gamma(u-\lambda) = -\Delta V \\ u(x) \to 0 \quad \text{as} \quad |x| \to \infty \\ \int \gamma(u-\lambda) = I \end{cases}$$

In order to solve $(\tilde{2})$ we first <u>freeze</u> $\lambda \geq 0$. For any <u>fixed</u> $\lambda \geq 0$ there exists a unique solution u_λ of the equation

$$\begin{cases} -\Delta u_\lambda + \gamma(u_\lambda - \lambda) = -\Delta V \\ u_\lambda(\infty) = 0 \end{cases}$$

and such that $\gamma(u_\lambda - \lambda) \in L^1$. This follows from a result of [3] :

<u>Lemma 1</u> (BBC). Assume $f \in L^1(\mathbb{R}^3)$ and $\beta: \mathbb{R} \to \mathbb{R}$ is any continuous, nondecreasing function with $\beta(0) = 0$. Then there exists a unique u solution of

$$\begin{cases} -\Delta u + \beta(u) = f \\ u(\infty) = 0 \end{cases}$$

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

Next, for every $\lambda \geq 0$ we set $I(\lambda) = \int \gamma(u_\lambda - \lambda)$. Problem $(\tilde{2})$ amounts to find a unique $\lambda \geq 0$ such that $I(\lambda) = I$ ($I > 0$ is given). Therefore we must study the function $\lambda \to I(\lambda)$:

<u>Lemma 2</u> The function $\lambda \to I(\lambda)$ is continuous nonincreasing on $[0,\infty)$. It is strictly decreasing on the set $\{\lambda \,;\, I(\lambda) > 0\}$. In addition $I(0) > 0$ and $I(\lambda) \to 0$ as $\lambda \to \infty$.

For the proof of Lemma 2 we refer to [2], [4]. It is essentially a consequence of the maximum principle. Note that $I(0) > 0$ follows from (5). Indeed suppose $I(0) = 0$, then $\gamma(u_0) = 0$ a.e. and $u_0 \leq 0$ a.e. Thus $-\Delta u_0 = -\Delta V$, and $u_0 = V$ a.e. — a contradiction with (5). Assertion (A) in Theorem 2 can be obtained from Lemma 2 with $I_0 = I(0)$.

Proof of Assertion (B)

Given $0 < I < I_0$ we have a unique $\lambda > 0$ such that $I(\lambda) = I_0$ and $\rho = \gamma(u_\lambda - \lambda)$. Since $\gamma \geq 0$ we have $-\Delta u_\lambda \leq -\Delta V$ and by the maximum principle $u_\lambda \leq V$. Therefore $\rho \leq \gamma(V - \lambda)$ and ρ has compact support since $V(x) \to 0$ as $|x| \to \infty$. When $I = I_0$, we have $\lambda = 0$ and $\rho = \gamma(u_0)$ with $-\Delta u_0 + \gamma(u_0) = -\Delta V$. Suppose $\int \gamma(u_0) > 0$ (otherwise $\rho = \gamma(u_0) \equiv 0$).

Choose R such that $\int_{|x|<R} \gamma(u_0) > 0$ and let

$$1_R(x) = \begin{cases} 1 & \text{if } |x| < R \\ 0 & \text{if } |x| \geq R . \end{cases}$$

Then $-\Delta u_0 + \gamma(u_0) 1_R \leq -\Delta V$ and so $u_0 \leq V - \frac{1}{|x|} * (\gamma(u_0) 1_R)$.

As $|x| \to \infty$, $\frac{1}{|x|} * \gamma(u_0) 1_R \sim \frac{C}{|x|}$ where $C = \int_{|x|<R} \gamma(u_0)$.

Since $\lim_{|x| \to \infty} |x|\, V(x) = 0$, it follows that $u_0 \leq 0$ far out and thus $\rho = \gamma(u_0) = 0$ far out.

Proof of Assertion (C).

We have $-\Delta u_0 + \gamma(u_0) = -\Delta V$. It follows from a result of [3] that $\int \gamma(u_0)^+ \leq \int (-\Delta V)^+$ (here no assumption about γ is needed). On the other hand we have $\int -\Delta u_0 + I_0 = \int -\Delta V$ and so we have to show that $\int \Delta u_0 \geq 0$. Suppose by contradiction that $\int \Delta u_0 < 0$. It follows that (in some weak sense)

$u_0(x) \sim \frac{C}{|x|}$ as $|x| \to \infty$ with $C = -\int \Delta u_0 > 0$.

Hence $\gamma(u_0) \sim \gamma\left(\frac{C}{|x|}\right)$ as $|x| \to \infty$. On the other hand if $j(\rho) \sim \rho^p$ as $\rho \to 0$ with $p \geq 4/3$, then

$\gamma\left(\frac{C}{|x|}\right) \notin L^1(|x| > 1)$ — a contradiction.

Proof of Assertion (D).

Using the same approach as above we must first solve the equation

$$\begin{cases} -\Delta u + \gamma(u - \lambda) = -\Delta V \\ u(\infty) = 0 \end{cases}$$

for fixed λ , with ΔV a measure. This is not always possible and we have to impose some restriction about the behavior of γ at infinity. The analogue of BBC lemma for measures is the following.

Lemma 3 Let $\beta: \mathbb{R} \to \mathbb{R}$ be a continuous nondecreasing function with $\beta(0) = 0$ and

(8) $\beta(\pm\frac{1}{|x|}) \in L^1 \; (|x| < 1)$

Then for every $\mu \in \mathcal{M}$, there exists a unique u solution of

(9) $$\begin{cases} -\Delta u + \beta(u) = \mu \quad \text{on } \mathbb{R}^3 \\ u(\infty) = 0 \end{cases}$$

For the proof of Lemma 3, see [2] or [4]. Replacing BBC Lemma by Lemma 3 we may now proceed with the same proof as above. Note that (8) is satisfied when $j(\rho) \sim \rho^p$ as $\rho \to \infty$ with $p > 4/3$.

Discussion of Lemma 3.

Assumption (8) is, in some sense, necessary for the solvability of (9). We may understand this in two ways :

(a) Suppose that $\mu = \delta$ = Dirac mass at 0 and suppose that (9) has a solution. Near $x = 0$, $\beta(u)$ is negligible compared to δ and thus $-\Delta u$ "feels" only δ . Therefore, $u(x) \sim \frac{1}{|x|}$ as $|x| \to 0$. Hense $\beta(u) \sim \beta(\frac{1}{|x|})$ near $x = 0$ and we must have $\beta(\frac{1}{|x|}) \in L^1 \; (|x| < 1)$.

(b) Suppose that $\mu = \delta$ and (for simplicity) that $\beta(u) = u^q$. Suppose that (9) has a solution u. Set $\Omega = \{ x \, ; \, |x| < 1 \}$. In particular $u \in L^q_{loc}(\Omega \setminus \{0\})$ and satisfies

$$-\Delta u + u^q = 0,$$

in the sense of distributions in $D'(\Omega \setminus \{0\})$. Such functions have been studied in [5], [6], [8]. The results are the following:

(i) If $q \geq 3$, then $u \in C^2(\Omega)$ and satisfies $-\Delta u + u^q = 0$ in Ω. In particular, it is impossible to have in Ω a solution of $-\Delta u + u^q = \delta$. The conclusion can also be expressed in the following way : "every isolated singularity of the equation $-\Delta u + u^q = 0$ is removable."

(ii) If $1 < q < 3$, then u may have a singularity at 0. The nature of the singularity can be completely described :

(α) either u is C^2 at 0

(β) or $u(x) \sim \frac{C}{|x|}$ as $|x| \to 0$, where $C > 0$ is an arbitrary constant

(γ) or $u(x) \sim \frac{C_q}{|x|^{\frac{2}{q-1}}}$ as $|x| \to 0$ where

$$C_q = \left[\left(\frac{2}{q-1} \right) \left(\frac{2q}{q-1} - 3 \right) \right]^{\frac{1}{q-1}}.$$

Such results show the importance of the study of singular solutions of nonlinear partial differential equations. A mumber of recent works have been devoted to this subject :

Gidas - Spruck (and Caffarelli) for singular solutions of $-\Delta u = u^q$, Uhlenbeck for singular solutions of Yang - Mills equations, Brezis - Friedman for singular solutions of nonlinear heat equations etc...

We conclude by mentioning a modification of the Thomas - Fermi problem studied in [1]. We consider Problem (1) with

$$\mathcal{E}(\rho) = \int |\nabla\sqrt{\rho}|^2 + \frac{1}{p}\int \rho^p - \int V\rho + \frac{1}{2}\iint \frac{\rho(x)\,\rho(y)}{|x-y|}\,dxdy .$$

Here $V(x) = \sum_{i=1}^{k} \frac{m_i}{|x-a_i|}$, $m_i > 0$, $a_i \in \mathbb{R}^3$.

The correction term $\int |\nabla\sqrt{\rho}|^2$ has been proposed by Van Weizsacker; we refer to this problem as Problem TFW. The main result of [1] is the following :

<u>Theorem 3</u> There is a critical value I_c such that

(a) If $0 < I \leq I_c$, there is a unique solution of Problem TFW.

(b) If $I > I_c$, there is no solution of TFW.

(c) When $p \geq 4/3$, then $I_c \geq I_0 = \sum_{i=1}^{k} m_i$.

(d) When $p \geq 5/3$ and $k = 1$, then $I_c > I_0$.

<u>Remarks</u>

1) A major difference between TF and TFW is that, even for $I < I_c$ the solution ρ of TFW does <u>not</u> have compact support.

2) It would be interesting to determine whether $I_c > I_0$ when $p \geq 5/3$ and $k \geq 2$ (molecular case).

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