A Remark on An Efficient Real Space Method for Orbital-Free Density-Functional Theory, by C.J. García-Cervera

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Abstract. In this short note we clarify some issues regarding the existence of minimizers for the Thomas-Fermi-von Weizsacker energy functional in orbital-free density functional theory, when the Wang-Teter corrections are included.

1 Introduction

In [1] it was claimed that there always exists a minimizer; however, the statement of Theorem 2.1 is incomplete. In this note we present the full statement, with a detailed proof.

The theorem stated in [1] holds as long as the number of electrons is below a certain critical value. The correct statement for the theorem in [1] is:

Theorem 1.1 (Existence of minimizers). Given $v \in C^\infty(\Omega)$, and $K_{WT} \in L^2_{loc}(\mathbb{R}^3)$, consider the problem

$$\inf_{u \in \mathcal{B}} F[u],$$

where $F$ and $\mathcal{B}$ are

$$F[u] = \frac{1}{2} \int_\Omega |\nabla u|^2 - \frac{7C_{TF}N^{2/3}}{25} \int_\Omega u^{10/3} + \frac{4C_{TF}N^{2/3}}{5} \int_\Omega |u|^{5/3} \left( K_{WT} * |u|^{5/3} \right) + \frac{N}{2} \int_\Omega u^2 \left( \frac{1}{|x|} * u^2 \right) - \frac{3}{4} \left( \frac{3N}{\pi} \right)^{1/3} \int_\Omega u^{8/3} + \int_\Omega u^2 \varepsilon(Nu^2) + \int_\Omega v(x)u^2(x) \, dx,$$ (1.2)

and

$$\mathcal{B} = \left\{ u \in H^1_0(\Omega) \left| u \geq 0, \int_\Omega u^2 = 1 \right. \right\}. $$ (1.3)

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In (1.2), the set $\Omega$ is open and bounded, and $\varepsilon$ is defined as

$$
\varepsilon(r_s) = \begin{cases} 
\frac{\gamma}{1+\beta_1 \sqrt{r_s} + \beta_2 r_s}, & r_s \geq 1, \\
A \ln(r_s) + B + C r_s \ln(r_s) + D r_s, & r_s \leq 1,
\end{cases}
$$

(1.4)

where $r_s = \left(\frac{3}{4\pi Nu^2}\right)^{1/3}$; the parameters used are $\gamma = -0.1423$, $\beta_1 = 1.0529$, $\beta_2 = 0.3334$, $A = 0.0311$, $B = -0.048$, and $C = 2.01915194062 \times 10^{-3}$ and $D = -1.163206637891 \times 10^{-2}$ are chosen so that $\varepsilon(r)$ and $\varepsilon'(r)$ are continuous at $r = 1$ [6].

Then, there exists $N_0 > 0$ such that:

1. If $N < N_0$ then $\exists u^* \in B$ such that

$$
F[u^*] = \min_{u \in B} F[u].
$$

(1.5)

2. If $N > N_0$ then

$$
\inf_{u \in B} F[u] = -\infty.
$$

(1.6)

Proof: The second part of the theorem was proved in [2,3]. We outline the proof here for completeness. Consider a compactly supported function $u_0 \in C^\infty_0(\Omega)$, such that

$$
\int_\Omega u_0^2 = 1.
$$

(1.7)

Given $x_0 \in \Omega$, $\exists \delta_0 > 0$ such that $B(x_0, \delta_0) \subset \Omega$. Consider the rescaling

$$
u_\delta(x) = \frac{1}{\delta^{3/2}} u_0 \left(\frac{x - x_0}{\delta}\right), \quad 0 < \delta < \delta_0.
$$

(1.8)

Then $u_\delta \in B$, and

$$
F[u_\delta] = \frac{1}{\delta^2} \left( \frac{1}{2} \int_\Omega |\nabla u_0|^2 - \frac{7C_{TF}N^{2/3}}{25} \int_\Omega u_0^{10/3} \right) + O \left( \frac{1}{\delta} \right).
$$

(1.9)

Define

$$
A_0 = \inf_{u \in H^1_0(\Omega), \|u\|_2 = 1} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^{10/3}} > 0.
$$

(1.10)

Then if $A_0/2 < \frac{7C_{TF}N^{2/3}}{25}$, we can choose $u_0$ so that the leading term in (1.9) is negative, and when $\delta \to 0$, the desired result follows.

For the existence of minimizers, assume that $N$ is such that such that $A_0/2 > \frac{7C_{TF}N^{2/3}}{25}$. By lemma 1.1, there exist $C > 0$, $\delta > 0$ such that

$$
F[u] \geq \frac{1}{2} \int_\Omega |\nabla u|^2 - \left( \frac{7C_{TF}N^{2/3}}{25} + \delta \right) \int_\Omega u^{10/3} - C
$$

\begin{align*}
&\geq \left( \frac{1}{2} - \frac{1}{A_0} \left( \frac{7C_{TF}N^{2/3}}{25} + \delta \right) \right) \int_\Omega |\nabla u|^2 \geq \tau \int_\Omega |\nabla u|^2 - C,
\end{align*}

(1.11)
where \( \tau > 0 \). Therefore the functional is coercive, and the result follows from now from standard arguments in the Calculus of Variations [4], involving the Sobolev Embedding, and the Rellich-Kondrachov compactness theorem. \( \square \)

**Remark 1.1.** Note that given \( \Omega \subset \mathbb{R}^3 \), then

\[
0 < A_0 = \inf_{u \in \mathcal{A}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^{10/3}},
\]

where

\[
\mathcal{A} = \left\{ u \in H^1_0(\Omega) | u \geq 0, \int_\Omega u^2 = 1 \right\}.
\]

By the Gagliardo-Nirenberg inequality, \( \exists C_1 > 0 \) such that

\[
\left( \int_\Omega u^6 \right)^{1/3} \leq C_1 \int_\Omega |\nabla u|^2.
\]

By the Riesz-Thorin theorem, since \( u \in L^2(\Omega) \cap L^6(\Omega) \), and

\[
\frac{3}{10} = \frac{\theta}{2} + \frac{1-\theta}{6},
\]

with \( \theta = 2/5 \), we get

\[
\left( \int_\Omega u^{10/3} \right)^{3/10} \leq \left( \int_\Omega u^2 \right)^{\theta/2} \left( \int_\Omega u^6 \right)^{(1-\theta)/6},
\]

and therefore, since \( \|u\|_2 = 1 \),

\[
\int_\Omega u^{10/3} \leq \left( \int_\Omega u^6 \right)^{5(1-\theta)/9} = \left( \int_\Omega u^6 \right)^{1/3} \leq C_1 \int_\Omega |\nabla u|^2.
\]

Therefore,

\[
\inf_{u \in \mathcal{A}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^{10/3}} \geq C_1^{-1} > 0.
\]

In [1] it was proved that \( K_{WT} \in L^2(\mathbb{R}^3) \). In the following lemma we establish the necessary inequalities to prove the coercivity of energy functional (1.2).

**Lemma 1.1.** Assume \( K_{WT} \in L^2(\mathbb{R}^3), v \in L^\infty(\Omega) \), and \( \varepsilon \) is defined as in 1.4. Then, there exist constants \( C_i, i = 1, \ldots, 5 \), dependent only on the domain \( \Omega \) and on \( N \), such that for all \( u \in H^1_0(\Omega) \) satisfying \( \|u\|_2 = 1 \),

1. \[
\left| \int_\Omega |u|^{5/3} (K_{WT} \ast |u|^{5/3}) \right| \leq C_1 \|u^{5/3}\|_2 \|u^{5/3}\|_1 \|K_{WT}\|_2.
\]
2. \[
\left| \int_{\Omega} \left( u^2 \ast \frac{1}{|x|} \right) u^2 \right| \leq C_2 \|u^2\|_{2}^{5/3} \|u\|_{2}^{7/3} .
\] (1.20)

3. \[
\left| \int_{\Omega} u^{8/3} \right| \leq C_3 \|u^{5/3}\|_{2} \|u\|_{2} .
\] (1.21)

4. \[
\left| \int_{\Omega} u^2 \epsilon(Nu^2) \right| \leq C_4 + C_5 \left( \int_{\Omega} |u|^{10/3} \right)^{3/4} .
\] (1.22)

Proof:

1. Since $K_{WT} \in L^2$, by the Cauchy-Schwarz inequality, followed by Young’s inequality:
\[
\left| \int_{\Omega} |u|^{5/3} \left( K_{WT} \ast |u|^{5/3} \right) \right| \leq \|u^{5/3}\|_{2} \|K_{WT} \ast |u|^{5/3}\|_{2} \leq C_1 \|u^{5/3}\|_{2} \|K_{WT}\|_{2} \|u^{5/3}\|_{1} .
\] (1.23)

Note that since $\|u\|_{2} = 1$, by Hölder’s inequality, $\|u^{5/3}\|_{1} \leq |\Omega|^{1/6}$.

2. This inequality was proved in [5] (Theorem IV.1, page 75).

3. This follows from the Cauchy-Schwarz inequality:
\[
\left| \int_{\Omega} u^{8/3} \right| = \left| \int_{\Omega} u^{5/3} u \right| \leq C \|u^{5/3}\|_{2} \|u\|_{2} .
\] (1.24)

4. From the definition of $\epsilon$, we get that
\[
\left| \int_{\Omega} u^2 \epsilon(Nu^2) \right| \leq C_1 + \tilde{C}_2 \left( \int_{|u| \geq 1} u^2 \log |u| \right) \leq C_1 + \tilde{C}_2 \left( \int_{\Omega} |u|^{5/2} \right) \leq C_1 + C_2 \left( \int_{\Omega} |u|^{10/3} \right)^{3/4} .
\] (1.25)

This concludes the proof.

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References


