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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 Weiszacker 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* $v \in C^\infty(\overline{\Omega})$, *and* $K_{WT} \in L^2_{loc}(\mathbb{R}^3)$, *consider the problem*

$$\inf_{u\in\mathcal{B}} F[u], \tag{1.1}$$

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

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

and

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

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In (1.2), the set Ω is open and bounded, and ε is defined as

$$\varepsilon(r_s) = \begin{cases} \frac{\gamma}{1+\beta_1\sqrt{r_s}+\beta_2 r_s}, & r_s \geq 1, \\ A\ln(r_s) + B + Cr_s\ln(r_s) + Dr_s, & r_s \leq 1, \end{cases} \tag{1.4}$$

where $r_s = \left(\frac{3}{4\pi N u^2}\right)^{1/3}$; the parameters used are $\gamma = -0.1423$, $\beta_1 = 1.0529$, $\beta_2 = 0.3334$, $A = 0.0311$, $B = -0.048$, and $C = 2.019151940622 \times 10^{-3}$ 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 $\exists u^* \in \mathcal{B}$ such that*

$$F[u^*] = \min_{u\in\mathcal{B}} F[u]. \tag{1.5}$$

2. *If $N > N_0$ then*

$$\inf_{u\in\mathcal{B}} F[u] = -\infty. \tag{1.6}$$

Proof: The second part of the theorem was proved in [2,3]. We outline the proof here for completeness. Consider a compactly supported function $u_0 \in C_0^\infty(\Omega)$, such that

$$\int_\Omega u_0^2 = 1. \tag{1.7}$$

Given $\mathbf{x}_0 \in \Omega$, $\exists \delta_0 > 0$ such that $B(\mathbf{x}_0, \delta_0) \subset \Omega$. Consider the rescaling

$$u_\delta(\mathbf{x}) = \frac{1}{\delta^{3/2}} u_0\left(\frac{\mathbf{x}-\mathbf{x}_0}{\delta}\right), \quad 0 < \delta < \delta_0. \tag{1.8}$$

Then $u_\delta \in \mathcal{B}$, and

$$F[u_\delta] = \frac{1}{\delta^2}\left(\frac{1}{2}\int_\Omega |\nabla u_0|^2 - \frac{7C_{TF}N^{2/3}}{25}\int_\Omega u_0^{10/3}\right) + O\left(\frac{1}{\delta}\right). \tag{1.9}$$

Define

$$A_0 = \inf_{u\in H_0^1(\Omega),\ \|u\|_2=1} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^{10/3}} > 0. \tag{1.10}$$

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

$$\begin{aligned} F[u] &\geq \frac{1}{2}\int_\Omega |\nabla u|^2 - \left(\frac{7C_{TF}N^{2/3}}{25} + \delta\right)\int_\Omega u^{10/3} - C \\ &\geq \left(\frac{1}{2} - \frac{1}{A_0}\left(\frac{7C_{TF}N^{2/3}}{25} + \delta\right)\right)\int_\Omega |\nabla u|^2 \geq \tau\int_\Omega |\nabla u|^2 - C, \end{aligned} \tag{1.11}$$

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 $\Omega \subset \mathbf{R}^3$, then

$$0 < A_0 = \inf_{u \in \mathcal{A}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^{10/3}}, \tag{1.12}$$

where

$$\mathcal{A} = \left\{ u \in H_0^1(\Omega) | u \geq 0, \int_\Omega u^2 = 1 \right\}. \tag{1.13}$$

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

$$\left(\int_\Omega u^6 \right)^{1/3} \leq C_1 \int_\Omega |\nabla u|^2. \tag{1.14}$$

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

$$\frac{3}{10} = \frac{\theta}{2} + \frac{1-\theta}{6}, \tag{1.15}$$

with $\theta = 2/5$, we get

$$\left(\int_\Omega u^{10/3} \right)^{3/10} \leq \left(\int_\Omega u^2 \right)^{\theta/2} \left(\int_\Omega u^6 \right)^{(1-\theta)/6}, \tag{1.16}$$

and therefore, since $\|u\|_2 = 1$,

$$\int_\Omega u^{10/3} \leq \left(\int_\Omega u^6 \right)^{5(1-\theta)/9} = \left(\int_\Omega u^6 \right)^{1/3} \leq C_1 \int_\Omega |\nabla u|^2. \tag{1.17}$$

Therefore,

$$\inf_{u \in \mathcal{A}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^{10/3}} \geq C_1^{-1} > 0. \tag{1.18}$$

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 ε is defined as in 1.4. Then, there exist constants C_i, $i = 1, \ldots, 5$, dependent only on the domain Ω and on N, such that for all $u \in H_0^1(\Omega)$ satisfying $\|u\|_2 = 1$,

1. $$\left| \int_\Omega |u|^{5/3} \left(K_{WT} * |u|^{5/3} \right) \right| \leq C_1 \|u^{5/3}\|_2 \|u^{5/3}\|_1 \|K_{WT}\|_2. \tag{1.19}$$

2.
$$\left|\int_\Omega \left(u^2 * \frac{1}{|\mathbf{x}|}\right) u^2\right| \leq C_2 \|u^2\|_{5/3}^{5/6} \|u\|_2^{7/3}. \tag{1.20}$$

3.
$$\left|\int_\Omega u^{8/3}\right| \leq C_3 \|u^{5/3}\|_2 \|u\|_2. \tag{1.21}$$

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

Proof:

1. Since $K_{WT} \in L^2$, by the Cauchy-Schwarz inequality, followed by Young's inequality:
$$\left|\int_\Omega |u|^{5/3} \left(K_{WT} * |u|^{5/3}\right)\right| \leq \|u^{5/3}\|_2 \|K_{WT} * |u|^{5/3}\|_2 \leq C_1 \|u^{5/3}\|_2 \|K_{WT}\|_2 \|u^{5/3}\|_1. \tag{1.23}$$
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:
$$\left|\int_\Omega u^{8/3}\right| = \left|\int_\Omega u^{5/3} u\right| \leq C \|u^{5/3}\|_2 \|u\|_2. \tag{1.24}$$

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

This concludes the proof.

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