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SHORT NOTE

A Remark on "An Efficient Real Space Method for Orbital-Free Density-Functional Theory"

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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.

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

$$\inf_{u\in\mathcal{B}} F[u], \tag{1}$$

where F and $\mathcal{B}$ are

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

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and

$$\mathcal{B}=\left\{u\in H_0^1(\Omega)\middle| u\geq 0,\ \int_\Omega u^2=1\right\}. \tag{3}$$

In (2), *the set* Ω *is open and bounded, and star-shaped with respect to* 0; ε *is defined as*

$$\varepsilon(Nu^2)=\begin{cases} \dfrac{\gamma}{1+\beta_1\sqrt{r_s}+\beta_2 r_s}, & r_s\geq 1,\\ A\ln(r_s)+B+Cr_s\ln(r_s)+Dr_s, & r_s\leq 1,\end{cases} \tag{4}$$

where $r_s=\left(4\pi Nu^2/3\right)^{-\frac{1}{3}}$; *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*

$$F[u^*]=\min_{u\in\mathcal{B}}F[u]. \tag{5}$$

2. *If* $N>N_0$ *then*

$$\inf_{u\in\mathcal{B}}F[u]=-\infty. \tag{6}$$

Proof. The second part of the theorem was proved in [2, 3]. We outline the proof here for completeness. Since $0\in\Omega$, $\exists\delta_0>0$ such that $B(0,\delta_0)\subset\Omega$. Consider a compactly supported function $u_0\in C_0^\infty(B(0,1))$, such that

$$\int_{\mathbb{R}^3}u_0^2=1, \tag{7}$$

and consider the rescaling

$$u_\delta(\mathbf{x})=\frac{1}{\delta^{3/2}}u_0\left(\frac{\mathbf{x}}{\delta}\right),\quad 0<\delta<\delta_0. \tag{8}$$

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

$$F[u_\delta]=\frac{1}{\delta^2}\left(\frac{1}{2}\int_\Omega|\nabla u_0|^2-\frac{7C_{TF}N^{2/3}}{25}\int_\Omega u_0^{10/3}\right)+\mathcal{O}\left(\frac{1}{\delta}\right). \tag{9}$$

Define

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

Then if $A_0/2<7C_{TF}N^{2/3}/25$, we can choose u_0 so that the leading term in (9) is negative, and when $\delta\to 0$, the desired result follows.

For the existence of minimizers, assume that N is such that $A_0/2 > 7C_{TF}N^{2/3}/25$. By Lemma 1, there exist $C>0$, $\delta>0$ such that

$$F[u] \geq \frac{1}{2}\int_\Omega |\nabla u|^2 - \left(\frac{7C_{TF}N^{2/3}}{25} + \delta\right)\int_\Omega u^{10/3} - C$$
$$\geq \left(\frac{1}{2} - \frac{1}{A_0}\left(\frac{7C_{TF}N^{2/3}}{25} + \delta\right)\right)\int_\Omega |\nabla u|^2 \geq \tau \int_\Omega |\nabla u|^2 - C, \tag{11}$$

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. Note that given $\Omega \subset \mathbf{R}^3$, then

$$0 < A_0 = \inf_{u\in\mathcal{A}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^{10/3}}, \tag{12}$$

where

$$\mathcal{A} = \left\{ u \in H_0^1(\Omega) | u \geq 0,\ \int_\Omega u^2 = 1 \right\}. \tag{13}$$

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

$$\left(\int_\Omega u^6\right)^{1/3} \leq C_1 \int_\Omega |\nabla u|^2. \tag{14}$$

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

$$\frac{3}{10} = \frac{\theta}{2} + \frac{1-\theta}{6}, \tag{15}$$

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

$$\left(\int_\Omega u^{10/3}\right)^{3/10} \leq \left(\int_\Omega u^2\right)^{\theta/2} \left(\int_\Omega u^6\right)^{(1-\theta)/6}, \tag{16}$$

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

$$\int_\Omega u^{10/3} \leq \left(\int_\Omega u^6\right)^{5(1-\theta)/9} = \left(\int_\Omega u^6\right)^{1/3} \leq C_1 \int_\Omega |\nabla u|^2. \tag{17}$$

Therefore,

$$\inf_{u\in\mathcal{A}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^{10/3}} \geq C_1^{-1} > 0. \tag{18}$$

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 (2).

Lemma 1. *Assume $K_{WT} \in L^2(\mathbb{R}^3)$, $v \in L^\infty(\Omega)$, and ε is defined as in (4). Then, there exist constants C_i, $i=1,\cdots,5$, dependent only on the domain Ω and on N, such that for all $u \in H_0^1(\Omega)$ satisfying $\|u\|_2 = 1$,*

$$\left| \int_\Omega |u|^{5/3} \left(K_{WT} * |u|^{5/3} \right) \right| \le C_1 \|u^{5/3}\|_2 \|u^{5/3}\|_1 \|K_{WT}\|_2; \tag{19}$$

$$\left| \int_\Omega \left(u^2 * \frac{1}{|\mathbf{x}|} \right) u^2 \right| \le C_2 \|u^2\|_{5/3}^{5/6} \|u\|_2^{7/3}; \tag{20}$$

$$\left| \int_\Omega u^{8/3} \right| \le C_3 \|u^{5/3}\|_2 \|u\|_2; \tag{21}$$

$$\left| \int_\Omega u^2 \epsilon(Nu^2) \right| \le C_4 + C_5 \left(\int_\Omega |u|^{10/3} \right)^{3/4}. \tag{22}$$

Proof. Since $K_{WT} \in L^2$, by the Cauchy-Schwarz inequality, followed by Young's inequality:

$$\begin{aligned} \left| \int_\Omega |u|^{5/3} \left(K_{WT} * |u|^{5/3} \right) \right| &\le \|u^{5/3}\|_2 \|K_{WT} * |u|^{5/3}\|_2 \\ &\le C_1 \|u^{5/3}\|_2 \|K_{WT}\|_2 \|u^{5/3}\|_1. \end{aligned} \tag{23}$$

Note that since $\|u\|_2 = 1$, by Hölder's inequality, $\|u^{5/3}\|_1 \le |\Omega|^{1/6}$. This gives (19). The inequality (20) was proved in [5] (Theorem IV.1, page 75). The estimate (21) follows from the Cauchy-Schwarz inequality:

$$\left| \int_\Omega u^{8/3} \right| = \left| \int_\Omega u^{5/3} u \right| \le C \|u^{5/3}\|_2 \|u\|_2. \tag{24}$$

From the definition of ϵ, we get that

$$\begin{aligned} &\left| \int_\Omega u^2 \epsilon(Nu^2) \right| \le C_1 + \widetilde{C}_2 \left| \int_{|u| \ge \frac{3}{4\pi N}} u^2 \log|u| \right| \\ \le\, & C_1 + \widehat{C}_2 \left| \int_\Omega |u|^{5/2} \right| \le C_1 + C_2 \left(\int_\Omega |u|^{10/3} \right)^{3/4}. \end{aligned} \tag{25}$$

This concludes the proof. $\square$

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