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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.