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On the minimizer of the Thomas-Fermi-Dirac-von Weizsäcker model

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Abstract. The energy functional of Thomas-Fermi-Dirac-von Weizsäcker model with external potential is studied. The minimizer for the functional is investigated. Furthermore, the value and some properties of the minimizer are estimated from the functional without solving the associate Euler-Lagrange equation.

1. Introduction

The Thomas-Fermi (TF) theory was proposed by Thomas and Fermi independently in 1927. Dirac in 1930 introduced the exchange correction to the theory so that the corrected model is called the Thomas-Fermi-Dirac (TFD). Then the gradient correction of the kinetic energy was added by von Weizsäcker in 1935. Those theories were placed on a firm mathematical footing by Lieb (1981) [1]. Although the Thomas-Fermi-Dirac-von Weizsäcker (TFDW) theory has not been extensively studied as the other theories, there exist some authors who studied it relativistically, such as Engel and Dreizler (1987) who discuss a systematic construction of the relativistic version of the TFDW model on the basis of field theory (QED) [2]. Moreover, Müller, Engel and Dreizler (1989) also presented an extension of the relativistic TFDW model to systems in arbitrary time-independent external four-potentials [3].

The existence of a minimizer is an interesting theme to be investigated. The existence of the minimizer for TFW model was proved by Benguria, Brezis and Lieb in 1981 [4]. The nonexistence of a minimizer for TFDW model for electrons with no external potential has been investigated by Lu and Otto [5]. They realized that the TFDW functional energy without external potential has no minimizer when the number of electrons exceed a certain positive integer. They also gave an estimation that the value of the functional is in the interval $[0, (4/5)^3]$. This current work is a part of our attempt to understand the properties of the minimizer for TFDW model of electrons in the influence of an external potential, without "touching" the associate Euler-Lagrange equation. The main result of our work here is proven by following partly the proof of a proposition in the work of Lu and Otto [5].

The TFDW energy functional for electrons with external potential V is given as

$$E(\phi) := \int_{\mathbb{R}^3} [|\nabla\phi|^2 + F(\phi^2)] dx + D(\phi^2, \phi^2) + \int_{\mathbb{R}^3} V\phi^2 dx, \quad (1)$$



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where $F(t) = t^{5/3} - t^{4/3}$ and $D(\cdot, \cdot)$ is the Coulomb interaction in \mathbb{R}^3 , i.e.

$$D(f, g) = \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x)g(y)}{|x - y|} dx dy.$$

The above functional can be rewritten as

$$E(\phi) := \int_{\mathbb{R}^3} [|\nabla\phi|^2 + \bar{F}(\phi^2)] dx + D(\phi^2, \phi^2), \tag{2}$$

where $\bar{F}(t) = t^{5/3} - t^{4/3} + Vt$.

The variational principle related to TFDW model is to find the minimizer of the TFDW functional energy, i.e. a function φ that minimizes $E(\phi)$ in the sense

$$E(\varphi) = \inf_{\phi \in X, \int \phi^2 = m} E(\phi), \tag{3}$$

for suitable function space X .

2. The estimation of the minimizer

Suppose the above functional (1) has a minimizer and we denote it by φ .

Proposition Let $b(x) = \left(\frac{4 + \sqrt{16 - 60V(x)}}{10}\right)^{3/2}$, where $V(x) \leq 4/15$ for all $x \in \mathbb{R}^3$. Then we have $\varphi(x) \in [0, b(x)]$ for a.e. $x \in \mathbb{R}^3$.

Proof. Since $E(|\varphi|) \leq E(\varphi)$, we may restrict to $\varphi \geq 0$. The $\text{argmin}_{t \geq 0} \bar{F}(t)$ is calculated as follows

$$\begin{aligned} \frac{\partial \bar{F}(t)}{\partial t} &= 0 \\ \frac{5}{3}t^{2/3} - \frac{4}{3}t^{1/3} + V &= 0 \end{aligned}$$

Let $t^{1/3} = \alpha$ then

$$\frac{5}{3}\alpha^2 - \frac{4}{3}\alpha + V = 0,$$

so we have the square root of the last equation as follows

$$\alpha_{1,2} = \frac{4 \pm \sqrt{16 - 60V}}{10},$$

and

$$t_{1,2} = \left(\frac{4 \pm \sqrt{16 - 60V}}{10}\right)^3. \tag{4}$$

Note that $V \leq 4/15$ ensures the value of critical points t to be a real number.

It is easy to show that the function $\bar{F}(t)$ assumes the minimum value at the critical point

$$t_1 = \left(\frac{4 + \sqrt{16 - 60V}}{10}\right)^3. \tag{5}$$

Take $\varphi_1 = \varphi \wedge \left(\frac{4+\sqrt{16-60V}}{10}\right)^{3/2}$ and let $m_1 = \int \varphi_1^2$. It is clear that $m_1 \leq m$. Since φ minimizes equation (1), we have

$$E(\varphi) \leq E(\varphi_1) + \inf_{\int \psi^2 = m - m_1} E(\psi). \quad (6)$$

Indeed, for any ψ with $\int \psi^2 = m - m_1$, let

$$\psi_L(x) = Z_L[\varphi_1(x) + \psi(x + Le_1)],$$

where $e_1 = (1, 0, 0) \in \mathbb{R}^3$ and Z_L is a normalization constant so that $\int \psi_L^2 = \int \varphi^2 = m$.

The value of the energy functional in ψ_L is given by

$$E(\psi_L) = \int_{\mathbb{R}^3} |\nabla \psi_L|^2 dx + \int_{\mathbb{R}^3} \bar{F}(\psi_L^2) dx + D(\psi_L^2, \psi_L^2). \quad (7)$$

The first term of (7) satisfies

$$\begin{aligned} \int_{\mathbb{R}^3} |\nabla \psi_L|^2 dx &= \int_{\mathbb{R}^3} |\nabla (Z_L[\varphi_1(x) + \psi(x + Le_1)])|^2 dx \\ &\leq Z_L^2 \left\{ \int_{\mathbb{R}^3} |\nabla \varphi_1(x)|^2 dx + \int_{\mathbb{R}^3} |\nabla \psi(x + Le_1)|^2 dx + \right. \\ &\quad \left. 2 \int_{\mathbb{R}^3} |\nabla \varphi_1(x)| |\nabla \psi(x + Le_1)| dx \right\}. \end{aligned}$$

When $L \rightarrow \infty$, then $Z_L \rightarrow 1$, $\int_{\mathbb{R}^3} |\nabla \psi(x + Le_1)|^2 dx = \int_{\mathbb{R}^3} |\nabla \psi(x)|^2 dx$, and $\int_{\mathbb{R}^3} |\nabla \varphi_1(x)| |\nabla \psi(x + Le_1)| dx \approx 0$ so that

$$\int_{\mathbb{R}^3} |\nabla \psi_L|^2 dx \leq \int_{\mathbb{R}^3} |\nabla \varphi_1(x)|^2 dx + \int_{\mathbb{R}^3} |\nabla \psi(x)|^2 dx. \quad (8)$$

Since $\bar{F}(t) = F(t) + tV$ and $\int V \psi_L^2(x) dx = \int V \varphi_1^2(x) dx + \int V \psi^2(x) dx$ when $L \rightarrow \infty$, then the second term of equation (7) satisfies

$$\int \bar{F}(\psi_L^2) dx \leq \int \bar{F}(\varphi_1^2(x)) dx + \int \bar{F}(\psi^2(x)) dx \quad (9)$$

The third term of (7) can be written as

$$\begin{aligned} D(\psi_L^2, \psi_L^2) &= \int \int \frac{\psi_L^2(x_1) \psi_L^2(x_2)}{|x_1 - x_2|^2} dx_1 dx_2 \\ &= Z_L^4 \int \int \frac{1}{|x_1 - x_2|^2} \{ \varphi_1^2(x_1) \varphi_1^2(x_2) + \varphi_1^2(x_1) \psi(x_2 + Le_1) + \\ &\quad 2\varphi_1^2(x_1) \varphi_1(x_2) \psi(x_2 + Le_1) + \\ &\quad \psi^2(x_1 + Le_1) \varphi_1^2(x_2) + \psi^2(x_1 + Le_1) \psi^2(x_2 + Le_1) + \\ &\quad 2\psi^2(x_1 + Le_1) \varphi_1(x_2) \psi(x_2 + Le_1) + \\ &\quad [2\varphi_1(x_1) \psi(x_1 + Le_1) \varphi_1^2(x_2) + 2\varphi_1(x_1) \psi(x_1 + Le_1) \psi^2(x_2 + Le_1) + \\ &\quad 4\varphi_1(x_1) \psi(x_1 + Le_1) \varphi_1(x_2) \psi(x_2 + Le_1)] \} dx_1 dx_2 \end{aligned}$$

Because of $\sigma(x)\psi(x + Le_1) = 0$ if $L \rightarrow \infty$ for every localized function σ , then

$$D(\psi_L^2, \psi_L^2) = D(\varphi_1^2, \varphi_1^2) + D(\psi^2, \psi^2) \quad (10)$$

Therefore, from equation (8), (9), and (10) we have

$$\limsup_{L \rightarrow \infty} E(\psi_L) = E(\varphi_1) + E(\psi) \tag{11}$$

We arrive at equation (6) as $E(\varphi) \leq E(\psi_L)$ for any L .

Consider the scaling $\psi_\eta = \eta^{-3/2}\psi(x/\eta)$, so $\int \psi_\eta^2 = \int \psi^2$. It is clear that $\psi_\eta \rightarrow 0$ as $\eta \rightarrow \infty$, as each term in equation (2) goes to zero. Therefore, we have $E(\varphi) \leq E(\varphi_1)$ as

$$\inf_{\int \psi^2 = m - m_1} E(\psi) \leq 0.$$

Suppose $|\{\varphi > \left(\frac{4+\sqrt{16-60V}}{10}\right)^{3/2}\}| > 0$, then as $\left(\frac{4+\sqrt{16-60V}}{10}\right)^3$ is the unique minimizer of $\bar{F}(t)$ for $t \geq 0$,

$$\int \bar{F}(\varphi_1^2) < \int \bar{F}(\varphi^2).$$

Note that $|\nabla\varphi_1| \leq |\nabla\varphi|$ and $D(\varphi_1^2, \varphi_1^2) < D(\varphi^2, \varphi^2)$, we arrive at a contradiction $E(\varphi_1) < E(\varphi)$. Therefore, $\varphi(x) \leq b(x)$ for $x \in \mathbb{R}^3$. □

For small illustration, in the case of negative Coulomb potential $V(x) = -|x|^{-1}$ we have the following graph of $b(x)$.

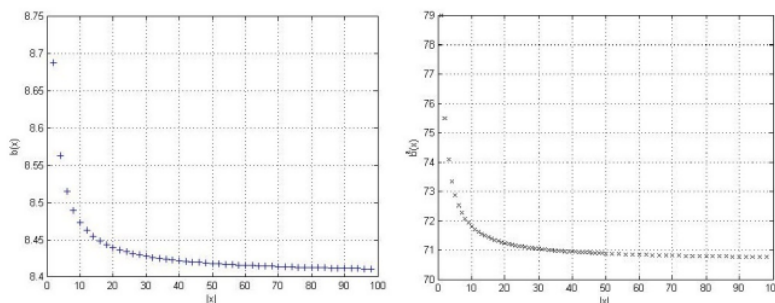


Figure 1. Left: The value of $b(x)$ with $V(x) = -|x|^{-1}$. Right: The value of $b^2(x)$ with $V(x) = -|x|^{-1}$.

3. Conclusion

The value of a minimizer is bounded from above by the "umbrella" function $b(x)$ which depends on the external potential $V(x)$.

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