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PROPERTIES OF THE POSITIVE SOLUTION OF A GENERALIZED THOMAS-FERMI-VON WEIZSÄCKER EQUATION

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I. Introduction. The Thomas-Fermi-von Weizsäcker (TFW) theory of atoms and molecules has been given a firm mathematical foundation, and many of the qualitative properties of the theory are understood and have been proven (see [19], Section VII, for a review on the subject, and references therein). In the TFW theory, the electrons are described by the positive solution of the following equation (in appropriate units)

$$-\Delta u + (cu^{4/3} - \phi)u = -\phi_0 u, \qquad \text{in } \mathbb{R}^3 \tag{1}$$

with $u \to 0$ as $|x| \to \infty$, where

$$\phi(x) = V(x) - \int \frac{u^2(y)}{|x-y|} dy \tag{2}$$

is the total electric potential and

$$V(x) = \sum_{i=1}^{k} \frac{z_i}{|x - R_i|} \tag{3}$$

is the electric potential of nuclei of charge $z_i > 0$ located at $R_i \in \mathbb{R}^3$. In equation (1), c is a positive constant and $\phi_0 \geqslant 0$ is the chemical potential. Given $u(x)$, the positive solution of (1), $u^2(x) \geqslant 0$ is the electronic density and $\int u^2\, dx$ is the total number of electrons. Here we will be concerned with the most negative ion, which corresponds to taking the chemical potential $\phi_0 = 0$ (see [19]).

It is known that equation (1), with ϕ given by (2), has a unique positive solution in

$$D = \{u \mid u(x) \geqslant 0,\ u \in L^6 \cap L^{10/3},\ \nabla u \in L^2,\ D(u^2, u^2) < \infty\},$$

where

$$D(f, f) \equiv \frac{1}{2} \int f(x) \frac{1}{|x-y|} f(y)\, dx\, dy \geqslant 0.$$

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