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Universality in the Thomas-Fermi-von Weizsäcker Model of Atoms and Molecules

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Abstract. We study the Thomas-Fermi-von Weizsäcker theory of atoms and molecules. The main result is to prove universality of the structure of very large atoms and molecules, i.e., proving that the structure converges as the nuclear charges go to infinity. Furthermore we uniquely characterize the limit density as the solution to a renormalized TFW-equation. This is achieved by characterizing the strong singularities of solutions to the non-linear TFW-system.

1. Introduction

The Thomas-Fermi-von Weizsäcker (TFW) theory for a molecule of K nuclei at positions $\mathscr{R}_1, \ldots, \mathscr{R}_K \in \mathbb{R}^3$ and with nuclear charges $z_1, \ldots, z_K \in \mathbb{R}_+$ is defined by the energy functional

$$\mathscr{E}(\psi; \underline{z}; \underline{\mathscr{R}}) = A \int_{\mathbb{R}^3} (\nabla \psi(x))^2 dx + \tfrac{3}{5}\gamma \int_{\mathbb{R}^3} (\psi(x)^2)^{5/3} dx - \sum_{j=1}^{K} z_j \int_{\mathbb{R}^3} \psi(x)^2 |x - \mathscr{R}_j|^{-1} dx + D(\psi^2, \psi^2), \tag{1}$$

where

$$D(f, g) = \tfrac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(x)^2 |x-y|^{-1} g(y)^2 dx dy. \tag{2}$$

Here $\underline{z} = (z_1, \ldots, z_K)$ and $\underline{\mathscr{R}} = (\mathscr{R}_1, \ldots, \mathscr{R}_K)$. $\mathscr{E}$ is defined on the set

$$G = \{\psi \in L^{10/3}(\mathbb{R}^3) | \psi \text{ real}, \nabla\psi \in L^2, D(\psi^2, \psi^2) < \infty\}. \tag{3}$$

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