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The Thomas–Fermi–von Weizsäcker Theory of Atoms and Molecules*

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Abstract. We place the Thomas–Fermi–von Weizsäcker model of atoms on a firm mathematical footing. We prove existence and uniqueness of solutions of the Thomas–Fermi–von Weizsäcker equation as well as the fact that they minimize the Thomas–Fermi–von Weizsäcker energy functional. Moreover, we prove the existence of binding for two very dissimilar atoms in the frame of this model.

Introduction

The Thomas–Fermi theory of atoms [1] (TF), attractive because of its simplicity, is not satisfactory because it yields an electron density with incorrect behavior very close and very far from the nucleus. Moreover, it does not allow for the existence of molecules. In order to correct this, von Weizsäcker [2] suggested the addition of an inhomogeneity correction

$$U_w(\rho) = C_w(\nabla\rho)^2/\rho \tag{1}$$

to the kinetic energy density. Here $c_w = h^2/(32\pi^2 m)$, where m is the mass of the electron. This correction has also been obtained as the first order correction to the TF kinetic energy in a semi-classical approximation to the Hartree–Fock theory [3].

The Thomas–Fermi–von Weizsäcker (henceforth TFW) energy functional for nuclei of charges $z_i > 0$ (which need not be integral) located at R_i, $i = 1, \ldots, k$ is defined by

$$\begin{aligned}\xi(\rho) = (3\pi^2)^{-2/3}\int(\nabla\rho^{1/2}(x))^2\,dx + \tfrac{3}{5}\int\rho(x)^{5/3}dx \\ - \int V(x)\rho(x)dx + \tfrac{1}{2}\iint\rho(x)\rho(y)|x-y|^{-1}dxdy,\end{aligned} \tag{2}$$

in units in which $h^2(8m)^{-1}(3/\pi)^{2/3} = 1$ and $|e| = 1$. Here $\rho(x) \geqq 0$ is the electron

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