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Analysis of the Thomas-Fermi-von Weizsäcker Equation for an Infinite Atom Without Electron Repulsion

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Abstract. The equation

$$\{-\Delta+|\psi(x)|^{2p-2}-|x|^{-1}\}\,\psi(x)=0$$

in three dimensions is investigated. Uniqueness and other properties of the positive solution are proved for $3/2<p<2$. There are two physical interpretations of this equation for $p=5/3$: (i) As the TFW equation for an infinite atom *without* electron repulsion; (ii) The positive solution, ψ, suitably scaled, is asymptotically equal to the solution of the TFW equation for an atom or molecule *with* electron repulsion in the regime where the nuclear charges are large and x is close to one of the nuclei.

I. Introduction

The equation to be analyzed here of primary physical interest is

$$\{-\Delta+|\psi(x)|^{4/3}-|x|^{-1}\}\,\psi(x)=0 \tag{1.1}$$

in three dimensions and with ψ real valued. (1.1) was introduced in [9], wherein it was asserted without proof that (1.1) has a unique, positive solution. The present paper contains that proof. If $z,\gamma,A>0$ and

$$\tilde{\psi}(z,\gamma,A,x)\equiv(z^2/A\gamma)^{3/4}\psi(zx/A), \tag{1.2}$$

then

$$\{-A\Delta+\gamma|\tilde{\psi}(x)|^{4/3}-z|x|^{-1}\}\,\tilde{\psi}(x)=0. \tag{1.3}$$

and conversely. Thus, (1.3) and (1.1) are equivalent problems.

(1.3) is to be compared with the Thomas-Fermi-von Weizsäcker (TFW) equation for a molecule [2–4, 9, 10, 13, 14]:

$$\{-A\Delta+\gamma|\hat{\psi}(x)|^{4/3}-V(x)+(|x|^{-1}*\hat{\psi}^2)(x)\}\,\hat{\psi}(x)=-\mu\hat{\psi}(x), \tag{1.4}$$

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