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On the Leading Energy Correction for the Statistical Model of the Atom: Interacting Case

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Abstract. Introducing the Hellmann-Weizsäcker functional for large angular momenta and the orbitals of the Bohr atom for small angular momenta we obtain an upper bound on the quantum mechanical ground state energy of atoms that proves Scott's conjecture.

1. Introduction

Let H be the hamiltonian of N electrons moving in the field of a nucleus of charge Z, i.e.

$$H=\sum_{i=1}^{N}\left(-\Delta_i-\frac{Z}{|\mathbf{r}_i|}\right)+\sum_{\substack{i,j=1\\ i<j}}^{N}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}$$

as a self-adjoint realization on $\bigwedge_{i=1}^{N}(L^2(\mathbb{R}^3)\otimes\mathbb{C}^q)$. In this paper we show for the ground state energy $E_Q(Z,N)$ of H:

Theorem 1.1.

$$E_Q(Z,Z)\leqq Z^{7/3}E_1^{\mathrm{TF}}(1)+\frac{q}{8}Z^2+o(Z^2),\tag{1.1}$$

where $E_Z^{\mathrm{TF}}(N)$ is the Thomas-Fermi energy of the above hamiltonian.

Combining this result with the reverse of (1.1), an inequality that has been claimed by Hughes [1], would imply

$$E_Q(Z,Z)=E_1^{\mathrm{TF}}(1)Z^{7/3}+\frac{q}{8}Z^2+o(Z^2).\tag{1.2}$$

Scott [2] claimed this result arguing that the leading energy which is given by the Thomas-Fermi energy (Lieb and Simon [3], Lieb [4], Thirring [5]) should be corrected in those regions where the assumptions of the statistical theory of the

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