BULLETIN (New Series) OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 23, Number 2, October 1990

ON THE ENERGY OF A LARGE ATOM

CHARLES L. FEFFERMAN AND LUIS A. SECO

We announce a proof of an asymptotic formula for the ground-state energy of a large atom. The early work of Thomas–Fermi, Hartree-Fock, Dirac, and Scott predicted that for an atomic number Z, the energy is $E(Z) \approx -c_0 Z^{7/3} + c_1 Z^2 - c_2 Z^{5/3}$ for known c_0, c_1, and c_2 (see [5]). Schwinger [7] observed an additional effect and set down the modified formula $E(Z) \approx -c_0 Z^{7/3} + c_1 Z^2 - \frac{10}{9} c_2 Z^{5/3}$. Our proof shows that Schwinger's formula is correct.

We give the precise formulation of the problem. For a fixed nucleus of charge Z and quantized electrons $x_1, \ldots, x_N \in \mathbf{R}^3$, the Hamiltonian $H_{N,Z}$ is the self-adjoint operator

$$\sum_{k=1}^{N} \left(-\Delta_{x_k} - \frac{Z}{|x_k|} \right) + \frac{1}{2} \sum_{i \neq j} \frac{1}{|x_i - x_j|}.$$

This operator acts on functions $\psi(x_1, \ldots, x_N)$ which satisfy the antisymmetry condition

$$\psi(x_1, \ldots, x_N) = (\operatorname{sgn} \sigma) \psi(x_{\sigma 1}, \ldots, x_{\sigma N})$$

for permutations σ. The ground-state energy $E(N, Z)$ is defined as the infimum of the spectrum of $H_{Z,N}$, and the ground-state energy of an atom is defined as $E(Z) = \inf_{N \geq 0} E(N, Z)$. We have ignored electron spin, which simplifies notation, alters no ideas, and causes some of our coefficients to differ from those in the physics literature. Our main result is as follows.

Theorem. $E(Z) = -c_0 Z^{7/3} + \frac{1}{8} Z^2 - \frac{10}{9} c_2 Z^{5/3} + O(Z^{(5/3)-a})$ *with* $a > 0$, *and* c_0, c_2 *to be described below.*

Hughes [1] and Siedentop–Weikard [9] recently proved the "Scott conjecture," i.e. $E(Z) = -c_0 Z^{7/3} + \frac{1}{8} Z^2 + O(Z^{2-a})$ with $a = 1/24$. (See also the early work of Lieb–Simon [6] on molecules,

Received by the editors May 7, 1990.
1980 *Mathematics Subject Classification* (1985 *Revision*). Primary 81G45, 81C15.
The first author is partially supported by a NSF grant at Princeton University.