Commun. Math. Phys. 116, 635-644 (1988)



Approximate Neutrality of Large-Z Ions*

Elliott H. Lieb¹, Israel M. Sigal², Barry Simon³ and Walter Thirring⁴

1 Departments of Mathematics and Physics, Princeton University, Princeton, NJ 08544, USA

2 Department of Mathematics, University of Toronto, Toronto, Canada M5S 1A1

3 Division of Physics, Mathematics and Astronomy, California Institute of Technology, Pasadena, CA 91125, USA

4 Institute for Theoretical Physics, University of Vienna, Vienna, Austria

Abstract. Let N(Z) denote the number of electrons which a nucleus of charge Z can bind in non-relativistic quantum mechanics (assuming that electrons are fermions). We prove that $N(Z)/Z \rightarrow 1$ as $Z \rightarrow \infty$.

1. Introduction

This paper is a contribution to the exact study of Coulombic binding energies in quantum mechanics. Let H(N, Z) denote the Hamiltonian

$$H(N,Z) = \sum_{i=1}^{N} \left(-\Delta_i - Z |x_i|^{-1} \right) + \sum_{i < j} |x_i - x_j|^{-1},$$

and let E(N, Z) denote its minimum over all fermion states (we suppose there are two spin states allowed, although any fixed number could be accommodated). For comparison purpose, we let $E_b(N, Z)$ denote the same minimum, but over all states (taken on a totally symmetric wave function, hence b for boson).

It is a fundamental result of Ruskai [9] for bosons, and Sigal [11] for fermions (see also Ruskai [10]) that there exists N(Z), $N_b(Z)$ so that, for all j = 0, 1, ...,

$$E(N(Z), Z) = E(N(Z) + j, Z); \quad E_b(N_b(Z), Z) = E_b(N_b(Z) + j, Z).$$

We let N(Z) (respectively $N_b(Z)$) denote the smallest number for which the first (respectively second) equality holds for all *j*. Sigal [12] showed that

$$\lim \left[N(Z)/Z \right] \le 2, \quad \lim \left[\ln N_b(Z)/\ln Z \right] \le 1, \tag{1.1}$$

and then Lieb [6,7] proved the bounds

$$N(Z) < 2Z + 1, \quad N_b(Z) < 2Z + 1 \tag{1.2}$$

which implies, in particular, that a doubly ionized hydrogen atom is unstable.

^{*} Research partially supported by the NSERC under Grant NA7901 and by the USNSF under Grants DMS-8416049 and PHY 85-15288-A01