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One-Electron Relativistic Molecules with Coulomb Interaction

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Abstract. As an approximation to a relativistic one-electron molecule, we study the operator $H = (-\Delta + m^2)^{1/2} - e^2 \sum_{j=1}^{K} Z_j |x - R_j|^{-1}$ with $Z_j \geqq 0$, $e^{-2} = 137.04$. H is bounded below if and only if $e^2 Z_j \leqq 2/\pi$, all j. Assuming this condition, the system is unstable when $e^2 \sum Z_j > 2/\pi$ in the sense that $E_0 = \inf \operatorname{spec}(H) \to -\infty$ as the $R_j \to 0$, all j. We prove that the nuclear Coulomb repulsion more than restores stability; namely $E_0 + 0.069 e^2 \sum_{i<j} Z_i Z_j |R_i - R_j|^{-1} \geqq 0$. We also show that E_0 is an increasing function of the internuclear distances $|R_i - R_j|$.

Introduction

The problem of "stability of matter" consists in proving that a system of charged particles (electrons and nuclei), interacting electromagnetically, does not collapse. In the framework of nonrelativistic Schrödinger quantum mechanics, with Coulomb interactions between the particles, a first proof of this was given by F. Dyson and A. Lenard [1]. A shorter proof, leading to a much better lower bound on the binding energy per electron, was later given by E. Lieb and W. Thirring [2]. The strategy these proofs followed was first to consider the nuclei fixed (i.e. with infinite mass); the general case (nuclei with finite mass) then follows easily. With the K nuclei at fixed positions $R_1, \ldots, R_K$, the problem then consists in proving that 1) the Hamiltonian describing N electrons and K nuclei (including also the repulsion terms between the electrons, and between the nuclei) is bounded below by a constant independent of the R_j; 2) the energy per particle, i.e. the ground state energy of the system of N

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