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One Electron Molecules with Relativistic Kinetic Energy: Properties of the Discrete Spectrum

Ingrid Daubechies*

Theoretische Natuurkunde, Vrije Universiteit Brussel, Pleinlaan 2, B-1050 Brussel, Belgium

Abstract. We discuss the discrete spectrum of the operator

$$H_K(c)=[-\hbar^2c^2\Delta+m^2c^4]^{1/2}-\sum_{k=1}^{K}Z_ke^2|x-R_k|^{-1}.$$

More specifically, we study 1) the behaviour of the eigenvalues when the internuclear distances contract, 2) the existence of a c-independent lower bound for $H_K(c)-mc^2$, 3) the nonrelativistic limit of the eigenvalues of $H_K(c)-mc^2$.

1. Introduction

This paper deals with the operator

$$H_K=(-\hbar^2c^2\Delta+m^2c^4)^{1/2}-\sum_{k=1}^{K}Z_ke^2|x-R_k|^{-1} \tag{1}$$

describing a relativistic charged particle with mass m in the presence of K fixed nuclei (Born-Oppenheimer approximation). The kinetic energy operator for the charged particle is obtained by straightforward "quantization" of the relativistic formula for the kinetic energy $[p^2c^2+m^2c^4]^{1/2}$; (1) can be considered as an alternative to the Klein-Gordon equation for a relativistic model neglecting spin effects. In what follows we shall, with a slight abuse of terminology, use the name "electron" for the charged particle described by (1).

For the case $K=1$ the above operator has been studied in detail by Herbst [1] and Weder [2]. One finds that

$$H_1=(-\hbar^2c^2\Delta+m^2c^4)^{1/2}-Ze^2|x|^{-1}$$

is bounded below if and only if the nuclear charge Z is less than a critical value Z_{crit}. This phenomenon is typical for relativistic atom models; the value for Z_{crit} in the

* "Wetenschappelijk medewerker" at the Interuniversitair Instituut voor Kernwetenschappen, Belgium