Progress on the Dirac Equation for the hydrogen molecular ion

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In the last few years, the spectroscopy of hydrogen molecular ions [1, 2] has advanced to a point where it can play a significant role in the determination of fundamental constants [3] and in placing tighter constraints on forces beyond the Standard Model [1, 4].

High-precision numerical resolution of the two-center Dirac Equation provides a path towards improving the theoretical predictions [5] via non-perturbative calculations of QED corrections. Major progress has been achieved recently, as the ground-state relativistic energy of H_2^+ was obtained with 20-digit accuracy [6, 7]. However, there is still room for improvement. In particular, calculations of QED corrections require evaluating the Dirac Green function, meaning that a numerical representation of the complete spectrum of the Dirac Hamiltonian has to be obtained. A method that gives one eigenstate at a time, such as the iterative method implemented in [6], would not be convenient for this purpose.

In this work [8], we write the Dirac Equation in a form suitable for complete diagonalization, which provides us with a numerical Green function. High-precision (27-32 digits) energy values are obtained using different kinetic balances. Furthermore, we were able to test our numerical Green function through the computation of relativistic sum rules, confirming that the representation of the Dirac spectrum is accurate and complete. The next step is the calculation of the one-loop self-energy correction.

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