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Calculations of the one-loop self-energy correction in one-electron systems with a numerical Green function

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Major progress in spectroscopy of ro-vibrational transitions of hydrogen molecular ions (HMI) has been achieved in the past few years, and the precision of these measurements can still be pushed further. In conjunction with further developments in the theory, this would yield tighter constraints on physics beyond the standard model and improved determinations of fundamental constants.

The theoretical precision is currently limited by the one-loop self-energy correction, which has been so far calculated perturbatively [1]. In order to evaluate this quantity in a fully relativistic approach we need the Dirac Green function of an electron in a two-center Coulomb potential, which is not known in analytic form. A numerical approximation of the Dirac Green function has been developed in our group [2] using the full spectrum of the Dirac equation obtained by a basis set method.

Having in mind the calculation of the one-loop self-energy in HMI, we perform calculations of this QED correction for H-like systems based on the algorithm developed by [3], except that we use a numerical Green function analogous to the one we obtained for HMI. Comparison with previous works that used the known analytical expression of the Dirac Green function [3, 4] allows evaluating the feasibility of extending this approach to HMI.

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