TOWARDS A FULLY RELATIVISTIC CALCULATION OF THE BETHE LOGARITHM FOR TWO-FERMION SYSTEMS

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Among the leading Quantum Electrodynamical (QED) corrections to atomic-molecular energy levels, the effect of transverse photon exchange and electron self-energy has proven to be the most challenging to compute. The calculation of these corrections boils down to the evaluation of the so-called Bethe logarithm $\ln(k_0)$ [1] [2].

For systems having small nuclear charges (such as H, He), calculation of $\ln(k_0)$ with the exact non-relativistic wave function leads to very accurate results, as done in the nrQED framework [3] [4] [5] [6] . However, the quality of this approach deteriorates as the nuclear charge increases or more complicated systems are considered, due to relativistic effects becoming too large to be treated as perturbations added to a non-relativistic zeroth-order solution. This problem necessitates a fully relativistic starting point to build QED corrections on.

In my poster I present our current progress towards the calculation of $\ln(k_0)$ with a relativistic two-electron wave function. The reference is a no-pair Dirac–Coulomb wave function obtained from an explicitly correlated variational procedure, providing an all-order description of (instantaneous, non-radiative) relativistic effects [7] [8] [9] . The relativistic generalization of the working formulae for $\ln(k_0)$ as well as the sixteen-component extension of the Hylleraas-functional based numerical techniques (for the actual evaluation of $\ln(k_0)$) are described, and pilot numerical results are showcased. The new challenges and obstacles associated with the relativistic generalization are also discussed.

[1] Bethe, Salpeter: *Quantum Mechanics of One- and Two-Electron Atoms*, Springer (1957)
[2] Sucher: *Energy-levels of the Two-Electron Atom, to Order α^3 Rydberg*, PhD, Columbia University (1958)
[3] Schwartz: *Phys. Rev.* **123** 1700 (1961)
[4] Pachucki: *J. Phys. B: At. Mol. Opt. Phys.* **31** 5123 (1998)
[5] Korobov: *Phys. Rev. A* **100** 012517 (2019)
[6] Ferenc, Mátyus: *J. Phys. Chem. A* **127 3** 627 (2023)
[7] Jeszenszki, Ferenc, Mátyus: *J. Chem. Phys.* **156** 084111 (2022)
[8] Ferenc, Jeszenszki, Mátyus: *J. Chem. Phys.* **157** 094113 (2022)
[9] Mátyus, Ferenc, Jeszenszki, Margócsy: *ACS Phys. Chem. Au* **3** 222-240 (2023)

p-number: p057 **Submitted on Fri, 09 Jun 2023 11:54:56 +0200**