TOWARDS A BOUND-STATE RELATIVISTIC QED APPROACH

P. JESZENSZKI, D. FERENC, and E. MÁTYUS,
ELTE, Eötvös Loránd University, Institute of Chemistry, Budapest, Hungary

Our overall goal is to develop a theoretical approach to describe atomic and molecular energy states with high accuracy. Numerical results of this theoretical framework can be used in comparison with precision spectroscopic experiments to test and further develop the fundamental theory of (atomic and molecular) matter, perhaps beyond the Standard Model. The current theoretical frontier, Non-Relativistic Quantum Electrodynamics (NRQED) [1] relies on a power expansion with respect to the fine-structure constant, α, and its nuclear-charge-number multiple, $Z\alpha$, about the non-relativistic reference. The current efforts in this direction are limited at most the $\alpha^5 E_\mathrm{h}$ ($m\alpha^7$) order. An alternative theoretical approach can be based on the Bethe–Salpeter equation [2], and its Salpeter–Sucher, exact, equal-time variant, a wave equation derived from relativistic QED [3, 4, 5]. For instantaneous interactions, the Salpeter–Sucher equation can be simplified to the so-called no-pair Dirac–Coulomb(–Breit) equation [4, 5] (with connections to relativistic quantum chemistry), for which we have developed solution techniques using explicitly correlated Gaussian functions [6, 7, 8, 9, 10]. We have demonstrated that the ground-state no-pair Dirac–Coulomb(–Breit) energy can be converged to $1 : 10^9$ relative precision within double precision arithmetic for He isoelectronic systems, H_2, HeH^+, and H_3^+ with clamped nuclei [6, 7, 8, 10], and to $1 : 10^{12}$ relative precision for a series of two-spin-1/2-fermion systems without external fields [11]. The α dependence of our relativistic energies reproduce the known NRQED corrections to high precision [7, 9, 10, 11]. Our ongoing work is focused at the application of the high-precision, relativistic wave functions for the evaluation of pair, retardation, and radiative corrections, also available from the Bethe–Salpeter–Sucher formalism in an operator form.

References

[1] V. A. Yerokhin, V. Patkóš, and K. Pachucki, *Phys. Rev. A* **107**, 012810 (2023).
[2] E. E. Salpeter and H. A. Bethe, *Phys. Rev. A* **84**, 1232 (1951).
[3] E. E. Salpeter, *Phys. Rev. A* **87**, 328 (1952).
[4] J. Sucher, *Ph. D. Thesis* (1958), Columbia University.
[5] E. Mátyus, D. Ferenc, P. Jeszenszki, Á. Margócsy, *ACS Phys. Chem. Au* **3**, 222 (2023).
[6] P. Jeszenszki, D. Ferenc, and E. Mátyus, *J. Chem. Phys.* **154**, 224110 (2021).
[7] P. Jeszenszki, D. Ferenc, and E. Mátyus, *J. Chem. Phys.* **156**, 084111 (2022).
[8] D. Ferenc, P. Jeszenszki, and E. Mátyus, *J. Chem. Phys.* **156**, 084110 (2022).
[9] D. Ferenc, P. Jeszenszki, and E. Mátyus, *J. Chem. Phys.* **157**, 094113 (2022).
[10] P. Jeszenszki and E. Mátyus, *J. Chem. Phys.* **158**, 054104 (2023).
[11] D. Ferenc and E. Mátyus, *Phys. Rev. A.* **107**, 052803 (2023).