Pre-Born–Oppenheimer Dirac–Coulomb–Breit computations for two-fermion systems

Dávid Ferenc, Edit Mátyus
ELTE, Eötvös Loránd University, Institute of Chemistry, Pázmány Péter sétány 1/A, Budapest, H-1117, Hungary

Positronium, muonium, hydrogen atom, and muonic-hydrogen are the simplest, yet some of the most extensively studied bound-state systems. High-precision spectroscopy experiments in combination with theoretical computations are proposed to test our fundamental understanding of ordinary matter in the low-energy range and to probe physics beyond the Standard Model. So far almost exquisitely relativistic and QED effects are treated within the non-relativistic quantum electrodynamics framework, which yields excellent agreement with experimentally measured transitions [1]. An alternative approach based on the relativistic Bethe–Salpeter wave equation was developed for the simplest two-fermion case in an external Coulomb field [2, 3, 4, 5, 6, 7]. The introduction of the equal-time wave function and separating a non-retarded interaction kernel gives rise to the no-pair Dirac–Coulomb(–Breit) equation, which is solved variationally to high precision. The advantage of the approach is that both correlation and special relativity are accounted for already in zeroth order. In this contribution, the extension of the Dirac–Coulomb(–Breit) framework is presented to pure two-body systems: positronium, muonium, hydrogen atom, and muonic-hydrogen as the first applications without the introduction of the Born–Oppenheimer approximation [8]. The numerical results show excellent agreement with the corresponding analytic relativistic perturbative energy contributions.

[1] G.S. Adkins, D.B. Cassidy and J. Pérez-Ríos, *Physics Reports* **975**, 1 (2022).
[2] P. Jeszenszki, D. Ferenc, and E. Mátyus, *J. Chem. Phys.* **154**, 224110 (2021).
[3] P. Jeszenszki, D. Ferenc, and E. Mátyus, *J. Chem. Phys.* **156**, 084111 (2022).
[4] D. Ferenc, P. Jeszenszki, and E. Mátyus, *J. Chem. Phys.* **156**, 084110 (2022).
[5] D. Ferenc, P. Jeszenszki, and E. Mátyus, *J. Chem. Phys.* **157**, 094113 (2022).
[6] P. Jeszenszki and E. Mátyus, *J. Chem. Phys.* **158**, 054104 (2023).
[7] E. Mátyus, D. Ferenc, P. Jeszenszki, and Á. Margócsy, *ACS Phys. Chem. Au* (2023).
[8] D. Ferenc and E. Mátyus, *Phys. Rev. A (under review)* arXiv:2301.13477 (2023).