

Pair corrections to the no-pair Dirac–Coulomb(–Breit) energy of heliumlike systems

Monday 10 June 2024 18:00 (2 hours)

The equal-time Bethe–Salpeter (Salpeter–Sucher) equation is the exact QED wave equation for a two-fermion system [1, 2, 3, 13, 14]. The equation containing only the instantaneous part of the interaction is the with-pair Dirac–Coulomb(–Breit) equation (wpDC(B)), which includes the double-pair correction to the no-pair DC(B) equation (npDC(B)). The numerical results for these equations can be converged within ppb to ppt relative precision using an explicitly correlated Gaussian (ECG) basis set approach [4]–[12].

While the double-pair correction is a non-hermitian, but ‘algebraic’ term, which leaves the DC(B) equation linear in energy, the single-pair correction, represented by the irreducible crossed–Coulomb(–Breit) interaction kernel, appears within a complicated, energy dependent operator in the Salpeter–Sucher equation. The inclusion of the crossed–Coulomb(–Breit) and other higher-order irreducible interaction kernels through this term renders the wave equation non-linear in energy.

A novel perturbative approach is therefore being considered for the treatment of these contributions, using the npDC(B) and wpDC(B) results as high-precision relativistic reference energies and wave functions [13, 14]. The results of this new *relativistic* QED (rQED) approach, including the single-pair correction, are expected to serve as a useful comparison to the well established *non-relativistic* QED (nrQED) methodologies, and the highest precision experimental results.

References

- [1] E. E. Salpeter and H. A. Bethe, Phys. Rev. A **84**, 1232 (1951).
- [2] E. E. Salpeter, Phys. Rev. A **87**, 328 (1952).
- [3] J. Sucher, Ph. D. Thesis (1958), Columbia University.
- [4] P. Jeszenszki, D. Ferenc, E. Mátyus, J. Chem. Phys. **154**, 224110 (2021).
- [5] P. Jeszenszki, D. Ferenc, E. Mátyus, J. Chem. Phys. **156**, 084111 (2022).
- [6] D. Ferenc, P. Jeszenszki, E. Mátyus, J. Chem. Phys. **156**, 084110 (2022).
- [7] D. Ferenc, P. Jeszenszki, E. Mátyus, J. Chem. Phys. **157**, 094113 (2022).
- [8] P. Jeszenszki and E. Mátyus, J. Chem. Phys. **158**, 054104 (2023).
- [9] D. Ferenc and E. Mátyus, Phys. Rev. A. **107**, 052803 (2023).
- [10] P. Hollósy, P. Jeszenszki, E. Mátyus, under review (2024).
- [11] P. Jeszenszki and E. Mátyus, in preparation (2024).
- [12] Á. Nonn, Á. Margócsy, E. Mátyus, under review (2024).
- [13] E. Mátyus, D. Ferenc, P. Jeszenszki, Á. Margócsy, ACS Phys. Chem. Au **3**, 222 (2023).
- [14] Á. Margócsy and E. Mátyus, arXiv:2312.13887 (2024)

Authors: NONN, Ádám (ELTE, Eötvös Loránd University, Institute of Chemistry, Budapest, Hungary); JESZENSZKI, Péter (ELTE, Eötvös Loránd University, Institute of Chemistry, Budapest, Hungary); MÁTYUS, Edit (ELTE, Eötvös Loránd University, Institute of Chemistry, Budapest, Hungary)

Presenter: NONN, Ádám (ELTE, Eötvös Loránd University, Institute of Chemistry, Budapest, Hungary)

Session Classification: Poster Session 1