ONE-PARTICLE OPERATOR REPRESENTATION OVER TWO-PARTICLE BASIS SETS FOR RELATIVISTIC QED COMPUTATIONS

P. HOLLÓSY, P. JESZENSZKI, and E. MÁTYUS,

ELTE, Eötvös Loránd University, Institute of Chemistry, Budapest, Hungary

This work is concerned with two(many)-spin-1/2-fermion relativistic quantum mechanics and it is about the construction of one-particle projectors and potentially, one-particle propagators, necessary for quantum-electrodynamics (QED) corrections [1], using an inherently two(many)-particle, 'explicitly correlated' basis representation, necessary for good numerical convergence of the results [2, 3, 4, 5]. It is demonstrated that a faithful representation of the one-particle operators, which appear in intermediate but essential computational steps, can be constructed over a many-particle basis set by accounting for the full Hilbert space, beyond the physically relevant anti-symmetric subspace. Applications of this development can be foreseen for the computation of quantum-electrodynamics corrections for a correlated relativistic reference state and for high-precision relativistic computations of medium-to-high Zhelium-like systems, for which other two-particle projection techniques are unreliable.

References

- [1] E. Mátyus, D. Ferenc, P. Jeszenszki, Á. Margócsy, ACS Phys. Chem. Au 3, 222 (2023).
- [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).