

One-Particle Operator Representation over Two-Particle Basis Sets for Relativistic QED Computation

Wednesday 12 June 2024 18:00 (2 hours)

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 Z helium-like systems, for which other two-particle projection techniques are unreliable.

References

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- [6] P. Jeszenszki and E. Mátyus, *J. Chem. Phys.* **158**, 054104 (2023).

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