Abstract Submitted
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Schrdinger and Dirac solutions to few-body problems[1] ANDREA MUOLO, MARKUS REIHER, ETH Zurich —

We elaborate on the variational solution of the Schrödinger and Dirac equations for small atomic and molecular systems without relying on the Born-Oppenheimer approximation. The all-particle equations of motion are solved in a numerical procedure that relies on the variational principle, Cartesian coordinates and parametrized explicitly correlated Gaussians functions. A stochastic optimization of the variational parameters allows the calculation of accurate wave functions for ground and excited states. Expectation values such as the radial and angular distribution functions or the dipole moment can be calculated. We developed a simple strategy for the elimination of the global translation that allows to generally adopt laboratory-fixed cartesian coordinates. Simple expressions for the coordinates and operators are then preserved throughout the formalism. For relativistic calculations we devised a kinetic-balance condition for explicitly correlated basis functions. We demonstrate that the kinetic-balance condition can be obtained from the row reduction process commonly applied to solve systems of linear equations. The resulting form of kinetic balance establishes a relation between all components of the spinor of an N-fermion system.

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