

Symmetry breaking and restoration by similarity transformation

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ABSTRACT

Symmetry conserving correlation methods perform well for weak correlation. In the strong correlation regime increasingly high levels of theory are needed to keep the same level of accuracy. This problem can seemingly be overcome by letting the reference state break symmetry. While giving accurate ground state energies at mean field cost, this sacrifices accuracy on most other properties in finite systems. Symmetry restoration can be performed by either increasing the level of theory or projection of the broken symmetry ground state into a multi-determinant wave function[1]. We have recently developed a method that expresses the symmetry projected wave function as a similarity transformation on the symmetry adapted reference state[2, 3], which links traditional coupled cluster style correlation methods to symmetry projection. I will present the key concepts, examples of performance for different hamiltonians and an outlook on the challenges and future developments.

References

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