

Title:

The role of electron pairing in challenging electronic structure problems

Authors:

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Abstract:

Accurate wave functions based on geminals or electron pairs have been developed for systems with strong pairing interactions. Specifically, we discuss configuration interaction methods based on an antisymmetrized geminal power (AGP) reference, a geminal product state with identical geminals. A systematic and mathematically rigorous scheme is devised to generate linearly independent AGPs, which are non-orthogonal by construction. This allows us to construct a hierarchy of linear combinations of AGPs (LC-AGPs) equivalent to geminal replacement models. We discuss the challenges and possibilities for developing LC-AGP-based methods for strong correlation beyond pairing.