Block-correlated coupled cluster methods for electronic structure calculations of strongly correlated systems

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Abstract:

I will report our recent advances in developing electronic structure methods for strongly correlated systems. We have developed an efficient algorithm for computing generalized valence bond (GVB) wave functions of large molecules in a black-box way.[1] With the GVB wave function as the reference function, block-correlated coupled cluster method (GVB-BCCC in short) is proposed and implemented at the *ab initio* level for strongly correlated systems.[2,3] The GVB-BCCC method in its present form is demonstrated to provide accurate descriptions for static correlation in strongly correlated systems. Our calculations on a number of typical systems have shown that GVB-BCCC3 (with up to three-pair correlation) can provide highly comparable results as the density matrix renormalization group method for systems with large active spaces. The GVB-BCCC method is expected to be a practical theoretical tool for electronic structure calculations of strongly correlated systems.

References

[1] Q. Wang, J. Zou, E. Xu, P. Pulay, S. Li, *J. Chem. Theory. Comput.* 2019, 15, 141.
[2] Q. Wang, M. Duan, E. Xu, J. Zou, S. Li, *J. Phys. Chem. Lett.* 2020, 11, 7536.
[3] J. Zou, Q. Wang, X. Ren, Y. Wang, H. Zhang, S. Li, *J. Chem. Theory Comput.* 2022, 18, 5276.