A simple and efficient adiabatic connection method with Cholesky decomposition for the correlation energy of strongly correlated systems

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Strong correlation can be essentially captured with multireference wavefunction methods such as complete active space (CAS) or, if dozens of active electrons are involved, with density matrix renormalization group (DMRG) technique. It is known that accurate description of electronic structure of strongly correlated systems requires accounting for the dynamic electron correlation, which CAS and DMRG largely miss. Second-order perturbation corrections are used to address the problem of dynamic correlation energy but they may be suffering from intruder states and lack of size consistency. They are also expensive, which precludes them from using with DMRG with very large number of active orbitals.

In my talk a new method for the correlation energy based on the adiabatic connection [1,2] will be presented. It employs the particle-hole multireference random phase approximation and a Cholesky decomposition technique. It is free from instability or intruder state problems and rigorously size-consistent. The computation cost of the method grows with the fifth power of the system size, which is unprecedentedly low comparing with other *ab initio* multireference dynamic correlation methods. I will show that the method combined with CASSCF and DMRG and applied to singlet and triplet states of organic biradicals leads to obtaining the ST gaps with the average error below 0.1 eV.

This development opens new perspectives for accurate calculations of systems with dozens of strongly correlated electrons..

[1] K. Pernal, *Phys. Rev. Lett.* **9**, 5534 (2018), *J. Chem. Phys.* **149**, 204101 (2018).
[2] P. Beran, M. Matoušěk, M. Hapka, K. Pernal, and L. Veis, *J. Chem. Theory Comput*. **17**, 7585 (2021).