Title: Explicitly-correlated higher-order coupled cluster CCk(F12) method

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Abstract: We present an explicitly correlated general-order coupled cluster CCk(F12) method for calculating electron correlation energies of closed-shell molecules. Higher-order coupled-cluster methods (beyond the perturbative triples correction) are required to achieve chemical accuracy. However, they suffer from a slow convergence of basis set error. This is corrected by a perturbative F12 correction. We compared the performance of explicitly-correlated general and approximate coupled cluster methods to a transcorrelated effective Hamiltonian. The higher-order coupled cluster equations are derived and spin-traced in SeQuant[(1)], a second-quantization toolkit for many-body methods, and the evaluation of cluster amplitudes and F12 intermediates in the MPQC v4[(2)] platform.

References:

(1) SeQuant 2.0: A C++ based second quantization toolkit Edward Valeev, Nakul Teke, Bimal Gaudel http://github.com/ValeevGroup/SeQuant2

(2) The Massively Parallel Quantum Chemistry Program (MPQC), Version 4.0.0-beta.1 Chong Peng, Cannada A. Lewis, Xiao Wang, Marjory C. Clement, Karl Pierce, Varun Rishi, Fabijan Pavošević, Samuel Slattery, Jinmei Zhang, Nakul Teke, Ashutosh Kumar, Conner Masteran, Andrey Asadchev, Justus A. Calvin, Edward F. Valeev *J. Chem. Phys*. 2020 153 (4), 044120. http://github.com/ValeevGroup/mpqc