Canonical Transformation and Renormalization Group for an Efficient Multireference Electronic Structure Method

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Canonical transformation (CT) for many-body theory [1-3] has been implemented to solve large-scale multireference quantum chemistry problems accurately. The theory constructs a renormalization structure of the high-level dynamic electron correlation in an effective Hamiltonian where the bare Hamiltonian is transformed by the unitary exponential correlation operator, which in parallel acts on the reference multi-configurational wavefunction that describes the substantial static correlation. A compact form of the high-level dynamic correlations is handled in CT for the efficient computation by exploiting robust truncations of higher-order perturbatives in three-particle operators and density matrices. We demonstrate large-scale multireference CT calculations performed with the computationally efficient implementation. The method has recently been able to be interfaced to the DMRG-CASSCF (Density Matrix Renormalization Group-Complete Active Space Self-Consistent Field) implementation [4-5] of Chan's group development, and resultantly the large-size multireference, which are statically correlated descriptions from the DMRG-CASSCF calculations with the unprecedentedly large CAS, have been handled in the subsequent CT calculations.

We present another implementation of the high-performance DMRG in which we have made some improvements that enhance applicability of DMRG to electronic structure study on transition metal complexes such as Cr2 or Cu2O2 core [6].

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