

Abstract Submitted
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Quadratic Scaling Local Canonical Transformation Method. DEBASHREE GHOSH, TAKESHI YANAI, GARNET KIN-LIC CHAN, Cornell University — Canonical transformation theory [1] can be used to describe the detailed dynamic correlation in bonding situations where there is significant non-dynamic, i.e. multireference character. This theory uses an exponential ansatz and is size-consistent. The computational cost of this method scales as N^6 which is about the same as in a single reference coupled cluster theory. We have devised a local Canonical transformation method for large systems. For large systems, we have been able to obtain quadratic scaling with the size of the system. Reduced and linear scaling algorithms for methods like MP2 and coupled cluster are well known. However, all these reduced scaling algorithms have been primarily developed for single reference correlation calculations. By combining the local canonical transformation method with, e.g. the quadratic scaling ab-initio Density Matrix Renormalization Group theory, we can now obtain a reduced-scaling description of dynamical and non-dynamical correlation in large multireference problems. [1] Takeshi Yanai, Garnet K.L. Chan, J. Chem. Phys. **124**, 194106, 2006.

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