

# Robust Least Square Tensor Hypercontraction for the Particle-Particle Ladder Term: Implementation, Efficiency, Accuracy

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One method of representing a high-rank tensor as a (hyper-)product of lower-rank tensors is the tensor hypercontraction (THC) method of Hohenstein et al. This strategy has been found to be useful for reducing the polynomial scaling of coupled-cluster methods by representation of a four dimensional tensor of electron-repulsion integrals in terms of five two-dimensional matrices. Pierce et. al. have already shown that the application of a robust form of THC to the particle-particle ladder term reduces the cost of this term in couple-cluster singles and doubles (CCSD) from  $O(n^6)$  to  $O(n^5)$  with negligible errors in energy with respect to the density-fitted variant. In this work we have implemented the least-squares variant of THC (LS-THC) which does not require a non-linear tensor factorization, including the robust form, for the calculation of the excitation and electron attachment energy using equation-of-motion coupled cluster methods EOM-EE-CCSD and EOM-EA-CCSD, respectively. We further analyze the efficiency of this implementation on regular alkane chains, and benchmark the accuracy of excited states energies as a function of the size of the molecular grid using the comprehensive QUEST database.