# Transcorrelated Coupled Cluster Methods and the xTC Approach

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Methods for calculating electronic correlation are often plagued by the necessity to use large basis-sets, which severely limits their applicability. In recent years transcorrelation has shown to be a promising alternative to more established methods to improve basis-set convergence, like F12-methods. In the transcorrelation approach the Hamiltonian is similarity-transformed by a Jastrow factor. In our work we use sophisticated Jastrow factors optimized system-specific by variational Monte Carlo. [5] This approach does not only accelerate basis-set convergence, but also compress the wave function and by doing so can ease the strong electron correlation problem.

The similarity transformation with a Jastrow factor introduces numerous three-electron integrals, which for a long time rendered the approach unattractive. Our work on transcorrelated coupled cluster [1, 2, 3] has shown that a majority of the correlation stemming from the three-electron integrals can be conveniently incorporated into the one and two-electron integrals without significant accuracy loses. Building on these findings we developed the transcorrelation method via exclusion of explicit three body correlation (xTC). [4]

The xC approach makes use of the concept of generalized normal-ordering pioneered by Kutzelnigg and Mukherjee in order to contract intermediates incorporating three-electron correlation with density matrices, resulting in a non-Hermitian Hamiltonian with no more than two-body integrals. The eigenvalues of the xTC transformed Hamiltonian can be obtained with any quantum chemistry method, which can accommodate non-Hermitian two-electron integrals, including coupled cluster methods with arbitrarily high excitations.

We will present the theory of transcorrelated coupled cluster with singles and doubles (TC-CCSD) and the xTC approach, followed by benchmark calculations justifying thexTC approximation with a comparison of the full transcorrelated TC-CCSD with approximate TC-CCSD, neglecting the three-electron integrals normal-ordered with respect to the HF determinant for atoms and molecules on the HEAT set. [2, 3] Calculations with xTC-CCSD, which can be used with a normal-ordering with respect to a non-HF reference function, are presented as well. [4] Additionally, we explore the benefits of using the distinguishable cluster approximation in transcorrelated coupled cluster methods, showing further improvements over traditional coupled cluster methods.

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