

# Exploring New Wavefunction Ansatzes for Quantum Chemistry

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Recent progress in modelling strong electronic correlation has mostly been achieved by the creation and refinement of new wavefunction ansatzes which go beyond the traditional single-reference paradigm. The flexible ansatzes for  $N$ -electron configuration interaction (FANCI) method is designed to facilitate the exploration of new wavefunction ansatzes, both mathematically and computationally. For example, using the FANCI's theoretical framework it is possible to characterize the set of wavefunctions that are size-consistent in a precise way, leading to the conception of new size-consistent wavefunction forms that subsume methods like geminal-product wavefunctions and traditional excitation-based coupled-cluster. Using FANCI's software implementations, PyCI and FanPy, it is possible to quickly test new wavefunction methods. Ongoing research (computing wavefunction properties, residual dynamic correlation, etc.) and troubling problems for future work (error estimates, orbital optimization) will be mentioned.