Symmetry breaking and restoration

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One of the fundamental challenges in modern electronic structure theory is the efficient incorporation of strong correlations at low computational cost. Despite more than 80 years of Schrodinger equation, this problem has remained unsolved. Brute force techniques that have combinatorial computational cost (exact diagonalization) are limited to small systems. Localizing the exchange hole and using symmetry broken orbitals in density functional theory are crucial to its success, and are effective steps towards achieving the goal of incorporating strong correlations. However, this is insufficient and unpleasant from the perspective that it goes hand in hand with the introduction of self-interaction error in an uncontrolled manner, one that has proven extremely difficult to overcome. Our recent work has focused on incorporating strong correlations via deliberate symmetry breaking followed by a restoration step. We will discuss a new model that leads to high-quality multi-reference wavefunctions with mean-field computational cost.