Two-Determinant Mixing with a Strong-Correlation Density Functional

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In recent papers [A.D. Becke, J. Chem. Phys. 138, 074109 (2013) and J. Chem. Phys. 138, 161101 (2013)] a density functional for strong correlations in quantum chemistry was introduced. The functional is designed to capture molecular dissociation limits using symmetry-restricted orbitals. Here we demonstrate that the functional describes, with good accuracy, two-determinant multi-reference states. The examples of this work involve 50/50 mixing of symmetry-equivalent Slater determinants at avoided crossings. We employ exactly-computed exchange and fractional spin-orbital occupancies. The connection with dissociated systems and *single*-determinant reference states is explained.