Branched variational procedure for finding the ground state of an interacting dimer

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We consider the asymmetric Hubbard dimer at half filling as a test case of our 'branched' variational procedure for finding the exact ground state energy of a many-body system. The procedure is designed to scale tractably regardless of the number of molecular orbitals in the system or the nature of the interactions. It proceeds by applying a rotation in charge space followed by a rotation in spin space to the local fermionic creation and annihilation operators of each molecular orbital. The characteristic angles of these rotations are taken as variational parameters. By minimizing the expectation value of the transformed Hamiltonian with respect to a single variational 'branch' as a function of all variational parameters, we obtain the correct ground state energy.