

Abstract Submitted
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Natural orbitals for a two-particle system in one dimension as a testbed for use in the nuclear many-body problem¹ MITCH A. MCNANNA, MARK A. CAPRIO, University of Notre Dame — Natural orbitals have been applied in atomic and molecular electronic-structure theory to increase the accuracy of calculations of observables for a many-particle system. However, unlike the electron-structure problem, the nuclear problem is translationally invariant. We created a testbed code to test the usefulness of natural orbitals as they may apply to translationally invariant problems. The relative Hamiltonian matrix of a two-particle system in one dimension is first calculated in a basis of antisymmetrized products of the harmonic oscillator eigenfunctions. The natural orbitals are then calculated for the resulting ground state, and the Hamiltonian matrix is recalculated using a two-particle basis built from the natural orbitals. The effect of basis size on the accuracy of the ground state energy calculation is explored.

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