NATURAL ORBITALS FOR THE NO-CORE CONFIGURATION
INTERACTION APPROACH

Abstract

by

Chrysovalantis Constantinou

Ab initio calculations face the challenge of describing a complex multiscale quantum many-body system. The nuclear wave function has both strong short-range correlations and long-range contributions.

Natural orbitals provide the means of adapting the single-particle basis for no-core configuration interaction (NCCI) calculations to better match the many-body wave function. Natural orbitals are obtained by diagonalizing the one-body density matrix from a calculation using an initial single-particle reference basis, such as the traditional harmonic oscillator basis. The natural orbital basis builds in contributions from high-lying oscillator shells, accelerating convergence of wave functions, energies, and other observables.

The convergence of the ground and excited state energies, radii, and electromagnetic observables of He, Li, and Be calculated using natural orbitals in ab initio NCCI calculations is discussed. It is found that electromagnetic observables involving the $M1$ operator fully converge, while the calculated energies, radii, and observables involving the $E2$ operator converge significantly faster with the natural orbital basis than with the harmonic oscillator basis. The use of infrared (IR) extrapolation schemes with the natural orbitals calculations is also explored.