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Natural Orbitals for the Equation of Motion Phonon Method

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We discuss the use of natural orbitals as single-particle basis states for the Equation of Motion Phonon Method (EMPM). They are obtained by computing a ground-state one-body density matrix in second-order many-body perturbation theory. We focus our attention on energy and proton point radius of ^{16}O and show that, with respect to Hartree-Fock, the new basis improves drastically the convergence of the two-phonon correlation energy.

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