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Natural Orbital Properties for Excited States

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Natural orbitals are defined as the eigenvectors one-body reduced density matrix. These orbitals are a highly convergent basis for the many-body problem. Here, some exact properties of the natural orbitals are discussed, particularly their similarities and differences for excited states with varying energy differences. These results are used to justify the behavior of entanglement renormalization techniques for excited states of both fermions and bosons. The results prove an upper bound on how different density matrices can be for excitations in a system with local correlations. A discussion of the relevance of symmetry on those solutions is also discussed and some examples are provided. I conclude with an outlook of how these results can be applied to real systems.

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