Abstract Submitted
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Using Wavelets to Make an Adapted Basis Set[1] THOMAS BAKER[2], GLEN EVENBLY, Department of Physics Astronomy, Univeristy of California Irvine, 92697, ANNA KESSELMAN, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel 76100, KIERON BURKE, Department of Chemistry and of Physics, Univeristy of California Irvine, 92697, STEVEN R. WHITE, Department of Physics Astronomy, Univeristy of California Irvine, 92697 — A wavelet transformation is a special type of filter usually reserved for image processing and other applications. We show that wavelets can be used to coarse grain a low-level calculation, such as density functional theory or Hartree-Fock, for use as a basis set in a high-level method, such as density matrix renormalization group or quantum Monte Carlo, in one dimension. The goal is to adapt a basis set to a given quantum chemical system using 2-3 basis functions per electron. We compare a variety of orthogonal wavelets such as coiflets, symlets, and daubechies wavelets as well as a new type of orthogonal wavelet with dilation factor three. Extending the method to three dimensions is also considered.

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Thomas Baker
Univ of California - Irvine

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