Abstract Submitted
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Investigating density functional theory with the density matrix renormalization group[1] THOMAS E. BAKER, STEVEN R. WHITE, Department of Physics & Astronomy, University of California, Irvine, KIERON BURKE, Department of Chemistry and of Physics, University of California, Irvine — Density functional theory (DFT) is an exact, low scaling method for the general purpose of solving quantum mechanical systems, especially computations used for quantum chemical systems. The difficulty in solving for many exact features of the theory in three dimensions can be revealed with analog calculations in one dimension [1,2], since the density matrix renormalization group (DMRG) gives numerically exact answers in one dimension with comparative ease. The current focus has involved constructing proofs of principle for efficient quantum algorithms. Recent progress will be discussed, including machine learning the universal density functional [3] and constructing optimized basis sets from a DFT orbital. [1] E.M. Stoudenmire, L.O. Wagner, K. Burke, and S.R. White *Phys. Rev. Lett.* **109**, 056402 (2012) [2] T.E. Baker, E.M. Stoudenmire, L.O. Wagner, K. Burke, and S.R. White *Phys. Rev. B* **91**, 235141 (2015) [3] L. Li, T.E. Baker, S.R. White, and K. Burke, arxiv:1609.03705

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