Abstract Submitted for the FWS15 Meeting of The American Physical Society

Probing the Structure of Density Functional Theory with Density Matrix Renormalization Group<sup>1</sup> THOMAS E. BAKER, LI LI, Department of Physics Astronomy, University of California, Irvine 92617, KIERON BURKE, Department of Chemistry and of Physics Astronomy, University of California, Irvine 92617, STEVEN R. WHITE, Department of Physics Astronomy, University of California, Irvine 92617 — Density Functional Theory (DFT) is a mathematically exact method for solving quantum system efficiently but that requires approximations. Making these approximations may exclude features seen in experiment or provide inadequate estimates. We may use Density Matrix Renormalization Group (DMRG) in one dimension to find exact DFT quantities [1,2] as a benchmark to test new functionals and to explore computational proof of principles [3,4]. [1] E.M. Stoudenmire, et. al., *Phys. Rev. Lett.* **109**, 056402 (2012) [2] Thomas E. Baker, et. al., *Phys. Rev. B* **91**, 235141 (2015) [3] Lucas O. Wagner, et. al., *Phys. Rev. Lett.* **111**, 093003 (2013) [4] Lucas O. Wagner, et. al., *Phys. Rev. B* **90**, 045109 (2014)

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