Abstract Submitted
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Exact density functionals for 1d systems[1] LUCAS WAGNER, E. STOUDENMIRE, Department of Physics and Astronomy, University of California, Irvine, KIERON BURKE, Department of Physics and Astronomy and Department of Chemistry, University of California, Irvine, STEVEN WHITE, Department of Physics and Astronomy, University of California, Irvine — The success of modern density functional theory (DFT) can be attributed to the Kohn-Sham (KS) scheme, for which density functional approximations are both practical and rather simple. We are often left in the dark, however, when trying to understand why certain approximations fail, or how well they approximate the true functional. To study such questions, an exact implementation of KS-DFT is required. Though exact KS-DFT is as difficult as solving the original many-body problem, the density matrix renormalization group (DMRG) gives us a powerful tool to do this. DMRG is a highly efficient wavefunction solver in 1d, which we use to solve model continuum systems with a long-range soft-Coulomb interaction between particles. Using DMRG, we implement exact KS-DFT and investigate its inner workings. Results for some atom chains are discussed and compared to HF and LDA calculations. Preprint at arXiv:1107.2394.

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