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Exact DFT with the density matrix renormalization group¹

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The density matrix renormalization group (DMRG) is a powerful, controlled numerical method traditionally applied to lattice models of strongly correlated electrons in 1D and 2D. By extending DMRG to simulate electronic structure models on a 1D quasi-continuum grid, we can compute exact Kohn-Sham (KS) potentials and even perform exact full KS calculations.² On their own, the continuum DMRG calculations provide significant insight into the structure of strongly correlated many-body wavefunctions both for smaller molecules and chains exceeding one hundred atoms. Combining DMRG with the machinery of density functional theory allows us to explore the reasons for the success or failure of standard DFT approximations and to better understand which many-body effects are faithfully reproduced by the KS system.

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²E.M. Stoudenmire, Lucas O. Wagner, Steven R. White, Kieron Burke, arXiv:1107.2394