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Comparing Exact Charge Gaps to Exact DFT and DFT Approximations for Extended 1D Continuum Systems[1] EDWIN MILES STOUDENMIRE, LUCAS O. WAGNER, STEVEN R. WHITE, KIERON BURKE, UC Irvine — With recent technical advances, the density matrix renormalization group (DMRG) can solve model electronic structure systems with long-range interactions in the 1D continuum exactly. We have been studying these systems as a laboratory for understanding and improving density functional theory (DFT). In this setting we can compute both the exact Kohn-Sham (KS) system and implement key DFT approximations. I will present exact data for charge gaps of extended chains of atoms and molecules driven through metal-insulator transitions, then compare various methods for computing these gaps in DFT. For example, we can compute the KS band gap exactly then compare to the KS band gap or integer gap computed within approximations such as LDA or LDA+U. Our results clarify how KS-DFT captures, or fails to capture, weakly and strongly correlated insuators and highlights the key challenges for improving approximate functionals.

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