Quantum Phase Transitions in One-Dimensional Nanostructures: A Comparison Between DFT and DMRG Methodologies

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In the realm of quantum chemistry, the accurate prediction of electronic structure and properties of nanostructures remains a formidable challenge. Density Functional Theory (DFT) and Density Matrix Renormalization Group (DMRG) have emerged as two powerful computational methods for addressing electronic correlation effects in diverse molecular systems. We compare ground-state energies (e0), density profiles (n) and average entanglement entropies (S) in metals, insulators and at the transition from metal to insulator, in homogeneous, superlattices and harmonically confined chains described by the fermionic one-dimensional Hubbard model. While for the homogeneous systems there is a clear hierarchy between the deviations, D%(S)<D%(e0)<D%(n), and all the deviations decrease with the chain size; for superlattices and harmonical confinement the relation among the deviations is less trivial and strongly dependent on the superlattice structure and the confinement strength considered. For the superlattices, in general increasing the number of impurities in the unity cell represents less precision on the DFT calculations. For the confined chains, DFT performs better for metallic phases, while the highest deviations appear for the Mott and band-insulator phases. This work provides a comprehensive comparative analysis of these methodologies, shedding light on their respective strengths, limitations, and applications.