Density Functional Optimizations for DFT Calculations in Fermi-Hubbard Model

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The advancement of experimental techniques for atom deposition in producing nanostructured materials has been crucial in quantum technology devices development, as quantum transistors [1]. To optimize such quantum technological applications, a theoretical investigation of their properties is essential, which invariably requires the quantum treatment of complex systems. Density Functional Theory (DFT) emerges as an efficient computation method for theoretical treatment of nanomaterial, solid, and cold atom properties. The efficiency of the electronic calculations *via* DFT depends however on the quality and precision of the density functionals used to describe the electronic correlations. For the one-dimensional Hubbard model, although we have robust analytical tools to obtain the ground-state energy of heterogeneous quantum systems *via* DFT in both non-magnetized [2] and magnetized systems [3], other quantities obtained from energy derivatives – such as magnetic susceptibility and chemical potential – are not well described by the current density functionals.

This study aims to enhance and optimize current density functionals for more precise DFT calculations of nanostructures described by the one-dimensional Hubbard model. Preliminary results for the ground-state energy reveal an overall reduction in relative average error across the interaction strength range (from $U = 0t$ to $U = 40t$, where t is the hopping term), with a 20% reduction in computational time. This initial improvement suggests the potential of our numerical code for functional optimizations to provide enhanced DFT calculations.

References

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