Density Functional Theory of Strongly Correlated Electrons: Exploiting the Links Between Ground-State Correlation Energy and Independent Fermion Entropy



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Introduction

The accurate many-particle description of systems exhibiting strong electronic correlations is one of the most challenging problems in current condensed-matter-physics research. From a theoretical perspective, the most widespread approach to electronic theory is density functional theory (DFT), which replaces the wave function by the electronic density as the fundamental variable of the quantum many-body problem. Although very successful in countless applications, the so far available approximations to the universal exchange-correlation functional of DFT are known to fail when strong electronic correlations play a central role. Our work aims to develop density-functional theoretical methods which are capable of accurately describing the properties of electrons interacting strongly in periodic lattices.

Methods

The ground-state properties of electrons in narrow bands are investigated in the framework of lattice density-functional theory (LDFT), by taking the Hubbard model as a particularly relevant example [1]. To this aim, the interaction energy W of the model is regarded as a functional of the spin-dependent single-particle

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density matrix. The periodicity of the lattice allows us to adopt a reciprocal-space perspective. Thus, W can be expressed as a functional of the occupation numbers of Bloch states having a well-defined wave vector k. By analyzing the limits of weak and strong correlations we were able to establish useful general links between W and the independent-fermion entropy S associated to the natural-orbital occupations. Exact numerical results for W provide additional support to the statistical analogy by revealing the approximate relation between W and S. A simple explicit linear ansatz has been proposed, which is suitable for extensive applications. The present reciprocal-space formulation constitutes an important alternative to previous real-space approaches to LDFT.

Results

A number of applications of the linear independent-fermion entropy (IFE) approximation have been performed for the Hubbard model on finite and infinite lattices having d = 1–3 dimensions as well as in the limit of d → ∞. Comparison with exact results and state-of-the-art numerical simulations, which are available for one- and two-dimensional systems, shows a good agreement as a function of the Coulomb-repulsion strength U/t from weak to strong correlations. Remarkably accurate are the IFE results in 1D, where in particular the strongly correlated Heisenberg limit is exactly reproduced. However, inaccuracies in the zero-field magnetic susceptibility χ are also observed in 1D for U/t → ∞.

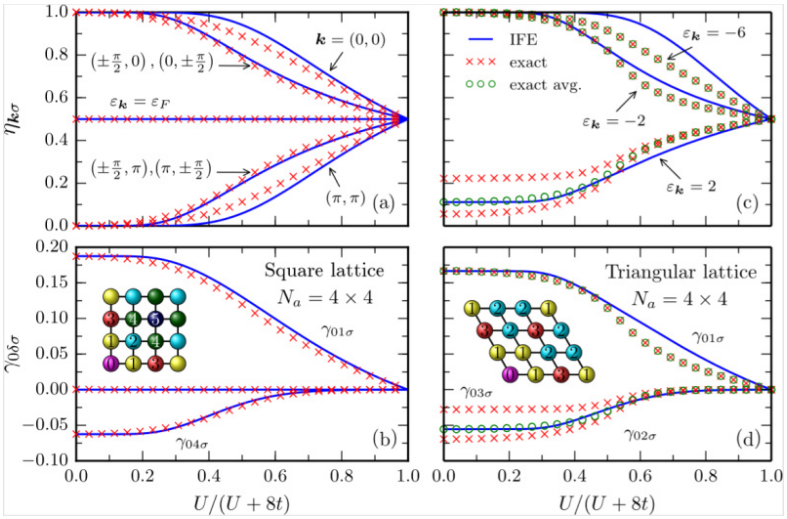
Concerning the trends for different lattice structures, one observes that the accuracy of the proposed approximation improves as the dimension or the coordination number of the system decreases. Thus, the 1D lattice is described more precisely than the 2D square lattice, which in turn is described more precisely than the triangular 2D lattice. Moreover, the accuracy improves with increasing system size both in the weakly and strongly correlated regimes, as illustrated, for example, by the calculations for finite and infinite triangular lattices. The statistical analogy underlying the IFE approach seems therefore more suitable for continuous single-particle spectra.

Outlook

The present investigations open a number of interesting perspectives for extensions and improvements. Future investigations concern mainly the transition from Luttinger-liquid to Fermi-liquid behavior occurring as the lattice dimension increases, the extension of the functional to systems showing non-uniform charge distributions, and the study of the Hubbard model with attractive local interactions which describes electronic pairing.

Figures





Reference

[1] T. S. Müller, W. Töws, and G. M. Pastor: Exploiting the links between ground-state correlations and independent-fermion entropy in the Hubbard model, Phys. Rev. B 98, 045135 (2018). https://doi.org/10.1103/PhysRevB.98.045135

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