

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Single-particle plus local reduced density matrix functional theory for Fermionic lattice models ZHENGQIAN CHENG, CHRIS MARIANETTI, Columbia Univ — We formulate a functional of the reduced density matrix (RDM) for interacting Fermionic lattice models, which depends on all local elements of the RDM (ie. all local N -body contributions); while the only nonlocal contributions are confined to the single-particle density matrix. We propose an ansatz for the unknown kinetic energy functional and evaluate it as compared to numerous exact results. In the one dimensional Hubbard model, the insulating state is properly obtained at infinitesimal U ; in addition to an accurate prediction of the ground state energy over a broad range of t/U . In the infinite dimension, single band Hubbard model, we properly find a finite- U metal-insulator transition with reasonable quantitative accuracy; in addition to the ground state energy. While our approach does not address frequency dependent observables, it has a negligible computational cost as compared to dynamical mean field theory and could be highly applicable in the context total energies of strongly correlated materials and molecules.

Zhengqian Cheng
Columbia Univ

Date submitted: 10 Nov 2016

Electronic form version 1.4