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Hubbard operator density functional theory for Fermionic lattice models ZHENGQIAN CHENG, CHRIS MARIANETTI, Columbia Univ — We formulate an effective action as a functional of Hubbard operator densities whose stationary point delivers all local static information of the interacting lattice model. Using the variational principle, we get a self-consistent equation for Hubbard operator densities. The computational cost of our approach is set by diagonalizing the local Fock space. We apply our method to the one and two band Hubbard model (including crystal field and on-site exchange) in infinite dimensions where the exact solution is known. Excellent agreement is obtained for the one-band model. In the two-band model, good agreement is obtained in the metallic region of the phase diagram in addition to the metal-insulator transition. 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.

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