Abstract Submitted
for the DAMOP11 Meeting of
The American Physical Society

Generalized Gradient Approximation for trapped ultracold atoms in optical lattices[1] JAMES FREERICKS, KARLIS MIKELSONS, Georgetown University, HULIKAL KRISHNAMURTHY, Indian Institute of Science — We present results of both quantum Monte Carlo calculations and exact analytic theories that employ corrections to the local density approximation for simulating realistic sized lattices (few million lattice sites, hundreds of thousands of particles). The QMC uses a continuous time impurity solver for inhomogeneous dynamical mean field theory. Applied to the Hubbard model, we analyze the relationship between the entropy and double occupancy for the experimental data on K^{40} measured by the ETH group. We also present results on mixtures of light and heavy atoms which are described by the Falicov-Kimball model. We find that both the LDA and the GGA work very well above the temperature where the homogeneous system first sees ordering. They can accurately correct approximations like the strong-coupling perturbation theory at low temperature, or for weak coupling, but the computational cost is dramatically higher. We also summarize how to go beyond the GGA to a full IDMFT implementation on large lattices using sparse matrix techniques.

[1]Supported under ARO Award W911NF0710576 with funds from the DARPA OLE Program and from the AFOSR MURI program under grant number FA9559-09-1-0617.

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Date submitted: 04 Feb 2011 Electronic form version 1.4