Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Configuration Interaction as an Impurity Solver: Benchmark Dynamical Mean-Field Theory for the Hubbard Model[1] ARA GO, ANDREW J. MILLIS, Department of Physics, Columbia University — The configuration interaction technique has been widely used in quantum chemistry to solve quantum many body systems with lower computational costs than exact diagonalization and was introduced by Dominika Zgid, Emanuel Gull, and Garnet Kin-Lic Chan [Phys. Rev. B **86**, 165128 (2012)] as a solver for the impurity models of dynamical mean field theory. We extend their work, demonstrating for the one and two dimensional Hubbard model how the method reproduces the known results and allows convergence with bath size to be studied in cluster dynamical mean field theory. As an example of the power of the method, cluster dynamical mean field studies of the three band copper-oxygen model are presented.

[1]This work was supported by the CMCSN program of the US Department of Energy.

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Date submitted: 08 Nov 2012 Electronic form version 1.4