Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Quantum impurity solver based on truncated ED (RASCI) wave function expansion[1] DOMINIKA ZGID, EMANUEL GULL, CHRIS MARIANETTI, ANDREW MILLIS, DAVID REICHMAN, Columbia University, GARNET CHAN, Cornell University — Quantum impurity models appear in many applications, including nanoscience and the dynamical mean field approximation (DMFT). Many physically relevant impurity models are too large to be solved by exact diagonalization (ED), lack the interaction and hybridization structure required for quantum Monte Carlo (QMC) simulations, or suffer from a severe sign problem. We present an alternative impurity solver inspired by configuration interaction (RASCI) techniques of quantum chemistry and based on a controlled truncation of a wave function expansion. The method can access larger impurity models (impurities with 5 d-orbitals and 20 bath orbitals can be easily calculated on a single processor) than can ED and avoids the sign problems of QMC methods. The performance is demonstrated for a cluster DMFT approximation to the two dimensional Hubbard model and for the problem of a Co adatom on a Cu(111) surface.

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

Dominika Zgid
Columbia University

Date submitted: 11 Nov 2011 Electronic form version 1.4