Abstract Submitted for the MAR09 Meeting of The American Physical Society

A linear in β solver for Cluster Dynamical Mean Field Theory EHSAN KHATAMI, MARK JARRELL, University of Cincinnati, CHE-RUNG LEE, National Tsing Hua University, RICHARD SCALETTAR, University of California, Davis — We develop a Quantum Monte Carlo (QMC) cluster solver for the Dynamical Cluster Approximation (DCA) which scales linearly in the inverse temperature, β , and has the same minus sign problem as conventional methods. Determinantal QMC (DQMC) used in this method is modified by adding non-interacting bands to mimic the coupling to the host. The DCA hybridization function is fitted to the non-interacting band parameters. We prove that the sign problem has the same statistics as in the Hirsch-Fye (HF) algorithm in the limit of a large number of bath bands (N_{α}) . Whereas the HFQMC scales as β^3 , this DQMC-based method scales linearly in β . We demonstrate rapid convergence of the sign to the HF result for different cluster sizes and model parameters as N_{α} increases. We also present results for the convergence of other physical quantities to their HFQMC counterparts. This method can be used to solve other embedded cluster problems including those in Dynamical Mean Field Theory (DMFT), and cellular DMFT.

> Ehsan Khatami University of Cincinnati

Date submitted: 20 Nov 2008

Electronic form version 1.4