Abstract Submitted for the MAR17 Meeting of The American Physical Society

Twisted Boundary Conditions for Lattice Monte Carlo Simulations JOSEPH PAKI, EMANUEL GULL, University of Michigan — Numerical simulations of spatially correlated lattice models have made progress via Dynamical Mean Field Theory and extensions such as the Dynamical Cluster Approximation, but are still hindered by computational costs that scale exponentially with lattice size. This presents a major barrier for applying modern many-body methods for correlated systems to real materials due to finite size errors. We present a method of addressing finite size errors in a computationally efficient manner by running simulations with twisted boundary conditions. The method is implemented with a continuous-time auxiliary spin impurity solver that Monte Carlo samples an interaction expansion series. Averaging over the twisted boundary conditions allows for thermodynamic extrapolation of certain physical quantities of interest without the cost associated with large system simulations.

> Joseph Paki University of Michigan

Date submitted: 11 Nov 2016

Electronic form version 1.4