Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

DCA$^+$: Incorporating self-consistently a continuous momentum self-energy in the Dynamical Cluster Approximation PETER STAAR, ETH Zurich, THOMAS MAIER, Oak Ridge National Lab, THOMAS SCHULTHESS, ETH Zurich, COMPUTATIONAL MATERIAL SCIENCE COLLABORATION — The dynamical cluster approximation (DCA) is a systematic extension beyond the single site approximation of dynamical mean field theory (DMFT) to include spatially non-local correlations in quantum many-body simulations using a finite size embedded cluster. In the last decade, the DCA has been very useful in describing and analyzing phase transitions in models of correlated electron systems such as the single-band Hubbard model. In the standard DCA algorithm, the single-particle self-energy is approximated by a step function in momentum space, with constant values in regions about the cluster momenta. As a consequence, results often depend sensitively on the topology and morphology of the chosen cluster and the corresponding cluster momenta. Here, we present an extension to the standard DCA that incorporates a self-energy with smooth, continuous momentum dependence self-consistently in the DCA algorithm. In this new algorithm, the influence of the cluster-geometry is significantly reduced and the self-energy converges much more rapidly as a function of cluster-size. We demonstrate the improved convergence of this algorithm for results of the pseudo-gap temperature T^* and the superconducting temperature T_c versus cluster-size.

Peter Staar
ETH Zurich

Date submitted: 11 Nov 2012 Electronic form version 1.4