

MAR15-2014-020269

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Simulations of high-T_c superconductors using the DCA⁺ algorithm

PETER STAAR, IBM Research Zurich

For over three decades, the high T_c-cuprates have been a gigantic challenge for condensed matter theory. Even the simplest representation of these materials, i.e. the single band Hubbard model, is hard to solve quantitatively and its phase-diagram is therefore elusive. In this talk, we present the recent algorithmic and implementation advances [1,2] to the Dynamical Cluster Approximation (DCA). The algorithmic advances allow us to determine self-consistently a continuous self-energy in momentum space, which in turn reduces the cluster-shape dependency of the superconducting transition temperature and thus accelerates the convergence of the latter versus cluster-size. Furthermore, the introduction of the smooth self-energy suppresses artificial correlations and thus reduces the fermionic sign-problem, allowing us to simulate larger clusters at much lower temperatures. By combining these algorithmic improvements with a very efficient GPU accelerated QMC-solver [3], we are now able to determine the superconducting transition temperature accurately and show that the Cooper-pairs have indeed a d-wave structure, as was predicted by Zhang and Rice.

[1] Peter Staar, Thomas A. Maier and Thomas C. Schulthess (Phys. Rev. B 88, 115101 (2013))

[2] Peter Staar, Thomas A. Maier and Thomas C. Schulthess (Phys. Rev. B 89, 195133 (2014))

[3] Peter Staar, Thomas A. Maier, Michael S. Summers, Gilles Fourestey, Raffaele Solca, and Thomas C. Schulthess. “Taking a quantum leap in time to solution for simulations of high-T_c superconductors.” (In Proceedings of SC13: International Conference for High Performance Computing, Networking, Storage and Analysis, SC '13, pages 1:1-1:11, New York, NY, USA, 2013. ACM.)