TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

INSTITUT FÜR FESTKÖRPERPHYSIK
Institute of Solid State Physics

Wiedner Hauptstraße 8-10/138, 1040 Wien, AUSTRIA – T: +43-1-5880113801 / F: +43-1-5880113899 – E: sekretariat@ifp.tuwien.ac.at

EINLADUNG zum IFP-SEMINAR

Thema: **Quasi-continuous-time impurity solver for the (cluster) dynamical mean-field theory with linear scaling in the inverse temperature**

Vortragender: **Daniel Rost**
Institut für Physik, KOMET 337, Johannes Gutenberg-Universität
Germany

Host: Karsten Held

Termin: **Dienstag, 3. Dezember 2013, 10:00 Uhr**

Ort: Institut für Festkörperphysik, TU Wien
Wiedner Hauptstraße 8-10, 1040 Wien
Seminarraum 138C, 9. OG (gelbe Leitfarbe)

Diagrammatic quantum Monte Carlo impurity solvers (CT-QMC) provide numerically exact solutions for (cluster) dynamical mean-field theory (DMFT), at a computational cost that scales cubically with the inverse temperature 1/T. In contrast, a recently proposed approach [1], based on a hamiltonian representation of the bath Green function and the BSS quantum Monte Carlo algorithm [2], scales linearly with 1/T, but introduces a bias due to Trotter discretization. We present an algorithm, based on multigrid extrapolations of Green functions, that combines the advantages of both methods: (i) it retains the superior linear scaling of BSS and (ii) is free of significant Trotter errors. We already established the high accuracy of this quasi continuous-time method for single-site DMFT, exploring the metal-insulator transition in the 1-band Hubbard model, in comparison with CT-QMC and exact diagonalization [3]. As extension to the single-site case, I present our recent developments on algorithms for cluster DMFT, retaining the superior linear scaling in the inverse temperature.

[1] E. Khatami et al., Phys. Rev. E 81, 056703 (2010).
[2] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24, 2278 (1981).
[3] D. Rost, F. Assaad and N. Blümer, Phys. Rev. E 87, 053305 (2013).