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: **Hund's coupling and spatial correlations: a cluster DMFT study**

Vortragender: **Yusuke Nomura**
Department of Applied Physics, University of Tokyo, Japan

Host: Karsten Held

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In strongly-correlated multi-orbital systems, both Hund's coupling and spatial correlations play a key role. The cluster extension of the dynamical mean-field theory (cDMFT) [1] is a powerful method which can treat them, however, due to its huge computational cost, its application has been highly limited.
In the present study, we develop a quantum Monte Carlo method which enables cDMFT calculation of strongly-correlated multi-orbital systems with full spin-rotational symmetry at rather low temperatures in a reasonable computational time [4]. We accomplished it by incorporating the submatrix update scheme (efficient sampling update algorithm) [2] into the continuous-time quantum Monte Carlo method based on the interaction expansion [3], and by developing a new sampling scheme which mitigates the sign problem coming from the spin-flip and pair-hopping terms [4].
We apply the method to two- and there-orbital Hubbard models defined on a square lattice. We found that Hund's coupling significantly affects the non-local correlations. We show this in the following settings [5]:
(i) three-orbital, <n>=2
(ii) two-orbital, <n>=1.5
Hund's coupling rearranges the filling among momenta such that a certain momentum patch becomes half-filling, which might result in a "patch-selective" state, where the Mott-insulating patch and the metallic patch coexist.

[1] T. Maier et al., Rev. Mod. Phys. 77, 1027 (2005).
[2] P. K. V. V. Nukala et al., Phys. Rev. B 80, 195111 (2009); E. Gull et al., Phys. Rev. B 83, 075122 (2011).
[3] A. N. Rubtsov et al., Phys. Rev. B 72, 035122 (2005).
[4] Y. Nomura, S. Sakai, and R. Arita, Phys. Rev. B 89, 195146 (2014).
[5] Y. Nomura, S. Sakai, and R. Arita, in preparation

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