

EINLADUNG zum IFP-SEMINAR

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

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Host: Karsten Held

Termin: **Dienstag, 24 Juni 2014, 10 Uhr**

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

Förderer: ERC-StG-306447 AbinitioDGA

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 three-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, $\langle n \rangle = 2$

(ii) two-orbital, $\langle n \rangle = 1.5$

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

