量子物理学・ナノサイエンス第 64 回特別セミナー

Downfolding and self-consistent GW+DMFT

講師　：　Professor Philipp Werner

University of Fribourg, Switzerland

日程　：　6 月 3 日（月）13:30–

場所　：　本館 2 階 284A 物理学系輪講室

概　要

The GW+DMFT method provides a consistent scheme for the description of correlation and screening effects in lattice systems and a powerful tool for the study of nonequilibrium states [1,2]. We will discuss the formalism and its implementation for simple lattice models (single-orbital Hubbard and three-orbital "d-p" model) and investigate the effect of dynamical screening on the local interaction and spectral function. For the d-p model of charge transfer insulators, we demonstrate that the GW contribution to the self-energy is not relevant in equilibrium, but crucially important for the description of photo-excited states [3]. These model-level studies are a first step in the development of parameter-free ab-initio simulation approaches for correlated materials.

[1] S. Biermann, F. Aryasetiawan, and A. Georges, Phys. Rev. Lett. **90**, 086402 (2003).
[2] D. Golez, L. Boehnke, M. Eckstein, and P. Werner, Phys. Rev. Lett. **118**, 246402 (2017).
[3] D. Golez, L. Boehnke, M. Eckstein, and P. Werner, arxiv:1808.02264 (2018).

連絡教員　物理学系　古賀　昌久（内線 2727）