A Selfenergy Cookbook — State-of-the-Art Computing for the NEGF Key Ingredient

Niclas Schlünzen[*1], **Jan-Philip Joost**[1], **Michael Bonitz**[1]

[1] *Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität, Kiel, Germany*

During the propagation of the Kadanoff−Baym equations the choice of selfenergy is crucial, both, from a physical point of view—as it incorporates all different classes of inter-particle effects and processes—as well as from the numercal view—since its determination readily dominates the computational effort. Entering the strong-coupling regime basically goes together with going beyond the second-Born level. There, a variety of many-body approximations becomes applicable—reaching from GW over the T matrix to the FLEX selfenergy [1].

In this talk, I will give an overview of the different selfenergy approximations, their respective strengths and weaknesses, as well as their computational demands. I will discuss the behavior for different basis sets and address parallelization possibilites.

[1] N. Schlünzen, S. Hermanns, M. Scharnke, and M. Bonitz, submitted for publication, arXiv:1902.07038 (2019)

---

* email: schluenzen@theo-physik.uni-kiel.de