

DMRG Spectral-functions for the Anderson-Impurity-Model

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Impurity models, in which there is a strongly interacting region coupled to a non-interacting bath, emerge in various situations in low temperature physics. The situations range from “real” impurities in metals, like Cobalt in Copper, over artificial created nanostructures coupled to leads, to Dynamical Mean Field Theory (DMFT) [1] for lattice models.

One of the most important theoretical models in this field is the Single Impurity Anderson Model (SIAM) [2]. Besides obtaining information about the ground-state of this model, it is desirable to calculate the single particle spectral function, as it can be directly measured in experiments, but is also needed for DMFT calculations.

In DMRG the ground-state can be obtained with very high precision, but information about excited states are rarely available, which is the major drawback of the method when trying to calculate dynamical correlation functions. For measuring these spectral functions one often uses the correction vector method [3, 4], resulting in a Lorentzian broadening. Unfortunately, it has turned out, that this broadening, especially for frequencies near the Fermi energy can give wrong results when using DMRG with DMFT.

Based on correction vectors, I will show, how a more detailed analysis, can provide additional information, from which arbitrary convolutions of the data is possible. Thus, it is also possible to analyze the spectral functions around the Fermi-energy in more detail.

References

- [1] A. Georges et al., Rev. Mod. Phys. **68** (1996), 13.
- [2] P.W. Anderson, Phys. Rev. **124** (1961), 41
- [3] T.D. Kuehner and S.R. White, Phys. Rev. B **60** (1999), 335.
- [4] E. Jeckelmann, Phys. Rev. B **66** (2002), 045114.