

Improving energy resolution in NRG calculations for dynamic quantities

Motivated by the question, to what extent one can, within NRG, obtain spectral information on a per mille level even for high-energy structures, we investigate the influence of the discretization and broadening procedures on the dynamical quantities for a single-impurity Anderson model. We observe several artifacts which are partly due to numerical issues, but partly also of systematic nature connected to the actual discretization scheme employed in the NRG. We present a way to remove at least the latter artifacts and present high-resolution spectra for single-impurity models as well as DMFT calculations.