Nonequilibrium steady-state transport through quantum impurity models – a hybrid NRG-DMRG treatment

FRAUKE SCHWARZ, JAN VON DELFT, ANDREAS WEICHSELBAUM, Ludwig-Maximilians Universitaet, Munich — Matrix Product State (MPS) methods, and in particular the Numerical Renormalization Group (NRG), have proven to be successful in describing interacting impurity models in equilibrium. For steady-state nonequilibrium, arising e.g. due to an applied voltage, we suggest to combine NRG with the Density Matrix Renormalization Group (DMRG): NRG is used to deal with virtual transitions to high-lying excitations, leading to a renormalized impurity problem, whereas DMRG is used to treat the nonequilibrium dynamics of the remaining low-lying excitations. Furthermore, we use a basis in which the thermal state of the noninteracting leads (decoupled from the impurity) is described by a product state resulting in a comparatively low entanglement. These two ideas enable us to deduce steady-state expectation values for the nonequilibrium Single Impurity Anderson Model (SIAM) based on quench calculations. In particular, we study the splitting of the Kondo resonance in the zero-bias peak as a function of increasing magnetic field. While our approach allows us to directly focus on the relevant low-energy regime in a properly designed closed system, it is also naturally suited to be extended to a truly open system by introducing Lindblad driving terms [F. Schwarz et al., PRB 94, 155142]