Sum-rule Conserving Spectral Functions from the Numerical Renormalization Group ANDREAS WEICHSELBAUM, JAN VON DELFT, Ludwig Maximilians University, Munich — We show how spectral functions for quantum impurity models, i.e. nanosystem embedded in fermionic or bosonic environment, can be calculated very accurately using a complete set of "discarded" numerical renormalization group (NRG) eigenstates, recently introduced by Anders and Schiller. The only approximation is to judiciously exploit energy scale separation. Our rigorous derivation avoids both the overcounting ambiguities and the single-shell approximation for the equilibrium density matrix prevalent in current methods including state of the art DM-NRG. The resulting procedure based on the full density matrix of the system (FDM-NRG) ensures that relevant sum rules hold rigorously and spectral features at energies below the temperature can be described accurately.

Andreas Weichselbaum
Ludwig Maximilians University, Munich