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Impurity Solvers for Dynamical Mean Field Theory using Matrix Product States MARTIN GANAHL, Perimeter Institute for Theoretical Physics, MARKUS AICHHORN, Graz University of Technology, PATRIK THUNSTROEM, Vienna University of Technology, FRANK VERSTRAETE, University of Vienna, KARSTEN HELD, Vienna University of Technology, HANS GERD EVERTZ, Graz University of Technology — We use the Time Evolving Block Decimation (TEBD) technique for for Matrix Product States to calculate spectral functions of impurity models. The resolution of the spectral function is improved using linear prediction. We apply the method as an impurity solver within the Dynamical Mean Field Theory (DMFT) for the single and two-band Hubbard model on the Bethe lattice. For the single band model we observe sharp features at the inner edges of the Hubbard bands. A finite size scaling shows that they remain present in the thermodynamic limit. We analyze the real time-dependence of the double occupation after adding a single electron and observe oscillations at the same energy as the sharp feature in the Hubbard band, indicating that they correspond to a long-lived, coherent superposition of eigenstates with different occupations. For a two-band Hubbard model we observe distinct features in the Hubbard bands which we interpret as multiplets originating from Hund's exchange.

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