November 28th, 2013 - 14:00

Seminar Room IV, CFEL (Bldg. 99)

CFEL SCIENCE

Max Planck Research Department for Structural Dynamics

SEMINAR

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Chebyshev expansion for Impurity Models using Matrix Product States

I present an improvement of a recently developed expansion technique for calculating spectral functions using matrix product states by postprocessing computed Chebyshev moments with linear prediction. This can be achieved at virtually no cost and, in sharp contrast to existing methods based on the dampening of the moments, improves the spectral resolution rather than lowering it. We validate the method for the exactly solvable resonant level model, and show that it is capable of resolving sharp Kondo resonances for the single impurity Anderson model as well as peaks within the Hubbard bands when employed as an impurity solver for dynamical mean-field theory (DMFT). We also propose an alternative expansion of $1 - \exp(-\tau H)$ instead of the usual H, which opens the possibility of using established methods for the time evolution of matrix product states to calculate spectral functions directly.

Host: Andrea Cavalleri, MPSD-CFEL