Tangent-space Krylov Approach for Matrix Product State Computation of zero-temperature, real-frequency spectral functions

We present a tangent-space Krylov (TaSK) method for efficient computation of zero-temperature real-frequency spectral functions on top of ground state (GS) matrix product states (MPS) obtained from the Density Matrix Renormalization Group. It relies on projecting resolvents to the tangent space of the GS-MPS, where they can be efficiently represented using Krylov space techniques. This allows for a direct computation of spectral weights and their corresponding positions on the real-frequency axis. We demonstrate the accuracy and efficiency of the TaSK approach by showcasing spectral data for various models. These include the 1D Haldane-Shastry and Heisenberg models as benchmarks. As an interesting application, we study the Hubbard model on a cylinder at half-filling, augmented by a density-assisted hopping (DAH) term. We find that DAH leads to particle-hole asymmetric single-particle mobilities and lifetimes in the resulting Mott insulator, and identify the responsible scattering processes. Further, we find that DAH influences the dispersion of Green's function zeros beyond its range, which has a frustrating effect on the Mott insulator studied here.

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