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Adaptively truncated Hilbert spaces for Hamiltonian-based impurity solvers[1] ARA GO, ANDREW MILLIS, Columbia Univ — We investigate truncations of the exponentially large Hilbert space in the exact diagonalization (ED) as an impurity solver for the dynamical mean-field theory (DMFT). A key issue is to maintain the high degree of numerical accuracy required in the construction of Greens functions. We test various truncation schemes with similar number of Slater determinants in both Hilbert spaces for the ground state and a particle- or a hole-excited state, and show that the excited states play an important role in accurate computation as well as the ground state. Appropriate truncation for both spaces enables us to compute the accurate self-energy of the impurity Hamiltonian with up to eight correlated orbitals hybridized with a sufficient number of bath orbitals to obtain converged solutions of the self-consistent equation in the DMFT, which is not solvable by the original ED. Application to spin-orbit coupled multi-orbital models and the one-dimensional Hubbard model and comparison to results from exact diagonalization and the configuration interaction based impurity solvers demonstrate the power of the method.

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Ara Go
Columbia Univ

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