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Adaptive Hilbert Space Truncation for Dynamical Mean-Field Impurity Models: Formalism and new results for the Hubbard model pseudogap[1] ARA GO, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, ANDREW MILLIS, Columbia University in the City of New York — An impurity solver based on adaptive truncation of a Hilbert space is shown to be a powerful new method for solving the equations of dynamical mean-field theory. Starting from an initial set of Slater determinants, the method performs an adaptive truncation followed by particle-hole substitutions, and then iterates the procedure to obtain an accurate ground state. A related process is used to define the excited state space needed for the Greens function. The reduced costs enable solutions of impurity models with 8 correlated orbitals. New results enabled by the method are presented including the spectral functions near the Mott transition and the fate of the pseudogap at large U in the 8-site dynamical mean-field approximation to the Hubbard model.

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