Hilbert space renormalization for the electron correlation problem

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We propose a new theoretical tool: Hilbert space renormalization, to describe many-electron correlations. It is inspired by the highly successful density matrix renormalization group (DMRG) algorithm that renormalizes many-body states in Fock space successively, and the traditional quantum chemical graphical representation of configuration space. By merging these two ideas, the Hilbert space renormalization provides a new way to classify and combine configurations. The underlying wavefunction, namely the Hilbert space matrix product state (HS-MPS), has a very rich and flexible mathematical structure. It provides low-rank tensor approximations to any configuration interaction (CI) space through restricting either the 'physical indices' or the coupling rules in the HS-MPS. Alternatively, simply truncating the 'virtual dimension' of the HS-MPS leads to a family of size-extensive wave function ansatz that can be used efficiently in variational calculations. We will also discuss the numerical comparisons between the HS-MPS, the traditional Fock-space MPS used in DMRG, and traditional CI approximations.