Tensor Product Selected CI for Strongly Correlated Systems

Vibin Abraham and Nicholas Mayhall

Virginia Tech,Blacksburg, VA

Strongly correlated systems have been a major challenge for a long time in the field of theoretical chemistry. For such systems, the relevant portion of the Hilbert space scales exponentially, preventing efficient simulation on large systems. We present the tensor product selected configuration interaction (TPSCI) method, where we partition the system into clusters such that the wavefunction can be represented using the tensor product of cluster states. The selected configuration interaction procedure is used to include important configurations in the tensor product basis. The Tucker decomposition technique is used to obtain compact local cluster states which reduces the number of tensor product configurations significantly. We present numerical results for a modified Hubbard model with different inter and intra cluster hopping term. We also studied molecular systems at bond breaking like: N_2, H_2O and CO. Numerical results show that TPSCI can be used to truncate the number of determinants in the variational space quite significantly as compared to other selected CI approaches.