Density-matrix based determination of low-energy model Hamiltonians from ab initio wavefunctions

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We propose a way of obtaining effective low-energy Hubbard-like model Hamiltonians from ab initio Quantum Monte Carlo calculations for molecular and extended systems. The Hamiltonian parameters are fit to best match the ab initio two-body density matrices and energies of the ground and excited states, and thus we refer to the method as "ab initio density matrix based downfolding" [1]. We present representative examples where we estimate effective parameters such as the Hubbard U and the Hund's coupling J, along with providing systematic tests of the validity of a given model. For molecules, such parameterizations enable calculation of excited states that are usually not accessible within ground state approaches. For solids, the effective Hamiltonian enables large scale calculations using techniques designed for lattice models.

[1] H. J. Changlani, H. Zheng, L. K. Wagner, J. Chem. Phys. 143, 102814 (2015).