

Dynamical Downfolding and Construction of Effective Hamiltonians for Correlated Systems

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There is wide and longstanding interest in reducing the computational cost for electronic structure calculations of correlated systems. Recently, Romanova et. al have developed a method of dynamical downfolding to map a large correlated problem onto a reduced subspace [Romanova et al., npj Computational Materials 9 (1), 126, 2023]. While this work succeeded in finding quantitative agreement with the experimental results, the limitations of this approach have not yet been explored. Using a solvable model system, we investigate under which conditions dynamical downfolding with renormalized 1-body terms can reliably provide a portion of the optical spectrum. Further, we relate this work to the method of exact downfolding by construction of a Schur complement. By studying the exact self-energy, we develop a language to understand how information about the many-body eigenvectors is lost through downfolding.