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Construction of low energy effective Hamiltonians from Ab Initio Quantum Monte Carlo[1] HITESH CHANGLANI, LUCAS WAGNER, University of Illinois at Urbana-Champaign — Solving the first principles quantum many-body Schroedinger equation can result in very high accuracy, but physical insight and generalization of the result can be hard to obtain. On the other hand, low energy effective model Hamiltonians often contain the essential physics of the problem, but may not provide sufficient accuracy needed to understand the properties of real materials. To connect the two approaches, we present a framework for obtaining low energy effective Hamiltonians from ab initio Quantum Monte Carlo calculations for molecular and extended systems. As a demonstration of the method, we focus on a few representative strongly correlated materials. We fit the Hamiltonian parameters to best reproduce the two body density matrix of the ground state obtained from ab initio calculations. We assess the accuracy of the resultant model, by comparing excited state properties to the original ab initio result. Such effective Hamiltonians are advantageous in reducing the computational complexity of the many-electron problem, and once generated, can be used for larger scale calculations using techniques designed for discrete systems.

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