

Symmetry-Projected Methods for Spin Lattices

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Spin Hamiltonians are of fundamental importance. For example, systems ranging from molecular magnets to iron-sulfur clusters relevant to nitrogen fixation can be treated via the Heisenberg spin model. In condensed matter physics, significant attention is paid to spin lattice models such as the XXZ and J_1 - J_2 Heisenberg Hamiltonians. While one can treat these problems with electronic structure methods designed for fermionic systems, it may be preferable to use techniques developed explicitly for Hamiltonians built from spin operators. In this talk, we will discuss how one can treat these spin lattice models with various symmetry-projected methods, including projected mean-field and coupled cluster theory, as well as their generalization to cluster-based approaches in which the fundamental objects are multi-site fragments instead of individual lattice sites.