Automatic generation of spin and spin-bath Hamiltonians

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Magnetism and spin physics is a true quantum mechanical effect and its description usually requires multi reference methods and can be hidden in the standard description of moelcules in quantum chemistry. Here we present a twofold approach to the description of spin physics in molecules and solid state physics for details see [1, 2]. First, we present a method that identifies the single-particle basis in which a given subset of the orbitals are equivalent with spin degrees of freedom for models and materials which feature significant spin physics. We introduce a metric for the spin-like character of a linear combinations of orbitals of which the optimization yields the optimal spin-like configurations. Second we demonstrate a generalized Schrieffer-Wolff transformation method to extract the effective Hamiltonian projected on the subspace of the Hilbert space in which the charge degree of freedom of electrons occupying the previously identified orbitals is negligible. The method then yields an effective spin or spin-bath Hamiltonian description for the system. This generalized Schrieffer-Wolff transformations is applicable to a wide range of Hamiltonians and has already been successfully employed with a selection of quantum chemistry Hamiltonians of molecules.

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[1] A method to derive material-specific spin-bath model descriptions of materials displaying prevalent spin physics (for simulation on NISQ devices); Benedikt M. Schoenauer, Nicklas Enenkel, Florian G. Eich, Michael Marthaler, Sebastian Zanker, and Peter Schmitteckert https://quantumsimulations.de/publications/white-paper-hqs-spin-mapper

[2] Understanding Radicals via Orbital Parities; Reza G. Shirazi, Benedikt M. Schoenauer, Peter Schmitteckert, Michael Marthaler, and Vladimir V. Rybkin, arXiv:2404.18787