Automated generation of spin-bath Hamiltonians for a wide range of interacting systems

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In simulating quantum materials one always has to extract the basic ingredients of a system into a model in order to describe the material under investigation. Here we describe an approach that allows us to extract the spin part of an interacting electronic system leading to a spin system coupled to a fermionic bath. To this end we first perform orbital transformations optimizing the separation of spin and fermionic degrees of freedom. We then perform a generalized Schrieffer-Wolff transformation that leads to the desired spin-bath system. Finally we present results starting with the well known single impurity Anderson model. We then discuss the calculation of the band structure of a two band Hubbard model. Finally we comment on the application to molecular systems.