Effective spin-bath models for solids and molecules

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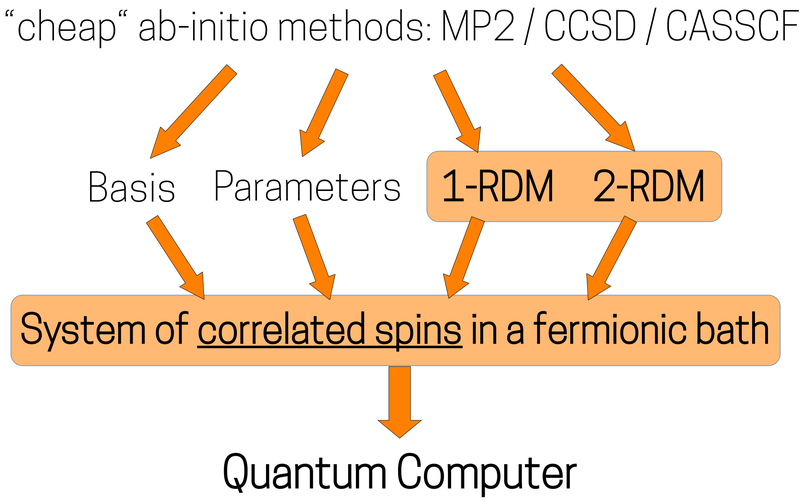
Introduction

Goal Derivation of an accurate spin-bath model descriptions from first principles and subsequent application to real materials that are relevant to our partners in QSOLID.



The spin physics of these spin-bath models can be studied using the quantum algorithms for noisy open systems developed by HQS.

Spin identification via parity optimization

We identify the *spin-like* character of a given basis orbital by its local parity.

$$P_i = (-1)^{n_{i\uparrow}+n_{i\downarrow}} = 1 - 2\left(c^\dagger_{i\uparrow}c_{i\uparrow} + c^\dagger_{i\downarrow}c_{i\downarrow}\right) + 4\,c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}c_{i\uparrow}$$

Local parity is computed from the one- and two particle reduced density matrices (1- / 2-RDM), calculated with ab-initio methods.

- Parity $P_i = -1$ $\Rightarrow$ perfect *single* occupancy of the orbital
- Local degree of freedom: spin of the electron

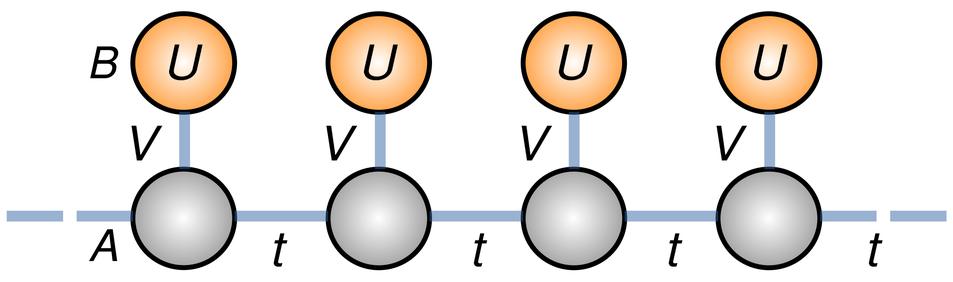
We use a sequence of pairwise orbital rotations to optimize the local parities. We select linear combinations of orbitals with sufficiently small parity as the ***spin-like orbitals*** of the effective spin-bath model.

Spins in lattice models for solids

We have compared our parity optimization approach to the conventional way of using the eigenstates of the 1-RDM, i. e. the "natural orbitals", with eigenvalue $\langle c^\dagger_q c_q\rangle = 1$.

A toy lattice model was constructed as benchmark. The orbitals B are designed to be highly *spin-like* due to a strong, repulsive Hubbard interaction U.

$$H = \sum_{i\sigma} t\left(c^\dagger_{i,A\sigma}c_{i+1,A\sigma} + \text{h.c.}\right) + V\left(c^\dagger_{i,B\sigma}c_{i,A\sigma} + \text{h.c.}\right) + U\sum_i \left(n_{i,B\uparrow} - \frac{1}{2}\right)\left(n_{i,B\downarrow} - \frac{1}{2}\right)$$



Natural orbitals are combinations of A and B orbitals. Their respective parities display no *spin-like* character.
Our optimization method subsequently recovers the orbitals A or B.

from the natural orbitals: $P_i = (+0.99 + 0.29 + 0.29 + 0.17 + 0.17 + 0.29 + 0.29 + 0.99)$

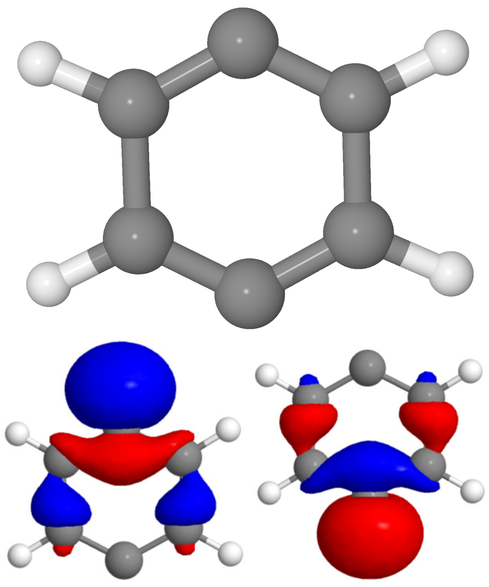
we recover parity optimized "original" local basis: $P_i = (\pm 0.00 \pm 0.00 - 0.13 - 0.13 - 0.99 - 0.99 - 0.99 - 0.99)$

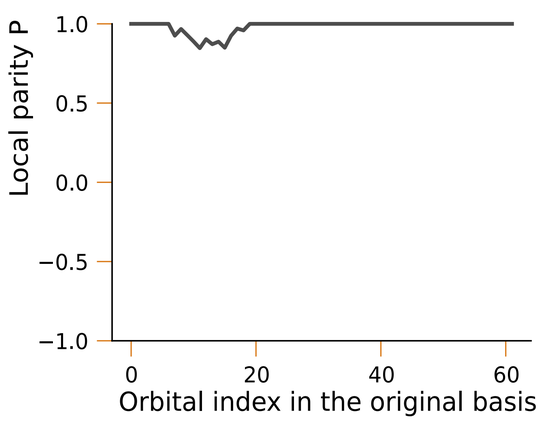
identify as bath — *identify as spins*

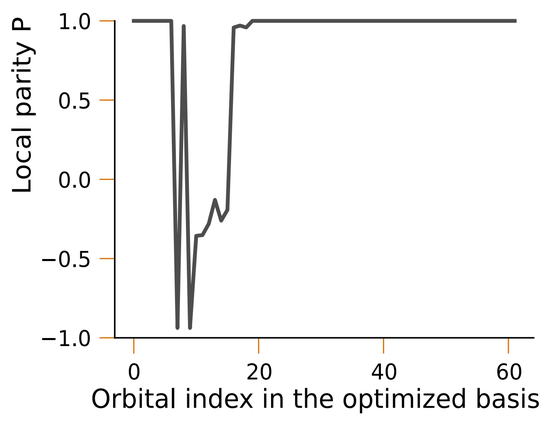
Spins in molecules

Our spin identification method was applied to a range of molecules of interest to our partners such as the *endiines*.

From initial ab-initio calculations we obtain the 1- and 2-RDM and the orbital basis. Our method identifies two linear combinations of orbitals with strong ***spin-like*** and **highly localized** character and strong local interaction.







Transformation to spin-bath models

We employ a generalized Schrieffer-Wolff transformation [1, 2] approach to integrate out undesirable terms V of the Hamiltonian. These terms V alter the occupancy of the orbitals previously identified as *spin-like*. This way ***spin-like*** orbitals become ideal ***spins***.

$$\tilde{H} = e^{S} H e^{-S} \simeq H + [S, H] + \mathcal{O}(S^2)$$

$$[S, H_0] = -V \quad \Rightarrow \quad \tilde{H} \simeq H_0 + \frac{1}{2}[S, V]$$

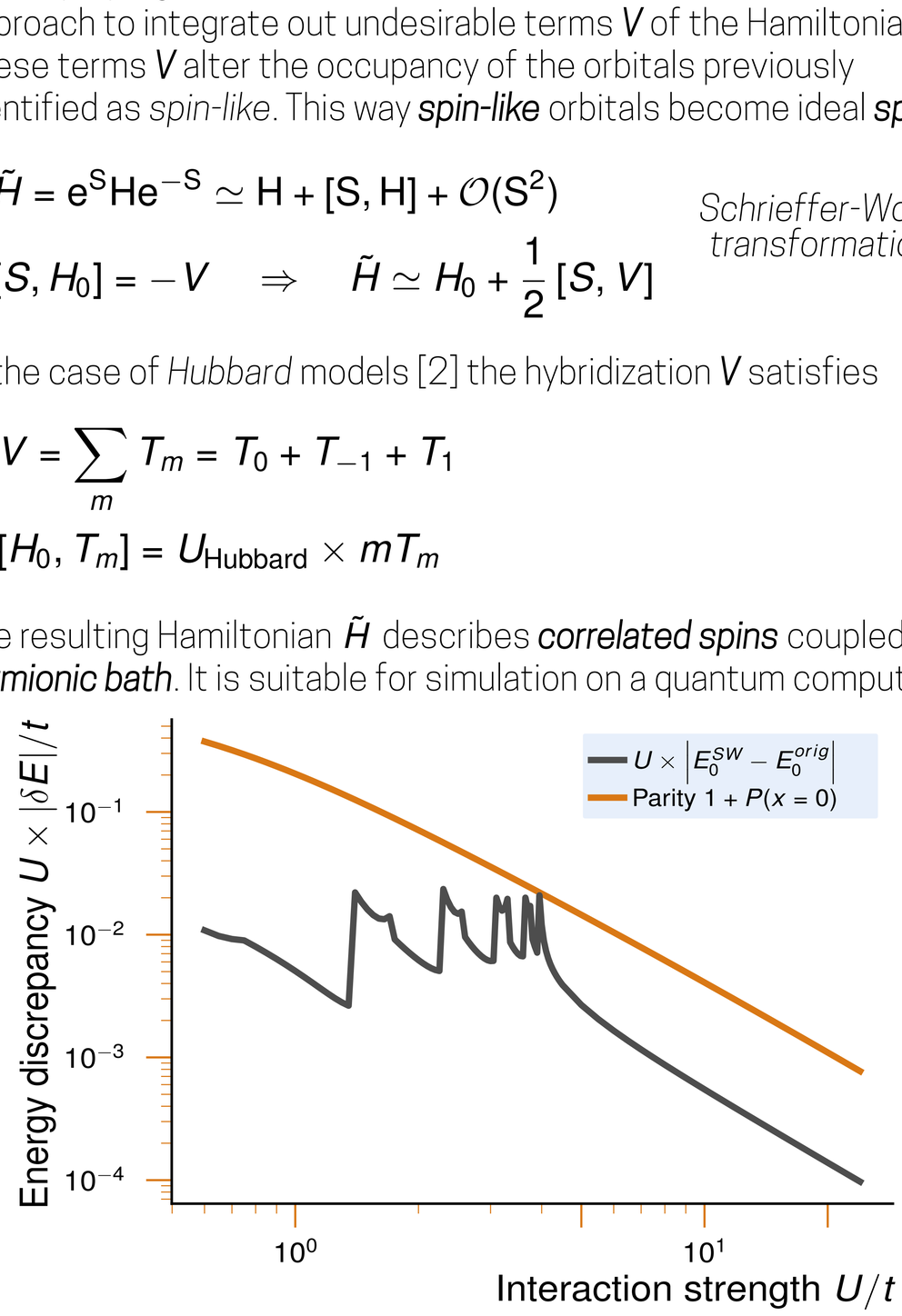
Schrieffer-Wolff transformation

In the case of *Hubbard* models [2] the hybridization V satisfies

$$V = \sum_m T_m = T_0 + T_{-1} + T_1$$

$$[H_0, T_m] = U_{\text{Hubbard}} \times m T_m$$

The resulting Hamiltonian $\tilde{H}$ describes ***correlated spins*** coupled to a ***fermionic bath***. It is suitable for simulation on a quantum computer.



Benchmark results for the single impurity Anderson model [1]

We find the parity to be a good indicator for the quality of the ***effective spin-bath model*** Hamiltonians derived with our method.

[1] J. Schrieffer and P. Wolff, Phys. Rev. 149, 491 (1966).
[2] A. H. MacDonald, S. M. Girvin, and D. Yoshioka, Phys. Rev. B 37, 9753 (1988).

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