Quantum computing in spin-adapted representations for efficient simulations of spin systems

Anthony Gandon
Alberto Baiardi
Max Rossmannek
Werner Dobrautz
Ivano Tavernelli

IBM Quantum, IBM Research – Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland
Institute for Theoretical Physics, ETH Zürich, Wolfgang-Pauli-Str. 27, 8093 Zürich, Switzerland
Department of Chemistry, Chalmers University of Technology, 41296 Gothenburg, Sweden
agandon@phys.ethz.ch

In this work, we propose a novel approach for implementing approximate quantum simulations in total-spin eigenbases. We show that the symmetric group approach [1] offers a natural framework for constructing spin-dapted quantum Hamiltonians [2] and corresponding time-evolution unitaries. This is accomplished through an encoding of spin eigenstates using a recursive coupling scheme, combined with a truncation of the permissible values for intermediate total spin variables. This truncation is justified by the remarkably fast convergence of the ground-state wavefunctions in the truncated subspaces toward the ground-state wavefunction in the complete spin-adapted subspace [3]. Combining this novel encoding and the truncation of height variables, we derive qubit Hamiltonians that are local and sparse, and well describe the low-energy spectrum of the Heisenberg model. Based on our newly-introduced hierarchy of Hamiltonians, we derive adiabatic schedules that interpolate between an easily prepared spin-adapted initial state and the exact ground state of the model. Compared to quantum algorithms that aim to preserve quantum numbers, the states prepared with our approach can be sampled directly in the eigenbasis of the total spin operator S^2, rather than in the eigenbasis of the projected spin operator S_z. We also show how to implement this adiabatic schedules can be implemented with shallow, hardware-friendly circuits.

References

[1] N. Flocke and J. Karwowski, Physical Review B 55, 8287 (1997).
[2] W. Dobrautz, S. D. Smart, and A. Alavi, The Journal of Chemical Physics 151, 094104 (2019).
[3] T. Vieijra and J. Nys, Physical Review B 104, 045123 (2021), ISSN 2469-9950

Figures

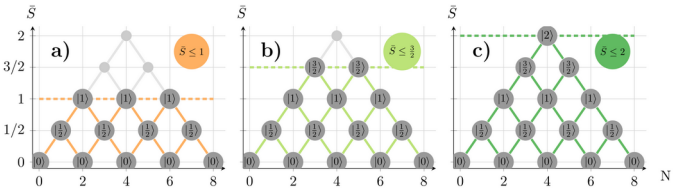

Figure 1: Truncation of the total-spin values allows a local and sparse qubit-encoding of the spin-adapted states and Hamiltonian.

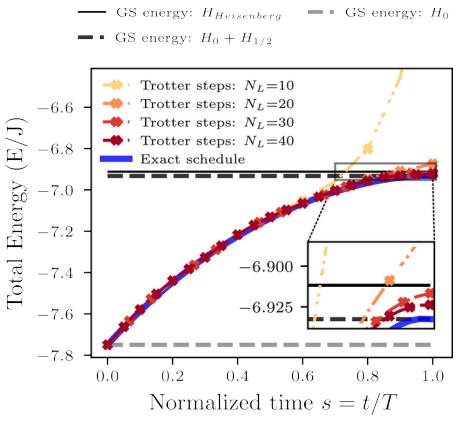

Figure 2: Simulation of an adiabatic state preparation schedule using the first non-trivial encoding. Our results (dashed) approximate the exact energy (full) with reduced circuit depth.