Quantum circuits for the preparation of spin eigenfunctions on quantum computers [1]

Alessandro Carbone [1,2]
Davide Emilio Galli, Mario Motta, Barbara Jones
[1] *Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland*
[2] *Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy*
alessandro.carbone@epfl.ch

The preparation of accurate and efficient approximations for Hamiltonian eigenstates on quantum computers is a crucial step for building the quantum advantage when studying many-body quantum systems. If we can describe molecules or materials with a coarse-grained spin Hamiltonian, spin eigenfunctions can be a useful starting point for simulations which aim to understand their electronic structure. On the other hand, if we do not know the spin model, the total spin eigenfunctions can be used to determine the coupling constants from first-principle calculations [2]. In particular the purpose of this work is to delve into the description of the quantum circuits which prepare total spin eigenfunctions in the case of spin-1/2 systems.

Previous approaches have typically concentrated on circuits encoding specific spin eigenstates, that have less generality, but require less quantum resources [3,4]. We investigate the balance between generality, accuracy, and computational cost in the encoding of spin eigenfunctions by quantum circuits without ancillary qubits, by pursuing two approaches: an exact recursive construction of spin eigenstates, and a heuristic variational construction of approximate spin eigenstates.

The former approach mimics the addition theorem of angular momenta. In general the circuits returned have an exponential scaling of the circuit depth with the system size. In the second approach we use the Variational Quantum Eigensolver (VQE) algorithm to minimize a suitable cost function and find the target circuits. The latter method has polynomial scaling of the circuit depth and it could lead to efficient implementations on hardware.

We have tested the described quantum circuits on the available IBM (classical) simulators and quantum devices through IBM Quantum Experience using IBM's open-source Python library for quantum computing, Qiskit [5]. In particular we show the fidelity values of several 3-spin and 5-spin quantum circuits with respect to the expected spin eigenstates, by focusing on both approaches.

References

[1] A. Carbone, D. E. Galli, M. Motta and B. Jones, arXiv: 2202.09479[quant-ph] (2022)
[2] R. Logemann, A. Rudenko, M. Katsnelson, and A. Kirilyuk, J. Phys. Cond. Mat, vol. 29, no. 33 (2017), p. 335801
[3] K. Sugisaki, S. Yamamoto, S. Nakazawa, K. Toyota, K. Sato, D. Shiomi, and T. Takui, Chem. Phys. Lett X, vol. 1 (2019), p. 100002
[4] A. Bärtschi and S. Eidenbenz, Fundamentals of Computation Theory (L. A. Gasieniec, J. Jansson, and C. Levcopoulos, eds.), Springer (2019), pp. 126–139
[5] G. Aleksandrowicz, T. Alexander, P. Barkoutsos, L. Bello, Y. Ben-Haim, D. Bucher, F. Cabrera-Hernández, J. Carballo-Franquis, A. Chen, C. Chen, et al., Zenodo, vol. 16 (2019)