Estimating exact energies in quantum simulation without Toffoli gates

Mark Steudtner[1] and Stephanie Wehner[2]
Phys. Rev. A **101**, 052329 (2020)

A quantum computer can essentially solve another quantum system by simulating the action of its Hamiltonian. The study of algorithms mimicking the effect of arbitrary Hamiltonians with a quantum computer is therefore an active field of research. First, a very simple such algorithm suggested discretizing the time evolution under a generic Hamiltonian in a stroboscopic fashion [1], but the accuracy of this approximation was not satisfying. Soon, more advanced algorithms were developed, that eventually culminated in an approach called *qubitization* [2]. Qubitization is a sophisticated quantum algorithm that can simulate a Hamiltonian exactly. However, advancing simulation algorithms further and further, we have strayed far away from the simplicity of the discretized time evolution. Just as other modern algorithms, qubitization requires complicated, Toffoli-like quantum gates operating on many qubits. The decomposition of these gates into native operations would either require a large number of additional resources or yield algorithms with a long runtime [3]. Even after attempts to simplify the qubitization routine the problem still persists [4]. In this work, however, we decompose the qubitization algorithm differently, and so eliminate Toffoli gates entirely. The resulting algorithm is so simple, it solely relies on operations similar to what has already been demonstrated in a large experiment [5]. By utilizing concepts from fermionic quantum computing, qubitization is now as simple as a discrete time evolution while still encoding an exact Hamiltonian simulation. `DOI: https://doi.org/10.1103/PhysRevA.101.052329`

[1] Lloyd, Science **273**, 1073 (1996).
[2] Low & Chuang, Quantum **3**, 163 (2019)
[3] Barenco et al., Phys. Rev. A **52**, 3457 (1995)
[4] Poulin et al., Phys. Rev. Lett. **121**, 010501 (2018)
[5] Google AI Quantum and Collaborators, arXiv:2004.04174 (2020)

---

[1] Dahlem Center for Complex Quantum Systems,
Freie Universität Berlin, 14195 Berlin, Germany
[2] Qutech, Delft University of Technology, 2628 CJ Delft, The Netherlands