

Improved Hardness Results for the Guided Local Hamiltonian Problem

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Ryu Hayakawa, Jordi Weggemans, Tomoyuki Morimae, Chris Cade, Marten Folkertsma, Sevag Gharibian and Francois Le Gall

Abstract: Estimating the ground state energy of a local Hamiltonian is a central problem in quantum chemistry. In order to further investigate its complexity and the potential of quantum algorithms for quantum chemistry, Gharibian and Le Gall (STOC 2022) recently introduced the guided local Hamiltonian problem (GLH), which is a variant of the local Hamiltonian problem where an approximation of a ground state (which is called a guiding state) is given as an additional input. Gharibian and Le Gall showed quantum advantage (more precisely, BQP-completeness) for GLH with 6-local Hamiltonians when the guiding state has fidelity (inverse-polynomially) close to $1/2$ with a ground state.

In this paper, we optimally improve both the locality and the fidelity parameter: we show that the BQP-completeness persists even with 2-local Hamiltonians, and even when the guiding state has fidelity (inverse-polynomially) close to 1 with a ground state. Moreover, we show that the BQP-completeness also holds for 2-local physically motivated Hamiltonians on a 2D square lattice or a 2D triangular lattice. Beyond the hardness of estimating the ground state energy, we also show BQP-hardness persists when considering estimating energies of excited states of these Hamiltonians instead. Those make further steps towards establishing practical quantum advantage in quantum chemistry.

Presenter: HAYAKAWA, Ryu

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