

Algorithmic improvements for adiabatic state preparation

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Finding the ground state of a general electronic structure Hamiltonian is one of the key problems in quantum chemistry. It is believed that quantum computers could be useful for solving this problem, due to their linear scaling with respect to the Hilbert space of a given system.

One of the first proposed methods to find good approximations to the ground state on a digital quantum computer in the gate model is adiabatic state preparation [1]. In the original implementation, the adiabatic evolution was performed using a discretisation of the time dependent Hamiltonian into sections where it is approximated as time independent, and the propagator is performed using Trotterization. The drawbacks of this method include a nonadiabatic error, which incurs due to finite simulation time, and large circuit depth due to the Trotterization of a non-local Hamiltonian.

However, since then there have been many improvements in the area of Hamiltonian simulation,

as well as our understanding of adiabatic processes. Here I will present a method which combines recent advances in Hamiltonian simulation [2], and a variational technique to counteract non-adiabatic effects [3], which has not yet been used for finding the ground state of an electronic structure problem. The former drastically improves the gate count in comparison to the more widely used Trotterization, while the latter mitigates the non-adiabatic errors. Finally, this method is applied to hydrogen and lithium hydride molecules together with phase estimation in an emulated quantum computer in order to show the advantage of the presented method.

References

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2. Campbell, Earl. "Random compiler for fast Hamiltonian simulation." *Physical Review Letters*, 123, 2019.
3. Pieter W. Claeys, Mohit Pandey, Dries Sels, and Anatoli Polkovnikov. "Floquet-Engineering Counterdiabatic Protocols in Quantum Many-Body Systems" *Phys. Rev. Lett.* 123, 2019.