Approximate quantum adiabatic Hamiltonian simulation on quantum computers

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Quantum evolution of a state is described by the Schrödinger equation: $i\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle, |\psi(0)\rangle = |\psi_0\rangle$, in which $H(t)$ is a time-dependent Hamiltonian operator. Formal solution of this problem is written as: $|\psi(t)\rangle = \mathcal{T}exp(-i\int_o^t H(t')dt')\,|\psi_0\rangle$, in which $\mathcal{T}exp$ is the so called T-exponent, resulting in a complicated iterative formula. Quantum adiabatic evolution (QAE) happens when $H(t)$ is a slowly varying function. QAE preserves an eigenstate. This can be used in quantum annealing for solving hard classical problems (see [4] and refs. therein), in holonomic quantum computing for manipulating qubits [2] or solving molecular and other electronic problems in material science [1].

We suggest a way to approximate QAE using piecewise constant Hamiltonians, see Fig. 1, the corresponding approximation (=AQAE) converges to the true QAE in the limit of small step-size. Such approximation can be implemented on a quantum gate computer. We made tests on solving the classical QUBO problem (e.g. number partitioning) and simulated the exotic quantum holonomy effect. Classical computers cannot effectively simulate QAE of large quantum systems and a quantum computer is needed as well as a gate implementation of the corresponding AQAE. Such capacity would be useful in simulating control of qubits in holonomic quantum computers and other quantum devices. For electronic structure simulations we suggest to use Hamiltonian matrices, which tend to be sparse and thus has an effective quantum gate implementation of AQAE. All concepts are tested on a small-scale using quantum gate computers like VTT's 5-qubit Helmi machine.

References

[1] W.Rodrigues, et al. Comput. Electron., 14(2015), 593-603
[2] P. Zanardi and M Rasetti, Physics Letters A, 264(1999), 94-99.
[3] T. Cheon, et al., Physics Letters A, 2(2009), 144-149
[4] H. Reittu, et al., In Proc. 2019 IEEE International Conf. on Big Data, Big Data 2019, 2457-2464

Figures

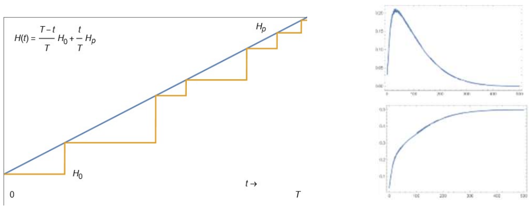

Figure 1: Left: QAE from H_0 to H_p, the blue line. The yellow line: a sequence of piecewise constant Hamiltonians approximating QAE (AQAE). AQAE can be effectively implemented as a sequence of quantum gates. AQAE for a QUBO – probability of a false state (top) vs of a solution (bottom).

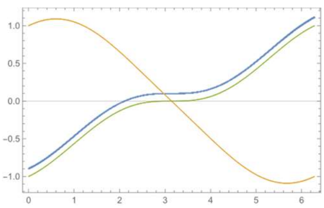

Figure 2: Exotic quantum holonomy in a two-level system [3], energies of two levels green and orange lines as a function of a parameter. Blue dots: energy found using QAE, points lie on the green line (a constant was added to each AQAE point to separate the plots).