AQAlg: Advanced Quantum Algorithms **2025 - 2026**

Lecture 5: Quantum simulation

Lecturer: Simon Apers (apers@irif.fr)

In previous lectures we discussed the use of quantum algorithms for solving essentially "non-quantum" problems such as factoring and optimization. However, the most natural (and maybe most promising) application of quantum computers is the simulation of quantum systems. For some given Hamiltonian H and time t, this corresponds to implementing the Hamiltonian evolution

$$|\psi\rangle \mapsto e^{iHt}|\psi\rangle .$$

1 Hamiltonian simulation

While the evolution e^{iHt} describes the "native dynamics" on certain (analog) quantum computing architectures, the leading architecture today is the quantum circuit model, and so we will look into simulating Hamiltonian evolution using a discrete circuit.

From last week's exercise, we know that any Hamiltonian H can be expanded as a sum of simpler Hamiltonians,

$$H = \sum_{j=1}^{m} H_j,$$

where the H_j's are n-qubit Pauli operators. In fact, looking at Hamiltonians of interest, they are often a linear combination of only $\text{poly}(n)$ k-local Pauli terms.[1] In the remainder, we will assume that

1. H is 2-local, and so H consists of $m \in O(n^2)$ 2-qubit terms.
2. We have access to the evolution $e^{iH_j\gamma}$ for all j and $\gamma > 0$, which are effectively just 2-qubit gates.

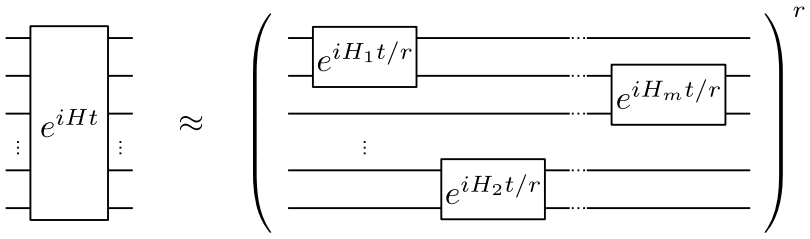
Unfortunately, since the H_j's do not generally commute, we have that

$$e^{iHt} = e^{i\sum_j H_j t} \neq e^{iH_1 t} \dots e^{iH_m t}.$$

However, by the so-called *Lie product formula*, we do have that

$$e^{iHt} = \lim_{r\to\infty} \left(e^{iH_1 t/r} e^{iH_2 t/r} \dots e^{iH_m t/r}\right)^r .$$

Crucially, for finite r, the expansion in the right hand side corresponds to a quantum circuit with mr gates of the form $e^{iH_j t/r}$. This hence yields a natural approach for doing Hamiltonian simulation:



[1] An n-qubit Pauli operator is k-local if it acts nontrivially on at most k qubits. E.g., the Max cut Hamiltonian from last week is 2-local.

In the following, we will bound the error incurred for finite r.

1. Assume $\|A_1\|, \|A_2\| \leq 1/2$. Use the Taylor series $e^B = I + B + O(\|B\|^2)$ for $\|B\| \leq 1$ to show that
$$e^{A_1+A_2} = e^{A_1}e^{A_2} + E, \quad \|E\| \in O(\|A_1\|^2 + \|A_2\|^2). \tag{1}$$

2. Assume $\|A_1\|, \ldots, \|A_m\| \leq \delta \leq 1/(2m)$. Use (1) to show that
$$e^{A_1+\cdots+A_m} = e^{A_1} \ldots e^{A_m} + E_m, \quad \|E_m\| \in O(m^2\delta^2). \tag{2}$$

3. Assume $\|H_1\|, \|H_2\| \leq 1/2$. For $r \geq t$, argue that
$$e^{i(H_1+H_2)t} = \left(e^{iH_1t/r}e^{iH_2t/r}\right)^r + E_r, \quad \|E_r\| \in O(t^2/r).$$

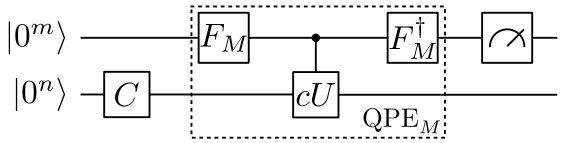
4. Assume $\|H_1\|, \ldots, \|H_m\| \leq 1$. For $r \geq 2mt$, argue that
$$e^{i(H_1+\cdots+H_m)t} = \left(e^{iH_1t/r} \ldots e^{iH_mt/r}\right)^r + E_r, \quad \|E_r\| \in O(m^2t^2/r).$$

Picking $r \in O(t^2m^2/\epsilon)$, it follows that we can ϵ-approximate the Hamiltonian evolution e^{iHt} using $mr \in O(t^2m^3/\epsilon)$ 2-qubit gates.

2 Ground state energy

A canonical problem in quantum chemistry is that of estimating the ground state energy of a molecular or condensed matter Hamiltonian. In full generality, this problem is QMA-hard (see lectures by A. Grilo), and so we do not expect to solve this efficiently even on a quantum computer. However, there is hope that more "natural" Hamiltonians do allow for efficient quantum algorithms, while still being hard for classical algorithms.

The most natural quantum algorithm for estimating the ground state energy of an n-qubit Hamiltonian H is based on quantum phase estimation. It corresponds to the following circuit:



Some details:

1. C is an n-qubit circuit that prepares an "ansatz state" $|\Psi_0\rangle$. Ideally this corresponds to a rough approximation of the ground state $|\phi_0\rangle$ of H.

2. The algorithm then applies quantum phase estimation on $|\Psi_0\rangle$ with operator $U = e^{iH}$ and precision $2^{-m} = 1/M$.

3. Finally, the phase estimation register is measured. The measurement result yields an estimate of the ground state energy.

Assume H has eigenvalue decomposition $H = \sum_{i=0}^{2^n-1} \lambda_i |\phi_i\rangle$, with eigenvalues $\lambda_0 \leq \cdots \leq \lambda_{2^n-1}$, and the ansatz has decomposition $|\Psi_0\rangle = \sum_i \alpha_i |\phi_i\rangle$. We can track the evolution in the circuit:

$$\begin{aligned} |0^m\rangle |0^n\rangle &\xrightarrow{C} |0^m\rangle |\Psi_0\rangle = \sum_i \alpha_i |0^m\rangle |\phi_i\rangle \\ &\xrightarrow{\mathrm{QPE}_M} \sum_i \alpha_i |\tilde{\lambda}_i\rangle |\phi_i\rangle \\ &\xrightarrow{\text{meas.}} |\tilde{\lambda}_i\rangle |\phi_i\rangle \quad \text{with probability} \quad p_i = |\alpha_i|^2. \end{aligned}$$

Here $\tilde{\lambda}_i$ is an estimate such that $|\tilde{\lambda}_i - \lambda_i| \leq 1/M$.

The *complexity* of the circuit is dominated by (i) the complexity of preparing the ansatz (i.e., implementing C), and (ii) the complexity of doing Hamiltonian simulation with Hamiltonian H for time $O(M)$.

Correctness of the algorithm hinges on the overlap $|\alpha_0|^2 = |\langle\Psi_0|\phi_0\rangle|^2$ of our ansatz state $|\Psi_0\rangle$ with the actual ground state $|\phi_0\rangle$. The probability of actually outputting an estimate of the ground state energy is $|\alpha_0|^2$. If this is sufficiently large (e.g., $|\alpha_0|^2$ constant), then after a constant number of iterations, the algorithm will output a correct estimate of the ground state energy. On the other hand, if we have no clue about the ground state $|\phi_0\rangle$, then we could pick as ansatz a uniformly random initial state, but then the overlap would only be $|\alpha_0|^2 = 1/2^n$ in expectation. The algorithm then returns an estimate of a uniformly random energy level of the Hamiltonian, which is typically useless.

Common ansatzes are based on the quantum adiabatic algorithm, variational quantum circuits, and classical approximations such as Hartree-Fock.