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Tutorial 6 (Quantum time evolution and simulation)
Physically, a (closed) quantum system is governed by a so-called *Hamiltonian* operator H (not to be confused with the Hadamard gate), which is a Hermitian matrix in finite dimensions. The eigenstates of H are referred to as energy eigenstates, and the corresponding eigenvalues as energies. The eigenstate with lowest energy is the *ground state*. In laboratory experiments, one often tries to prepare a quantum state near the ground state by cooling the physical system.

H also governs how a quantum state $|\psi\rangle$ changes over time via the following linear differential equation:

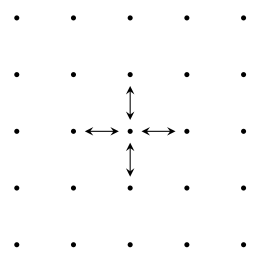
$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = H|\psi(t)\rangle. \tag{1}$$

This is the famous Schrödinger equation. The argument t denotes the time dependence of $|\psi\rangle$, and $\hbar$ is the reduced Planck constant (a fundamental physical constant), which we will absorb into H such that effectively $\hbar = 1$.

In case H does not itself depend on time, the solution of Eq. (1) is

$$|\psi(t)\rangle = U_t|\psi(0)\rangle \quad \text{with} \quad U_t = \mathrm{e}^{-iHt}.$$

U_t is the unitary *time evolution operator*.
For typical physical systems, H can be written as sum over many local interactions: $H = \sum_{k=1}^{L} H_k$. An example are particles arranged on a regular lattice, which interact solely with nearest neighbors and an external magnetic field. Specifically, a well-studied model is the Ising Hamiltonian



$$H = -J \sum_{j,\ell \text{ nn}} Z_j\, Z_\ell - h \sum_j X_j$$

where J and h are parameters, j and ℓ label lattice sites, the first sum is over nearest neighbors, Z_j is the Pauli-Z matrix acting on lattice site j, and analogously X_j the Pauli-X matrix acting on site j.

Here we investigate how to simulate the quantum time evolution using quantum circuits. Rewriting H as a sum over local terms is useful because, even though e^{-iHt} is difficult to compute, $\mathrm{e}^{-iH_k t}$ acts on a smaller subsystem and is easier to handle. In general, $\mathrm{e}^{i(A+B)t} \neq \mathrm{e}^{iAt}\mathrm{e}^{iBt}$ unless A and B commute. However, even for non-commuting operators, the following Trotter formula holds:

$$\mathrm{e}^{i(A+B)t} = \lim_{n\to\infty} \left(\mathrm{e}^{iAt/n}\, \mathrm{e}^{iBt/n}\right)^n. \tag{2}$$

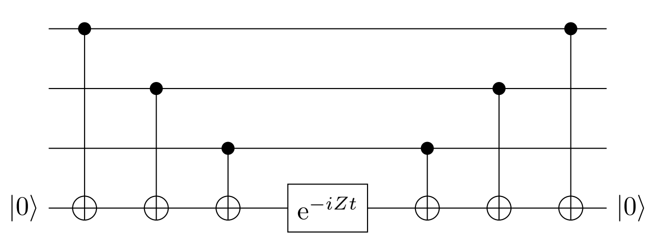
Thus we can approximate a time step Δt via $\mathrm{e}^{i(A+B)\Delta t} \approx \mathrm{e}^{iA\Delta t}\, \mathrm{e}^{iB\Delta t}$ and similarly $\mathrm{e}^{-iH\Delta t} \approx \mathrm{e}^{-iH_1\Delta t} \cdots \mathrm{e}^{-iH_L\Delta t}$.

(a) Prove the Trotter formula in Eq. (2), and discuss the corresponding simulation algorithm.

In some cases it is even possible to simulate systems where the Hamiltonian is not a sum of local interactions. For example, consider

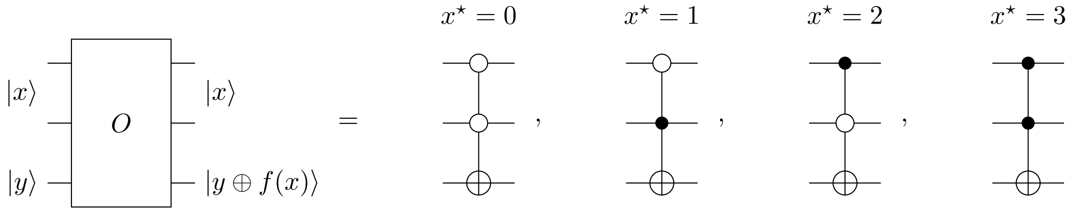
$$H = Z_1 \otimes Z_2 \otimes \cdots \otimes Z_n. \tag{3}$$

(b) How would a quantum state evolve under H in Eq. (3)? Argue that the circuit on the right is an exact implementation of the time evolution operator e^{-iHt}, illustrated for $n = 3$.



Exercise 6.1 (Two-bit quantum search)
We consider the quantum search (Grover's) algorithm described in tutorial 6 for the special case $n = 2$, i.e., a search space with $N = 4$ elements, and $M = 1$ (exactly one solution). The solution is denoted $x^\star$, and correspondingly $f(x^\star) = 1$, $f(x) = 0$ for all $x \neq x^\star$.

The oracle, which is able to recognize the solution, can be realized as follows (depending on $x^\star$):

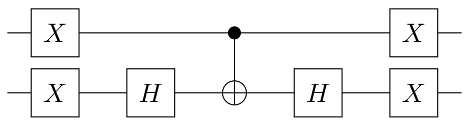


The rightmost gate for $x^\star = 3$ is the *Toffoli* gate, a generalization of CNOT: the first and second qubits act as controls, and the third qubit as target, which is flipped precisely if both controls are set to 1. The empty circles in the gates for $x^\star = 0, 1, 2$ mean that the control is activated by 0 (instead of 1).

As derived in tutorial 6, the Grover operator G performs a rotation by angle θ in the plane spanned by the orthonormal states $|\alpha\rangle$ and $|\beta\rangle$; thus k applications to the initial equal superposition state $|\psi\rangle = \cos(\frac{\theta}{2})|\alpha\rangle + \sin(\frac{\theta}{2})|\beta\rangle$ results in

$$G^k|\psi\rangle = \cos\left((\tfrac{1}{2} + k)\theta\right)|\alpha\rangle + \sin\left((\tfrac{1}{2} + k)\theta\right)|\beta\rangle.$$

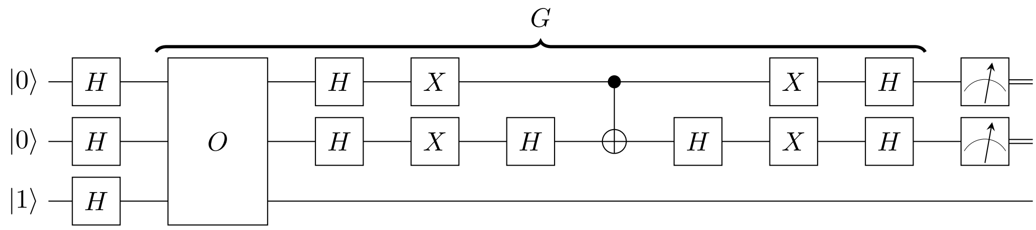
(a) Show that the following circuit implements the negated phase gate appearing in the Grover operator, that is, $-(2|00\rangle\langle 00| - I)$:



The global factor (-1) does not influence the final quantum measurement results and will be ignored from now on.

(b) Compute the angle θ defined via $\sin(\frac{\theta}{2}) = \sqrt{M/N}$. Why is a single application of G sufficient to reach the desired solution state $|\beta\rangle$ exactly, that is, $G|\psi\rangle = |\beta\rangle$?

In summary, the quantum search circuit with one use of G and the above realization of the phase gate is:



(c) Assemble this circuit in the IBM Q Circuit Composer for one of the four possible oracles of your choice, and verify that the final measurement indeed yields the solution $x^\star$.

Hint: You can use the Pauli-X gate to initialize the oracle qubit to $|1\rangle$. The Toffoli gate is available in the Circuit Composer.

Exercise 6.2 (Bloch sphere for mixed state qubits[1])

(a) Show that an arbitrary density operator ρ for a qubit may be written as

$$\rho = \frac{I + \vec{r} \cdot \vec{\sigma}}{2}, \tag{4}$$

where $\vec{r} \in \mathbb{R}^3$ is a real vector such that $\|\vec{r}\| \leq 1$. ($\vec{r}$ is called the *Bloch vector* of ρ.)

Hint: Recall from tutorial 1 that $\{I, \sigma_1, \sigma_2, \sigma_3\}$ forms a basis of 2×2 matrices. Argue that the corresponding coefficients to represent a density matrix are real. Why is the coefficient of I equal to $\frac{1}{2}$? Finally, compute the eigenvalues of the representation in Eq. (4) and use the positivity of ρ to derive the condition $\|\vec{r}\| \leq 1$.

(b) Show that a state ρ is pure if and only if $\|\vec{r}\| = 1$.

(c) Verify that for pure states $\rho = |\psi\rangle\langle\psi|$, the above definition of the Bloch vector $\vec{r}$ coincides with the Bloch vector of $|\psi\rangle$ (cf. exercise 2.1).

Hint: Insert $|\psi\rangle = e^{i\gamma}(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle)$ into $|\psi\rangle\langle\psi|$, read off the entries of $\vec{r}$ based on $|\psi\rangle\langle\psi| = (I + \vec{r}\cdot\vec{\sigma})/2$, and verify that $\vec{r} = (\cos(\varphi)\sin(\theta), \sin(\varphi)\sin(\theta), \cos(\theta))$.

[1] M. A. Nielsen, I. L. Chuang: *Quantum Computation and Quantum Information*. Cambridge University Press (2010), Exercise 2.72