Quantum Information Theory
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Sheet 4

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Quantum simulation

Graded exercises

Problem 1. We are given a set of unitaries $U_1, \ldots, U_M$ acting on n qubits. Furthermore, there is another register (called the clock register), with states $|t\rangle$ with $t = 0, \ldots, M$. Consider the Hamiltonian

$$H = -|0^n\rangle\langle 0^n| \otimes |0\rangle\langle 0| - \mathrm{id} \otimes |M\rangle\langle M| - \sum_{t=0}^{M-1} \left(U_{t+1} \otimes |t+1\rangle\langle t| + \mathrm{h.c.}\right) .$$

Note that 'h.c.' means *Hermitian conjugate*, and is used to denote the Hermitian conjugates of the terms that appear just before. We would like to investigate the ground state of this Hamiltonian. Consider the operator W,

$$W = \mathrm{id} \otimes |0\rangle\langle 0| + \sum_{t=1}^{M} U_t \ldots U_2 U_1 \otimes |t\rangle\langle t| .$$

1. Show that W is unitary.
2. Compute the Hamiltonian $H' = W^* H W$.
3. Show that the state

$$|G\rangle = \frac{1}{\sqrt{M+1}} \left(\sum_{t=1}^{M} U_t \ldots U_2 U_1 |0^n\rangle |t\rangle + |0^n\rangle |0\rangle \right)$$

is the ground state of the Hamiltonian H.

Hint: To compute the ground state of H, do it first for H' and use the relation between H and H'.
Hint 2: If you need it, you can assume that the clock register is large enough, such that the boundary at $t = 0$ and $t = M$ can be neglected.

Problem 2. Consider the unitary $U = \exp(i(X + Z)t)$. Show that

1. $U \neq \exp(iXt)\exp(iZt)$. In particular, show that

$$\|U - \exp(iXt)\exp(iZt)\| \leq O(t^2),$$

where, for a matrix M, the norm we are taking is $\|M\| = \sup_{|\psi\rangle \neq 0} \|M|\psi\rangle\| / \||\psi\rangle\|$, and $\||\psi\rangle\| = \sqrt{|\psi_1|^2 + \ldots + |\psi_n|^2}$.

2. Consider the unitary U_M given by

$$U_M = \left(\exp\left(iX\frac{t}{M}\right)\exp\left(iZ\frac{t}{M}\right)\right)^M .$$

Using the result from the previous part, show that

$$\|U - U_M\| \leq O(t^2/M) .$$

Problem 3. Consider the two-qubit Heisenberg Hamiltonian

$$H(t) = J(t)\vec{S_1}\cdot\vec{S_2} = \frac{J(t)}{4}\left[X_1X_2 + Y_1Y_2 + Z_1Z_2\right] .$$

1. Show that a SWAP operation (denoted by U) can be implemented by turning on $J(t)$ for an appropriate amount of time τ, to obtain $U = \exp(-i\pi\vec{S_1}\cdot\vec{S_2})$.

   Hint: Compute the eigenvalues of the SWAP gate, as well as those of $\vec{S_1}\cdot\vec{S_2} = \frac{X_1X_2+Y_1Y_2+Z_1Z_2}{4}$*, and compare them. Set* $J(t) = 1$ *for time* π *for simplicity.*

2. Compute the gate that we obtain by turning on $J(t)$ for time $\tau/2$, which we denote by $\sqrt{SWAP}$. Together with arbitrary single qubit gates, the $\sqrt{SWAP}$ gate is universal for quantum computation.

Challenge exercise

Problem 4. Here, we are going to prove that Grover's algorithm can be derived from a Schrödinger time evolution equation governed by a certain Hamiltonian H. For simplicity, we assume that there is a single solution $x \in \{0, \ldots, N-1\}$ to Grover's problem with N elements and we start from an arbitrary initial state $|\psi\rangle$. It turns out that the Hamiltonian

$$H = |x\rangle\langle x| + |\psi\rangle\langle\psi|$$

achieves a transition from $|\psi\rangle$ to $|x\rangle$ for a certain time t^*, i.e. $\mathrm{e}^{-iHt^*}|\psi\rangle = |x\rangle$. To understand it, first note that the time dynamics under H never leave the two-dimensional space spanned by $|x\rangle$ and $|\psi\rangle$. Consider a vector $|y\rangle$ such that $\{|x\rangle, |y\rangle\}$ forms an orthonormal basis of this subspace, and represent $|\psi\rangle = \alpha|x\rangle + \beta|y\rangle$ with coefficients $\alpha, \beta \in \mathbb{C}$, with $|\alpha|^2 + |\beta|^2 = 1$. For simplicity, let us assume that the phases of $|x\rangle, |y\rangle$ and $|\psi\rangle$ are such that α and β are real.

1. Show that the matrix representation of H within this subspace is given by

$$H = I + \alpha(\beta X + \alpha Z) .$$

2. From the previous expression, we obtain $\mathrm{e}^{-iHt} = \mathrm{e}^{-it}\,\mathrm{e}^{-i\alpha t(\beta X + \alpha Z)}$, where the factor e^{-it} appears from the identity matrix in the representation. Use the single-qubit maps for rotations to verify that

$$\mathrm{e}^{-iHt} = \mathrm{e}^{-it}(\cos(\alpha t)I - i\sin(\alpha t)(\beta X + \alpha Z)) .$$

3. Show that $(\beta X + \alpha Z)|\psi\rangle = |x\rangle$. Jointly with the previous part, obtain

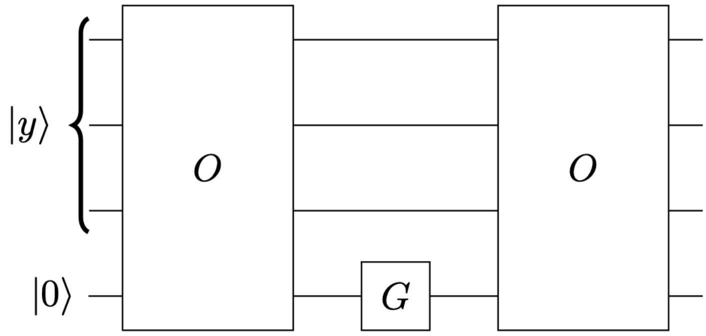
$$\mathrm{e}^{-iHt}|\psi\rangle = \mathrm{e}^{-it}(\cos(\alpha t)|\psi\rangle - i\sin(\alpha t)|x\rangle) .$$

4. Specify a time t^* such that $e^{-iHt^*} |\psi\rangle = |x\rangle$, up to a phase factor.
5. Since the required time t^* depends on $\alpha = \langle x|\psi\rangle$ and thus seemingly on the solution x (which, a priori, we do not know), a natural question is how to determine t^*. To solve this equation, one can choose $|\psi\rangle$ to be the equal superposition state. Compute α in this case, assuming that $|\psi\rangle$ is normalized.

   Now, we are going to approximate the effect of the Hamiltonian via the Trotter formula:

   $$\lim_{n\to\infty} \left(e^{-iH_1 t/n}\, e^{-iH_2 t/n}\right)^n = e^{-i(H_1+H_2)t} \ .$$

   For that, we are going to consider a small time step $\Delta t = t/n$ and $H_1 = |x\rangle\langle x|$ and $H_2 = |\psi\rangle\langle\psi|$.
6. Show that the following circuit implements $e^{-iH_1\Delta t}$:



   where G is given by $G = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\Delta t} \end{pmatrix}$ and O is an oracle that maps $|y\rangle|0\rangle$ to $|y\rangle|1\rangle$ if $x = y$, and leaves it invariant otherwise.

   Hint: Represent the input in the following form:

   $$|y\rangle|0\rangle = (I - |x\rangle\langle x|)|y\rangle|0\rangle + |x\rangle\langle x|y\rangle|0\rangle$$

   and use the series expansion of the exponential to show

   $$e^{-i|x\rangle\langle x|\Delta t} = I - |x\rangle\langle x| + e^{-i\Delta t}|x\rangle\langle x| \ .$$

7. Modify the oracle to design a circuit analogous to the one above that implements the time evolution with respect to $|\psi\rangle\langle\psi|$ instead, for the cases:
   a) $|\psi\rangle = |+\rangle^{\otimes 3}$.
   b) $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)|1\rangle$.
8. Identify the circuits from the last two parts for a time step $\Delta t = \pi$ with the building blocks of the circuit diagram of Grover's algorithm.