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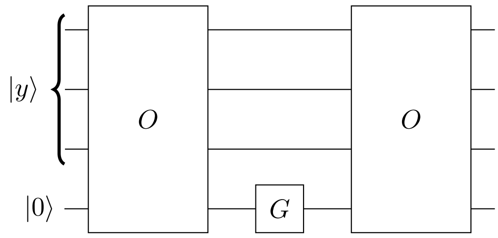
Exercise 10.2 (Quantum search as quantum simulation, part 2)
Continuing from exercise 9.2, the goal here is to *simulate* the time evolution governed by the Hamiltonian $H = |x\rangle\langle x| + |\psi\rangle\langle\psi|$ on a quantum computer. For that purpose, we can decompose $H = H_1 + H_2$ with $H_1 = |x\rangle\langle x|$ and $H_2 = |\psi\rangle\langle\psi|$, and approximate its effect via the Trotter formula, based on the identity:

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

In our case, we can apply H_1 and H_2 in an alternating fashion using a small time step $\Delta t = t/n$ for some large n.

(a) Show that the following circuit implements $e^{-iH_1\Delta t}$, where $G = \left(\begin{smallmatrix}1 & 0\\ 0 & e^{-i\Delta t}\end{smallmatrix}\right)$ and the oracle O is defined as in exercise 9.1, i.e., O maps $|y\rangle|0\rangle \mapsto |y\rangle|1\rangle$ precisely if $y = x$, and leaves $|y\rangle|0\rangle$ invariant otherwise.



Hint: Represent the input as

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

and use the series expansion of the exponential to derive that $e^{-i|x\rangle\langle x|\Delta t} = I - |x\rangle\langle x| + e^{-i\Delta t}|x\rangle\langle x|$.

(b) Modify the oracle to design a circuit analogous to part (a) that implements the time evolution with respect to $H_2 = |\psi\rangle\langle\psi|$ for the cases

(i) $|\psi\rangle = |+\rangle^{\otimes 3}$, i.e., $|\psi\rangle$ the equal superposition state
(ii) $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)\,|1\rangle$

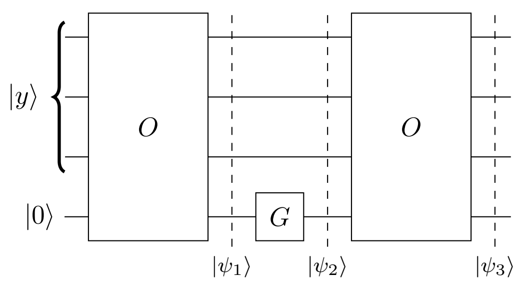
(c) Identify the circuits from (a) and (b) for a time step $\Delta t = \pi$ with the building blocks of the circuit diagram of Grover's algorithm.

Solution

(a) We first expand the term $e^{-i|x\rangle\langle x|\Delta t}$ via the matrix exponential series:

$$\begin{aligned}
e^{-i|x\rangle\langle x|\Delta t} &= \sum_{k=0}^{\infty}\frac{(-i\,|x\rangle\langle x|\,\Delta t)^k}{k!}\\
&= I + \sum_{k=1}^{\infty}\frac{(-i\Delta t)^k}{k!}\,|x\rangle\langle x|\\
&= I - |x\rangle\langle x| + \underbrace{\sum_{k=0}^{\infty}\frac{(-i\Delta t)^k}{k!}}_{e^{-i\Delta t}}\,|x\rangle\langle x|\\
&= I - |x\rangle\langle x| + e^{-i\Delta t}\,|x\rangle\langle x|\,.
\end{aligned}$$

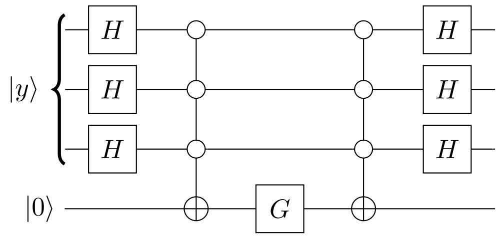
We then break down the circuit into individual steps:



$$
\begin{aligned}
|\psi_1\rangle &= (I - |x\rangle\langle x|)\,|y\rangle\,|0\rangle + |x\rangle\langle x\,|\,y\rangle\,|1\rangle \\
|\psi_2\rangle &= (I - |x\rangle\langle x|)\,|y\rangle\,|0\rangle + e^{-i\Delta t}\,|x\rangle\langle x\,|\,y\rangle\,|1\rangle \\
|\psi_3\rangle &= (I - |x\rangle\langle x|)\,|y\rangle\,|0\rangle + e^{-i\Delta t}\,|x\rangle\langle x\,|\,y\rangle\,|0\rangle \\
&= (I - |x\rangle\langle x| + \mathrm{e}^{-i\Delta t}\,|x\rangle\langle x|)\,|y\rangle\,|0\rangle \\
&= e^{-i|x\rangle\langle x|\Delta t}\,|y\rangle\,|0\rangle\,.
\end{aligned}
$$

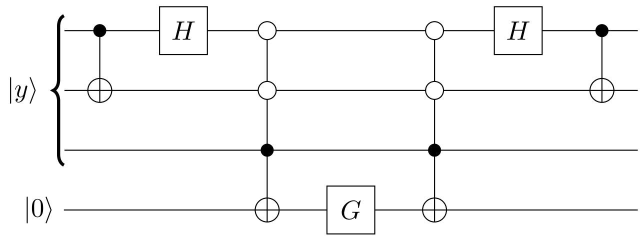
(b) Analogous to part (a), we note that the required effect of the to-be modified oracle is to flip the last qubit if the input $|y\rangle$ is equal to $|\psi\rangle$, and leave the last qubit invariant for any state orthogonal to $|\psi\rangle$. Different from (a), $|\psi\rangle$ is not a computational basis state here, but we can use Hadamard gates to perform as base change and then proceed as for computational basis states.

(i) Since $(H \otimes H \otimes H)\,|\psi\rangle = |000\rangle$, after the base change we need to recognize the state $|000\rangle$. This results in the overall circuit



The right half is a mirrored version of the left half to "uncompute" its action. The overall effect is to apply the phase factor $e^{-i\Delta t}$ precisely for input $|\psi\rangle$, as required.

(ii) We need an oracle which recognizes a Bell state in the leading two qubits:



(c) Note that $\mathrm{e}^{-i\pi} = -1$ corresponds to a sign flip. The circuit from part (b), case (i) (equal superposition state) can be identified with the Hadamard-phase-Hadamard block from Grover's algorithm, since it sends $|\psi\rangle \mapsto -|\psi\rangle$. The circuit from part (a) corresponds to the oracle application with the "oracle qubit" initialized to $|-\rangle$, since this likewise effects a sign flip precisely if the input is the sought solution $|x\rangle$.