Quantum Computation and Simulation

Exercise set 1

Exercise 1

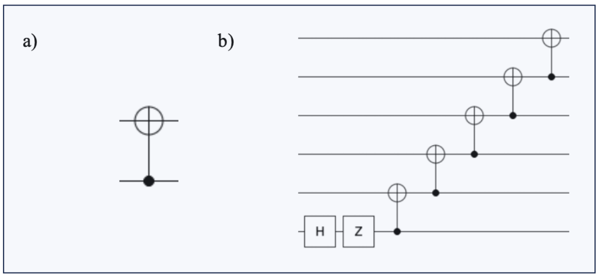
On circuit theory.

a) Write down the unitary that represents the upside-down CNOT gate in Fig. a)

b) What is the state resulting from the circuit shown in Fig. b) to $|0\rangle^{\otimes 6}$?

c) What is the result of measuring the X operator on the first qubit of that state?

d) How would you perform the $X^{\otimes n}$ measurement in practice? (i.e. assuming your quantum computer can only measure in the computational basis)



Solution 1

a)

$$U = CNOT_{2\to 1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

b)

$$U_{\text{tot}} = (CNOT_{2\to 1} \otimes \mathbb{I}_{3456})\,(CNOT_{3\to 2} \otimes \mathbb{I}_{1456})\,(CNOT_{4\to 3} \otimes \mathbb{I}_{1256})\,(CNOT_{5\to 4} \otimes \mathbb{I}_{1236})$$
$$(CNOT_{6\to 5} \otimes \mathbb{I}_{1234})\left(\mathbb{I}^{\otimes 5} \otimes Z_6 H_6\right)$$

$$
\begin{aligned}
|\psi'\rangle &= U_{\text{tot}} |0\rangle^{\otimes 6} \\
|\psi_1\rangle &= \left(\mathbb{I}^{\otimes 5} \otimes Z_6 H_6\right) |0\rangle^{\otimes 6} = |00000\rangle \otimes Z_6 H_6 |0\rangle = |00000\rangle \otimes Z_6 \frac{|0\rangle + |1\rangle}{\sqrt{2}} = |00000\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \\
&= \frac{1}{\sqrt{2}} \left(|000000\rangle - |000001\rangle\right) \\
|\psi_2\rangle &= (CNOT_{6\to 5} \otimes \mathbb{I}_{1234}) |\psi_1\rangle = \frac{1}{\sqrt{2}} \left(|000000\rangle - |000011\rangle\right) \\
|\psi_3\rangle &= (CNOT_{5\to 4} \otimes \mathbb{I}_{1236}) |\psi_2\rangle = \frac{1}{\sqrt{2}} \left(|000000\rangle - |000111\rangle\right) \\
|\psi_4\rangle &= (CNOT_{4\to 3} \otimes \mathbb{I}_{1256}) |\psi_3\rangle = \frac{1}{\sqrt{2}} \left(|000000\rangle - |001111\rangle\right) \\
|\psi_5\rangle &= (CNOT_{3\to 2} \otimes \mathbb{I}_{1456}) |\psi_4\rangle = \frac{1}{\sqrt{2}} \left(|000000\rangle - |011111\rangle\right) \\
|\psi'\rangle &= (CNOT_{2\to 1} \otimes \mathbb{I}_{3456}) |\psi_5\rangle = \frac{1}{\sqrt{2}} \left(|000000\rangle - |111111\rangle\right)
\end{aligned}
$$

c) The two possible outcomes of measuring X are $|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ and $|-\rangle = \frac{|0\rangle-|1\rangle}{\sqrt{2}}$. Suppose we measure $|+\rangle$:

$$
\begin{aligned}
|\psi_{\text{after}}\rangle &\propto (\mathbb{I}_{23456} \otimes |+\rangle\langle+|) |\psi\rangle = \frac{1}{\sqrt{2}} \left(|00000+\rangle \langle +|0|+|0\rangle - |11111+\rangle \langle +|1|+|1\rangle\right) \\
&\propto \frac{1}{2} \left(|00000\rangle - |11111\rangle\right) \otimes |+\rangle
\end{aligned}
$$

The associated probability is :

$$
\mathbb{P}[|+\rangle] = \langle \psi_{\text{after}} | \psi_{\text{after}} \rangle = \frac{1}{4} \left(1 - (-1)\right) \cdot 1 = \frac{1}{2}
$$

Now suppose we measure $|-\rangle$:

$$
\begin{aligned}
|\psi_{\text{after}}\rangle &\propto (\mathbb{I}_{23456} \otimes |-\rangle\langle-|) |\psi\rangle = \frac{1}{\sqrt{2}} \left(|00000-\rangle \langle -|0|-|0\rangle - |11111-\rangle \langle -|1|-|1\rangle\right) \\
&\propto \frac{1}{2} \left(|00000\rangle + |11111\rangle\right) \otimes |-\rangle
\end{aligned}
$$

The associated probability is :

$$
\mathbb{P}[|-\rangle] = \langle \psi_{\text{after}} | \psi_{\text{after}} \rangle = \frac{1}{4} \left(1 + 1\right) \cdot 1 = \frac{1}{2}
$$

Therefore the average measure on X is :

$$
\langle X \rangle_{\psi'} = \langle \psi' | X | \psi' \rangle = \frac{1}{2} \cdot (+1) + \frac{1}{2} \cdot (-1) = 0
$$

d) If we were to measure $X^{\otimes 6}$, we need to add gates such that the measurement in the computational basis corresponds effectively to a measurement in the X basis. Remember that $X = ZHZ$. Since we are interested in computing quantity of the form $\langle\psi| X |\psi\rangle$, we can rewrite this formula such that :

$$\langle\psi| X^{\otimes 6} |\psi\rangle = \underbrace{\langle\psi| H^{\otimes 6}}_{\langle\psi'|} Z^{\otimes 6} \underbrace{H^{\otimes 6} |\psi\rangle}_{|\psi'\rangle} = \langle\psi'| Z^{\otimes 6} |\psi'\rangle$$

How to interpret this equation ? Well it correponds to adding an Hadamard layer (one Hadamard gate for each qubit). Our new final state is $|\psi'\rangle = H^{\otimes 6} |\psi\rangle$ which is measured in the computational basis. But effectively, this corresponds to measure our "wanted" final state $|\psi\rangle$ in the X basis for each of its qubit (i.e. $X^{\otimes 6}$)

Exercise 2

Bernstein–Vazirani's algorithm. Consider a vector $\mathbf{a} = (a_1, \ldots, a_n) \in \{0,1\}^n$ and the function $f : \{0,1\}^n \to \{0,1\}$ defined by

$$f(x) = \mathbf{a} \cdot x \pmod 2 = a_1x_1 + \cdots + a_nx_n \pmod 2 = a_1x_1 \oplus \cdots \oplus a_nx_n, \quad x \in \{0,1\}^n.$$

Classically, n evaluations of f are needed to discover $\mathbf{a}$.

a) Show that, assuming a quantum oracle U_f with $n+1$ input and output qubits (as in Deutsch–Jozsa), one can discover $\mathbf{a}$ with probability 1 using a single call to U_f.

b) Now let $f(x) = b \oplus (\mathbf{a} \cdot x)$ with unknown $b \in \{0,1\}$. *(i)* With the same circuit, can you still determine $\mathbf{a}$ with probability 1 in one query to U_f? *(ii)* What about b?

Solution 2

a) From lecture notes, we can retrieve the final expression of Deutsch-Josza Algorithm with the function $f(x) = \mathbf{a} \cdot x \mod 2$:

$$|\psi_{\text{out}}\rangle = \sum_{y_1 \ldots y_n} \left\{ \frac{1}{2^n} \sum_{x_1 \ldots x_n} (-1)^{x \cdot a \bmod 2} (-1)^{x \cdot y \bmod 2} |y_1 \ldots y_n\rangle \right\} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$= \sum_{y_1 \ldots y_n} \left\{ \frac{1}{2^n} \sum_{\vec{x} \in \mathbb{F}_2^n} (-1)^{x \cdot (y \oplus a) \bmod 2} |y_1 \ldots y_n\rangle \right\} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$\text{Prob}[|\vec{y} = \vec{a}\rangle] = \frac{1}{2^{2n}} \left| \sum_{\vec{x} \in \mathbb{F}_2^n} (-1)^{x \cdot (y \oplus a) \bmod 2} \right|^2$$

$$= \frac{1}{2^{2n}} \left| \sum_{\vec{x} \in \mathbb{F}_2^n} (-1)^{2 \sum_i x_i a_i \bmod 2} \right|^2 \quad \text{if } \vec{a} = \vec{y}$$

$$= \frac{1}{2^{2n}} \left| \sum_{\vec{x} \in \mathbb{F}_2^n} 1 \right|^2 = \frac{1}{2^{2n}} |2^n|^2 = 1.$$

b) We can proceed similarly to the previous question by just reconsidering :

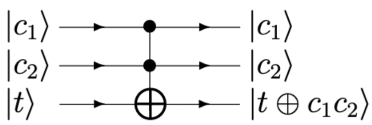
$$f(x) = b \oplus a \cdot x$$

$$\begin{aligned}
\text{Prob}[\,|y = a\rangle\,] &= \frac{1}{2^{2n}} \left| \sum_{\vec{x} \in \mathbb{F}_2^n} (-1)^{b \oplus x \cdot a \bmod 2 \oplus x \cdot y \bmod 2} \right|^2 \\
&= \frac{1}{2^{2n}} \left| \sum_{\vec{x} \in \mathbb{F}_2^n} (-1)^{b \oplus 2 \sum_i x_i a_i \bmod 2} \right|^2 \\
&= \frac{1}{2^{2n}} \left| \sum_{\vec{x}} (-1)^{b \oplus 0} \right|^2 \\
&= \frac{|(-1)^b|^2 2^{2n}}{2^{2n}} = 1.
\end{aligned}$$

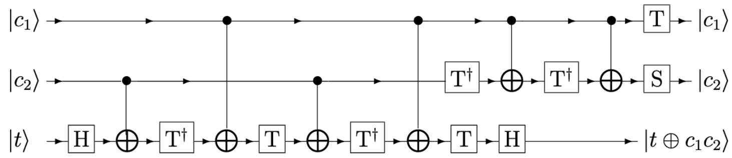
Since b appears only as a sign factor, it does not affect the probability, so we cannot determine it and only a can be retrieve.

Exercise 3

Construction of the Toffoli gate with CNOT**,** H**,** T**, and** S**.** Verify that the controlled-controlled-NOT (Toffoli) gate, mapping $|c_1, c_2, t\rangle \mapsto |c_1, c_2, t \oplus c_1 c_2\rangle$, is equivalent to the following



circuit built from CNOT, H, T, and S gates



Solutions 4

Using the first hint, we see that the circuit outputs the tensor product state $|\psi\rangle$ given by

$$|\psi\rangle = T\,|c_1\rangle \otimes SX^{c_1}TX^{c_1}T^\dagger\,|c_2\rangle \otimes HTX^{c_1}T^\dagger X^{c_2}TX^{c_1}T^\dagger X^{c_2}H\,|t\rangle\,.$$

We then verify explicitly all the cases of c_1 and c_2. The calculation largely uses the fact that all the quantum gates here are unitary (e.g., $TT^\dagger = T^\dagger T = I$); in particular, the gates X and H are involutory, i.e., $X^2 = H^2 = I$.

For $c_1 = 0$, we have

$$\begin{aligned}
|\psi\rangle &= T\,|0\rangle \otimes ST^\dagger T^\dagger\,|c_2\rangle \otimes HTT^\dagger X^{c_2}TT^\dagger X^{c_2}H\,|t\rangle \\
&= |0\rangle \otimes |c_2\rangle \otimes H(TT^\dagger)(X^{c_2}(TT^\dagger)X^{c_2})H\,|t\rangle = |0\rangle \otimes |c_2\rangle \otimes |t\rangle\,.
\end{aligned}$$

For $c_1 = 1$ and $c_2 = 0$, let us follow the second hint:

$$XT^\dagger X = \begin{pmatrix} e^{-i\pi/4} & 0 \\ 0 & 1 \end{pmatrix} = e^{-i\pi/4} T$$

and use this to compute

$$\begin{aligned}
|\psi\rangle &= T|1\rangle \otimes SXT^\dagger XT^\dagger|0\rangle \otimes HTXT^\dagger TXT^\dagger H|t\rangle \\
&= e^{i\pi/4}|1\rangle \otimes S(XT^\dagger X)T^\dagger|0\rangle \otimes H(T(X(T^\dagger T)X)T^\dagger)H|t\rangle \\
&= e^{i\pi/4}|1\rangle \otimes e^{-i\pi/4} STT^\dagger|0\rangle \otimes |t\rangle \\
&= e^{i\pi/4}|1\rangle \otimes e^{-i\pi/4}|0\rangle \otimes |t\rangle = |1\rangle \otimes |0\rangle \otimes |t\rangle\,.
\end{aligned}$$

Finally, for $c_1 = c_2 = 1$, we compute, using repeatedly (1):

$$\begin{aligned}
|\psi\rangle &= T|1\rangle \otimes SXT^\dagger XT^\dagger|1\rangle \otimes HTXT^\dagger XTXT^\dagger XH|t\rangle \\
&= e^{i\pi/4}|1\rangle \otimes e^{-i\pi/4} STT^\dagger|1\rangle \otimes e^{-i\pi/2} HT^4H|t\rangle \\
&= e^{i\pi/4}|1\rangle \otimes e^{i\pi/4}|1\rangle \otimes e^{-i\pi/2} X|t\rangle
\end{aligned}$$

as

$$T^4 = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and therefore

$$HT^4H = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = X$$

Finally, this gives

$$|\psi\rangle = |1\rangle \otimes |1\rangle \otimes |\bar{t}\rangle$$

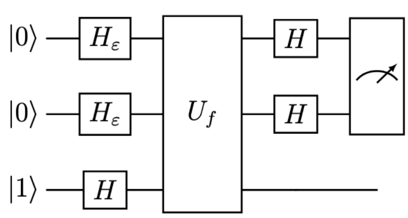
as expected.

Exercise 4

Deutsch–Jozsa with imperfect Hadamards. Recall that the goal of the DJ algorithm is to decide if $f : \{0, \}^n \mapsto \{0, 1\}$ is balanced or constant. Here we analyze a variation of this problem with imperfect Hadamard gates. For simplicity we take $n = 2$. The imperfect Hadamard gates H_ε are defined as

$$H_\varepsilon|0\rangle = \sqrt{\tfrac{1+\varepsilon}{2}}|0\rangle + \sqrt{\tfrac{1-\varepsilon}{2}}|1\rangle, \quad H_\varepsilon|1\rangle = \sqrt{\tfrac{1-\varepsilon}{2}}|0\rangle - \sqrt{\tfrac{1+\varepsilon}{2}}|1\rangle.$$

and consider the Deutsch-Josza circuit: Verify that H_ϵ is unitary. Then analyze this circuit and



compute the success probability of the algorithm.

Solutions 4

a) First observe that $H_g' = H_e$, so

$$H_\varepsilon H_\varepsilon^\dagger = H_\varepsilon^2 = \frac{1}{2}\begin{pmatrix}\sqrt{1+\epsilon} & \sqrt{1-\epsilon}\\ \sqrt{1-\epsilon} & -\sqrt{1+\epsilon}\end{pmatrix}^2 = \frac{1}{2}\begin{pmatrix}(1+\epsilon+1-\epsilon) & 0\\ 0 & (1-\epsilon+1+\epsilon)\end{pmatrix} = I$$

b) The state of the system after the first passage of the Hadamard gates is given by

$$\begin{aligned}|\psi_1\rangle &= H_\varepsilon|0\rangle \otimes H_\varepsilon|0\rangle \otimes H|1\rangle\\ &= \frac{1}{2}(\sqrt{1+\epsilon}\,|0\rangle + \sqrt{1-\epsilon}\,|1\rangle) \otimes (\sqrt{1+\epsilon}\,|0\rangle + \sqrt{1-\epsilon}\,|1\rangle) \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}\\ &= \frac{1}{2}((1+\epsilon)\,|00\rangle - \sqrt{1-\epsilon^2}(|01\rangle + |10\rangle) + (1-\epsilon)\,|11\rangle) \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}\end{aligned}$$

Let us write this state as

$$|\psi_1\rangle = \sum_{x\in\{0,1\}^2} \beta_x|x\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

where $\beta_{00} = \frac{1+\epsilon}{2}$, $\beta_{01} = \beta_{10} = \frac{\sqrt{1-\epsilon^2}}{2}$ and $\beta_{11} = \frac{1-\epsilon}{2}$. Then the output of the circuit (before the measurement) is given by

$$|\psi_4\rangle = \frac{1}{2}\sum_{y\in\{0,1\}^2}\left(\sum_{x\in\{0,1\}^2}\beta_x(-1)^{f(x)+x\cdot y}\right)|y\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

So the probability that the output state is $|00\rangle$ when f is constant is given by

$$|\alpha_{00}|^2 = \left(\frac{(1+\epsilon) + 2\sqrt{1-\epsilon^2} + (1-\epsilon)}{4}\right)^2 = \left(\frac{1+\sqrt{1-\epsilon^2}}{2}\right)^2$$

c) From the above expression, using successively the approximations $\sqrt{1-x} \simeq 1 - \frac{x}{2}$ and $(1-x)^2 \simeq 1 - 2x$, both valid for x small, we obtain

$$|\alpha_{00}|^2 \simeq \left(1 - \frac{\epsilon^2}{4}\right)^2 \simeq 1 - \frac{\epsilon^2}{2}$$

So the error probability $\delta \simeq \frac{\epsilon^2}{2}$. In order to ensure $\delta \leq 0.1$, ϵ should be taken less than 0.33; for $\delta \leq 0.01$, $\epsilon \leq 0.14$ is needed.

Exercise 5

An algorithm involving the Quantum Fourier Transform. Let $M = 2^m$. For $x \in \{0, \ldots, M-1\}$ an integer, recall that the quantum Fourier transform (QFT) is defined as

$$\mathrm{QFT}\,|x\rangle = \frac{1}{\sqrt{M}}\sum_{y=0}^{M-1} e^{2\pi i xy/M}\,|y\rangle\,.$$

Let $f : \{0, \ldots, M-1\} \to \{0, \ldots, M-1\}$ be an arithmetic function, and let V_f be the $M \times M$ matrix defined by

$$V_f\,|x\rangle = e^{-2\pi i f(x)/M}\,|x\rangle\,.$$

a) What are the matrix elements of both QFT and V_f in the basis $\{|x\rangle\,,\, x = 0, \dots, M-1\}$? Prove that these two matrices are unitary.

b) Let

$$|\Psi\rangle = (\mathrm{QFT})\, V_f\, H^{\otimes m}\, |0\rangle\,,$$

where $|0\rangle$ is the state corresponding to the integer $0 \in \{0, \dots, M-1\}$. Explain how to represent this identity by a quantum circuit, specifically, how to represent the various states with qubits and how many qubits are needed, and then draw the circuit.

c) Compute the state at each stage in the circuit, and in particular the output state $|\Psi\rangle$.

d) Let $A, B \in \{0, \dots, M-1\}$ and define $f(x) = Ax + B \bmod M$. After measuring the state in the computational basis:

   (i) What is the minimum number of measurements needed to determine the value of A?

   (ii) Can we also determine B by this process?

Solutions 5

a) The matrix elements of V_f are

$$\langle y|V_f|x\rangle = e^{-\frac{2\pi i}{M}f(x)}\langle y|x\rangle = \begin{cases} e^{-\frac{2\pi i}{M}f(x)} & \text{if } x = y \\ 0 & \text{if } x \neq y \end{cases}$$

i.e., the matrix is diagonal and one checks trivially that $V_f V_f^\dagger = V_f^\dagger V_f = I$. For the QFT matrix, we have

$$\langle y|QFT|x\rangle = \frac{1}{\sqrt{M}}\sum_{y'=0}^{M-1} e^{\frac{2\pi i}{M}xy'}\langle y|y'\rangle = \frac{1}{\sqrt{M}}e^{\frac{2\pi i}{M}xy} \quad \text{since } \langle y|y'\rangle = \delta_{y,y'}$$

The inner product between two lines is given by

$$\frac{1}{M}\sum_{y=0}^{M-1} e^{\frac{2\pi i}{M}(x-x')y} = \begin{cases} 1 & \text{if } x = x' \\ 0 & \text{otherwise} \end{cases}$$

so $(QFT)(QFT)^\dagger = (QFT)^\dagger(QFT) = I$.

b) A state $|x\rangle$ is represented by

$$|x\rangle = |x_0\rangle \otimes |x_1\rangle \otimes \cdots \otimes |x_{m-1}\rangle$$

where $x = x_0 + 2x_1 + \cdots + 2^{m-1}x_{m-1}$, $x_i \in \{0,1\}$ is represented in base 2. The Hilbert space is $(\mathbb{C}^2)^{\otimes m}$. The initial state is $|x=0\rangle = |0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle$.

c) AAfter the Hadamard gates, the state is

$$\frac{1}{2^{m/2}}\sum_{b_1 \dots b_M} |b_1\rangle \otimes |b_2\rangle \otimes \cdots \otimes |b_M\rangle = \frac{1}{\sqrt{M}}\sum_{x=0}^{M-1}|x\rangle$$

After the V_f gate, the state is

$$\frac{1}{\sqrt{M}} \sum_{x=0}^{M-1} e^{-\frac{2\pi i}{M} f(x)} |x\rangle$$

After the QFT gate, the state is

$$\begin{aligned} |\Psi\rangle &= \frac{1}{\sqrt{M}} \sum_{x=0}^{M-1} e^{-\frac{2\pi i}{M} f(x)} \frac{1}{\sqrt{M}} \sum_{y=0}^{M-1} e^{\frac{2\pi i}{M} xy} |y\rangle \\ &= \frac{1}{\sqrt{M}} \sum_{y=0}^{M-1} \left\{ \frac{1}{\sqrt{M}} \sum_{x=0}^{M-1} e^{-\frac{2\pi i}{M} f(x)} e^{\frac{2\pi i}{M} xy} \right\} |y\rangle \end{aligned}$$

d) For $f(x) = Ax + B$, the coefficients of $|\Psi\rangle$ in the computational basis are

$$\frac{1}{M} \sum_{x=0}^{M-1} e^{-\frac{2\pi i}{M} Ax} e^{-\frac{2\pi i}{M} B} e^{\frac{2\pi i}{M} xy} = e^{-\frac{2\pi i}{M} B} \frac{1}{M} \sum_{x=0}^{M-1} e^{\frac{2\pi i}{M} (y-A)x}.$$

The probability to observe a given state $|y\rangle$ after the measurement is

$$\mathbb{P}(y) = \frac{1}{M^2} \left| \sum_{x=0}^{M-1} e^{\frac{2\pi i}{M} (y-A)x} \right|^2$$

For $y = A$, $\mathbb{P}(y) = 1$ and for $y \neq A$, $\mathbb{P}(y) = 0$. Therefore, a single measurement suffices to retrieve the value of A. On the other hand, B only appears as a global phase and cannot therefore be determined.

Exercise 6

Simulating quantum dynamics of a spin system. Consider the following Hamiltonian defined on two qubits:

$$\hat{\mathcal{H}} = \hat{\sigma}_1^x \hat{\sigma}_2^x + \hat{\sigma}_1^y \hat{\sigma}_2^y,$$

where we use the standard definition for the Pauli matrices:

$$\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

a) Write $\hat{\mathcal{H}}$ as a 4x4 matrix in the standard basis $|0,0\rangle$, $|0,1\rangle$, $|1,0\rangle$, $|1,1\rangle$. Find the smallest eigenvalue and the corresponding eigenstate.

b) Consider the problem of simulating quantum dynamics starting from the initial state $|0,0\rangle$ using a quantum computer. Show that the FSIM(θ, ϕ) gate (as implemented on Google hardware, for example) can be used to obtain $|\psi(t)\rangle = \exp\left(-it\hat{\mathcal{H}}\right)|0,0\rangle$. Determine what values of θ and ϕ are necessary. Recall that the FSIM gate is defined as

$$\text{FSIM}(\theta, \phi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & -i\sin(\theta) & 0 \\ 0 & -i\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}$$

c) Now consider the problem of approximating the ground state of $\hat{\mathcal{H}}$ using a variational ansatz. We will consider the ansatz

$$|\Psi(\gamma_1, \gamma_2)\rangle = \text{CNOT} \times \text{RY}_1(\gamma_1) \times \text{RY}_2(\gamma_2)|0, 0\rangle$$

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

and

$$\text{RY}(\gamma) = \exp(-i\hat{\sigma}^y\gamma/2) = \begin{bmatrix} \cos(\gamma/2) & -\sin(\gamma/2) \\ \sin(\gamma/2) & \cos(\gamma/2) \end{bmatrix}$$

Find the expression of the energy as a function of the parameters γ_1 and γ_2. For what values of the parameters do you recover the exact ground-state energy computed at point 1?

Solutions 6

a) **Hamiltonian.**

$$\hat{H} \;=\; \sigma_1^x\sigma_2^x \;+\; \sigma_1^y\sigma_2^y.$$

Tensor notation and matrices (computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$).

$$\hat{H} \;=\; \hat{X}_1 \otimes \hat{X}_2 \;+\; \hat{Y}_1 \otimes \hat{Y}_2,$$

$$\hat{X}_1 \otimes \hat{X}_2 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \qquad \hat{Y}_1 \otimes \hat{Y}_2 = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix},$$

$$\Rightarrow \quad \hat{H} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Projector (ladder–flip) form.

$$\hat{H} \;=\; 2(|01\rangle\langle 10| + |10\rangle\langle 01|) \;=\; 2(|0\rangle\langle 1| \otimes |1\rangle\langle 0| + |1\rangle\langle 0| \otimes |0\rangle\langle 1|)\,.$$

Eigenstates and eigenvalues.

$$\hat{H}\,|00\rangle = 0 \cdot |00\rangle\,, \qquad \hat{H}\,|11\rangle = 0 \cdot |11\rangle\,,$$

$$\hat{H}\,\frac{|01\rangle + |10\rangle}{\sqrt{2}} = +2\,\frac{|01\rangle + |10\rangle}{\sqrt{2}}, \qquad \hat{H}\,\frac{|01\rangle - |10\rangle}{\sqrt{2}} = -2\,\frac{|01\rangle - |10\rangle}{\sqrt{2}}.$$

b) We will use the property $f(\hat{O}) = \sum_i f(\lambda_i)\,|\lambda_i\rangle\,\langle\lambda_i|$:

$$e^{-it\hat{H}} = e^{-2it}\left(\frac{|01\rangle + |10\rangle}{\sqrt{2}}\right)\left(\frac{\langle 01| + \langle 10|}{\sqrt{2}}\right) + e^{+2it}\left(\frac{|01\rangle - |10\rangle}{\sqrt{2}}\right)\left(\frac{\langle 01| - \langle 10|}{\sqrt{2}}\right)$$
$$+\,|00\rangle\langle 00| + |11\rangle\langle 11|\,.$$

Expanding,

$$e^{-it\hat{H}} = \frac{e^{-2it}}{2}\big(\,|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|\,\big) + \frac{e^{2it}}{2}\big(\,|01\rangle\langle 01| - |01\rangle\langle 10| - |10\rangle\langle 01| + |10\rangle\langle 10|\,\big)$$
$$+ |00\rangle\langle 00| + |11\rangle\langle 11|\,,$$

hence

$$e^{-it\hat{H}} = \cos(2t)\big(\,|01\rangle\langle 01| + |10\rangle\langle 10|\,\big) - i\sin(2t)\big(\,|01\rangle\langle 10| + |10\rangle\langle 01|\,\big) + |00\rangle\langle 00| + |11\rangle\langle 11|\,.$$

In the ordered basis $\{|00\rangle\,, |01\rangle\,, |10\rangle\,, |11\rangle\}$, the unitary $U(t) = e^{-it\hat{H}}$ is

$$U(t) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2t) & -i\sin(2t) & 0 \\ 0 & -i\sin(2t) & \cos(2t) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \quad \text{and we want} \quad \mathrm{FSIM}(\theta,\phi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & -i\sin(\theta) & 0 \\ 0 & -i\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}$$

By identification we find :

$$\boxed{\theta = 2t}, \qquad \boxed{\phi = 2k\pi,\ k \in \mathbb{Z}}$$

c)

$$|\psi(\gamma_1,\gamma_2)\rangle \;=\; \mathrm{CNOT} \cdot RY_1(\gamma_1) \cdot RY_2(\gamma_2)\,|00\rangle$$

$$=\; \mathrm{CNOT} \begin{bmatrix} \cos(\gamma_1/2) \\ \sin(\gamma_1/2) \end{bmatrix} \otimes \begin{bmatrix} \cos(\gamma_2/2) \\ \sin(\gamma_2/2) \end{bmatrix}$$

$$=\; \mathrm{CNOT}\Big((\cos(\gamma_1/2)\,|0\rangle + \sin(\gamma_1/2)\,|1\rangle) \otimes (\cos(\gamma_2/2)\,|0\rangle + \sin(\gamma_2/2)\,|1\rangle)\Big)$$

$$=\; \mathrm{CNOT}\big(\,\cos(\gamma_1/2)\cos(\gamma_2/2)\,|00\rangle + \cos(\gamma_1/2)\sin(\gamma_2/2)\,|01\rangle + \sin(\gamma_1/2)\cos(\gamma_2/2)\,|10\rangle$$
$$+ \sin(\gamma_1/2)\sin(\gamma_2/2)\,|11\rangle\,\big)$$

$$\Rightarrow\; |\psi(\gamma_1,\gamma_2)\rangle = \cos(\gamma_1/2)\cos(\gamma_2/2)\,|00\rangle + \cos(\gamma_1/2)\sin(\gamma_2/2)\,|10\rangle$$
$$+ \sin(\gamma_1/2)\cos(\gamma_2/2)\,|11\rangle + \sin(\gamma_1/2)\sin(\gamma_2/2)\,|10\rangle\,.$$

$$\hat{H}\,|\psi(\gamma_1,\gamma_2)\rangle = 2\big(\,|01\rangle\langle 10| + |10\rangle\langle 01|\,\big)\,|\psi(\gamma_1,\gamma_2)\rangle = 2\Big(\,\cos(\gamma_1/2)\sin(\gamma_2/2)\,|10\rangle + \sin(\gamma_1/2)\sin(\gamma_2/2)\,|01\rangle\,\Big).$$

$$\langle\psi(\gamma_1,\gamma_2)|\hat{H}|\psi(\gamma_1,\gamma_2)\rangle = 2\Big[\,\cos(\gamma_1/2)\sin(\gamma_1/2)\sin^2(\gamma_2/2) + \cos(\gamma_1/2)\sin(\gamma_1/2)\sin^2(\gamma_2/2)\Big]$$

$$\boxed{\langle\psi(\gamma_1,\gamma_2)|\hat{H}|\psi(\gamma_1,\gamma_2)\rangle = 2\,\sin(\gamma_1)\,\sin^2(\gamma_2/2)}$$

The ground state is reached for $\gamma_1 = \frac{3\pi}{2}$ and $\gamma_2 = \pi$, because we obtain -2.