Quantum Computing Basics: Qubits and Quantum Gates

Basis set of a two-dimensional vector space

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix};\ |1\rangle = \begin{bmatrix}0\\1\end{bmatrix} \tag{1}$$

Qubit = vector

$$|\psi(\theta,\phi)\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}|1\rangle;\ \theta \in [0,\pi], \phi \in [0,2\pi] \tag{2}$$

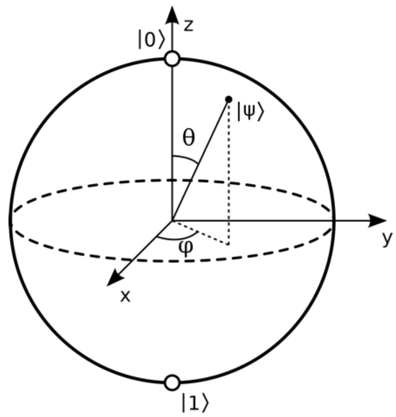

Fig. 1: Bloch sphere representation of a qubit.

(Example)

Classical bits: $|\psi(0,0)\rangle = |0\rangle$; $|\psi(\pi,0)\rangle = |1\rangle$

Superposed states: $\left|\psi(\frac{\pi}{2},0)\right\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$; $\left|\psi(\frac{\pi}{2},\pi)\right\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

Quantum gate = matrix

Pauli X (NOT) gate

$$X = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}, \tag{3}$$

thus

$$X|0\rangle = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}0\\1\end{bmatrix} = |1\rangle;\ X|1\rangle = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}1\\0\end{bmatrix} = |0\rangle. \tag{4}$$

Hadamard (H) gate

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix} \tag{5}$$

thus

$$H|0\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix};\ H|1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}. \tag{6}$$

Two-qubit state = tensor product

$$|x\rangle \otimes |y\rangle = |x\rangle|y\rangle = |xy\rangle =$$
$$(x = a|0\rangle + b|1\rangle)(y = c|0\rangle + d|1\rangle) = ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle. \tag{7}$$

Flat vector representation of tensor product uses the following basis set

$$\begin{bmatrix}1\\0\\0\\0\end{bmatrix} = |00\rangle;\ \begin{bmatrix}0\\1\\0\\0\end{bmatrix} = |01\rangle;\ \begin{bmatrix}0\\0\\1\\0\end{bmatrix} = |10\rangle;\ \begin{bmatrix}0\\0\\0\\1\end{bmatrix} = |11\rangle \tag{8}$$

and thus

$$\begin{array}{cc}\begin{bmatrix}a\\b\end{bmatrix} & \begin{array}{l}|0\rangle\\|1\rangle\end{array}\end{array} \otimes \begin{array}{cc}\begin{bmatrix}c\\d\end{bmatrix} & \begin{array}{l}|0\rangle\\|1\rangle\end{array}\end{array} = \begin{array}{cc}\begin{bmatrix}ac\\ad\\bc\\bd\end{bmatrix} & \begin{array}{l}|00 = 0\rangle\\|01 = 1\rangle\\|10 = 2\rangle\\|11 = 3\rangle\end{array}\end{array}. \tag{9}$$

Both binary and decimal indices are shown for the flat vector representation of the tensor-product state in Eq. (9).

Two-qubit gate: Controlled NOT (CNOT or controlled *X*)

$$|x\rangle|y\rangle \xrightarrow{\text{CNOT}} \text{CNOT}\left(\overbrace{|x\rangle}^{\text{control qubit}} \quad \overbrace{|y\rangle}^{\text{target qubit}}\right) = |x\rangle|x \oplus y\rangle \quad , \tag{10}$$

x	y		x⊕y
0	0	y	0
0	1		1
1	0	¬y	1
1	1		0

where $\oplus$ is the logical exclusive OR operator (defined by the truth table, in which $\neg$ is the logical negation operator), or more specifically

$$\text{CNOT}(|00\rangle) = |00\rangle;\ \text{CNOT}(|01\rangle) = |01\rangle;\ \text{CNOT}(|10\rangle) = |11\rangle;\ \text{CNOT}(|11\rangle) = |10\rangle; \tag{11}$$

Matrix notation of CNOT

$$U_{\text{CNOT}} = \begin{array}{cc} \begin{array}{cccc}00 & 01 & 10 & 11\end{array} & \\ \begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\\0 & 0 & 1 & 0\end{bmatrix} & \begin{array}{c}00\\01\\10\\11\end{array}\end{array} = \begin{bmatrix}I & 0\\0 & X\end{bmatrix}, \tag{12}$$

where I is the 2×2 identity matrix. The last notation represents the 4×4 matrix as 2×2 blocks, with each block being a 2×2 matrix.

Fig. 2: Operation of CNOT gate.

In Eq. (12), the most|least significant bit in a binary matrix row or column index (*i.e.*, 00, 01, 10, 11) specifies inter|intra-block index for the first|second qubit.

Circuit example (try it at https://quantum-computing.ibm.com using Composer)

This circuit generates a correlated 2-qubit state, $(|00\rangle + |11\rangle)/\sqrt{2}$, called Bell state.

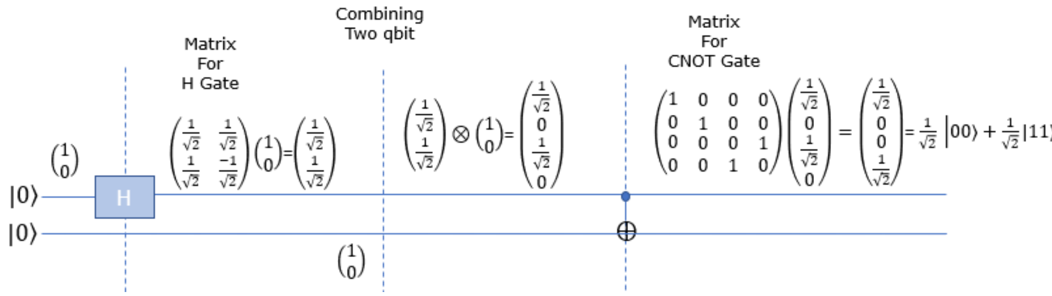

Fig. 3: Hadamard and CNOT gates example.

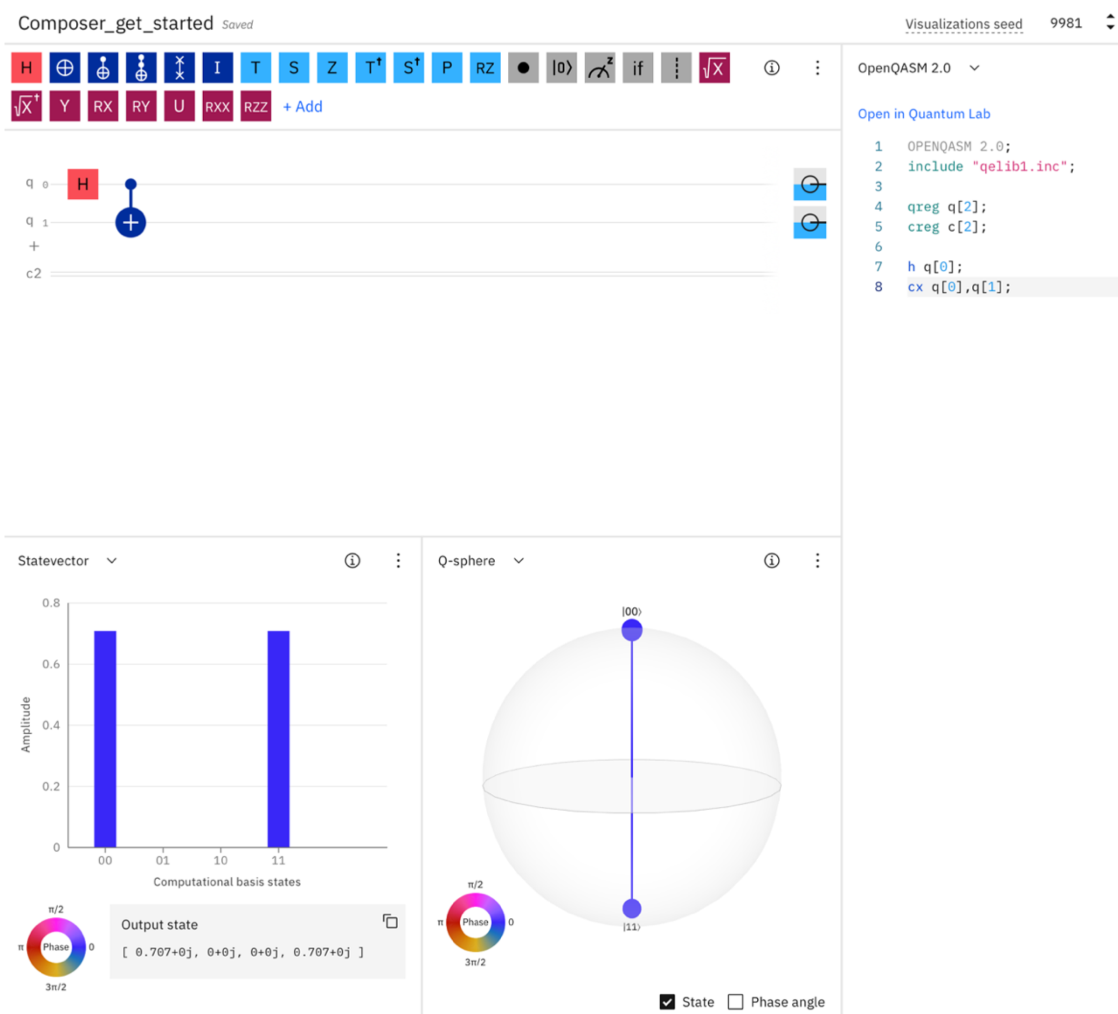

Fig. 4: Hadamard and CNOT gates example using IBM Q Composer.

Q-sphere (it's not the 1-qubit Bloch sphere) visually represents a state of n (≤ 5) qubits. The north|south pole signifies the state where all qubits are 0|1 (*e.g.*, $|000\rangle$|$|111\rangle$), and the latitude is the Hamming distance from the all-zero state (*i.e.*, how many qubits are not zero).

Tensor product of one-qubit quantum gates (matrices)

Consider quantum gates A and B independently operating on the first and second qubits:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}; B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

$$\Rightarrow A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{bmatrix}. \tag{13}$$

See Appendix for detailed explanation of Eq. (13).

(Example) $H \otimes H$ where $H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

$$H \otimes H = \frac{1}{\sqrt{2}} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \tag{14}$$

This circuit transforms a pure state to a superposition of all possible states, which is a way to achieve quantum parallelism, *e.g.*, $H \otimes H|00\rangle = \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$.

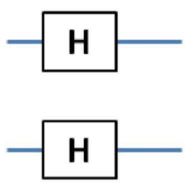

Fig. 5: An example tensor product of quantum operators.

(Application for quantum circuit reduction)

$$\Lambda = \frac{1}{2} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & X \end{bmatrix} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} = \frac{1}{2} \begin{bmatrix} H & HX \\ H & -HX \end{bmatrix} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} = \frac{1}{2} \begin{bmatrix} I + HXH & I - HXH \\ I - HXH & I + HXH \end{bmatrix} \tag{15}$$

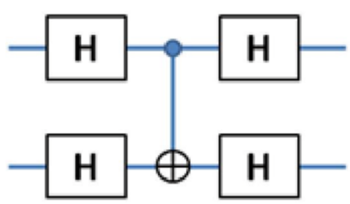

Fig. 6: Quantum circuit Λ in Eq. (15).

Here, we have used the identity,

$$H^2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I, \tag{16}$$

i.e., H is a symmetric orthogonal matrix ($H = H^T$ and $H^T H = HH^T = I$).

In Eq. (15),

$$HXH = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = Z, \tag{17}$$

where Z denotes Pauli Z gate.

Substituting Eq. (17) to (15), we obtain

$$\Lambda = \frac{1}{2}\begin{bmatrix} H & H \\ H & -H \end{bmatrix}\begin{bmatrix} I & 0 \\ 0 & X \end{bmatrix}\begin{bmatrix} H & H \\ H & -H \end{bmatrix} = \frac{1}{2}\begin{bmatrix} I+Z & I-Z \\ I-Z & I+Z \end{bmatrix} = \begin{array}{c c} \begin{array}{cccc} 00 & 01 & 10 & 11 \end{array} & \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} & \begin{array}{c} 00 \\ 01 \\ 10 \\ 11 \end{array} \end{array}, \tag{18}$$

where we have used the relation

$$\frac{1}{2}(I \pm Z) = \frac{1}{2}\begin{bmatrix} 1 \pm 1 & 0 \\ 0 & 1 \mp 1 \end{bmatrix} = \begin{cases} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \end{cases}. \tag{19}$$

Equation (18) states that

$$\Lambda|00\rangle = |00\rangle;\ \Lambda|10\rangle = |10\rangle;\ \Lambda|01\rangle = |11\rangle;\ \Lambda|11\rangle = |01\rangle \tag{20}$$

or

$$\Lambda(x, y) = x \oplus y, y \tag{21}$$

which is CNOT gate, where the second qubit acts as the conditional qubit. Graphically, thus

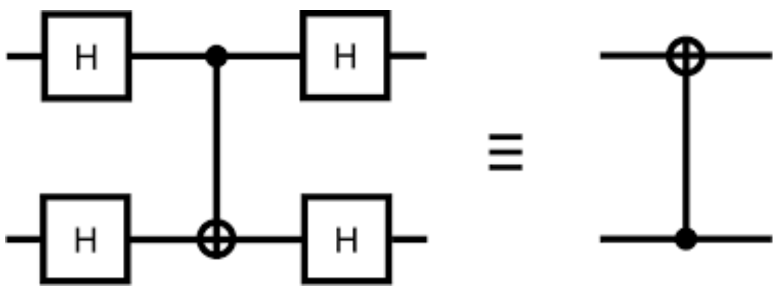

Fig. 7: Quantum-circuit equivalence.

Measurement gate

Measurement operator M projects a qubit $|\psi\rangle$ to the Z basis, *i.e.*, eigenvectors $|0\rangle$ and $|1\rangle$ with corresponding eigenvalues 1 and -1.

$$M|\psi\rangle = |z\rangle\langle z|\psi\rangle = \psi(z)|z\rangle \tag{22}$$

Each measurement gate irreversibly returns the measured value, $z = 0$ or 1, with the probability

$$\langle\psi|M|\psi\rangle = \langle\psi|z\rangle\langle z|\psi\rangle = |\psi(z)|^2 = P(z). \tag{23}$$

Measurement example (try it at https://quantum-computing.ibm.com using Composer)

Consider a two-qubit circuit, where both qubits (named q_0 and q_1) are initialized to $|0\rangle$ by default. This is simply the equivalent circuit in Fig. 7, after q_1 was flipped to $|1\rangle$. The CNOT gate conditional to q_1 then flips q_1 to $|1\rangle$. The measurements thus show both qubits are 100% in $|1\rangle$, as $\Lambda|01\rangle = |11\rangle$ shown in Eq. (20).

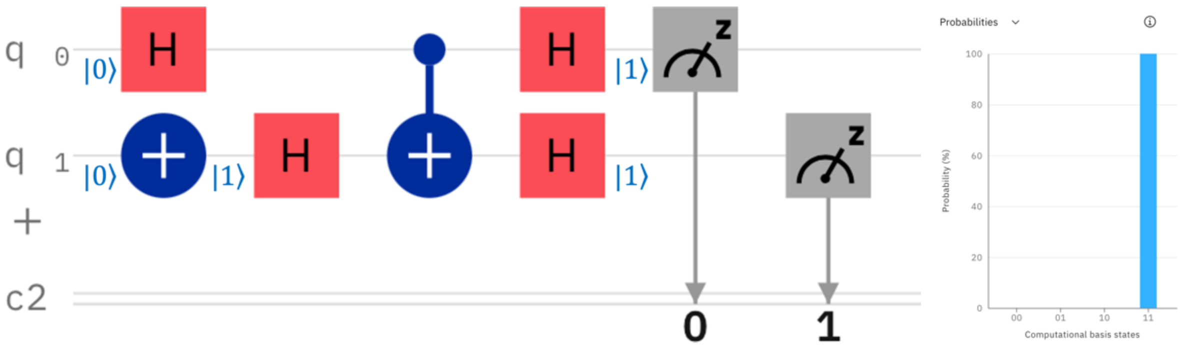

Fig. 8: (Left) Operation of the equivalent quantum circuit in Fig. 7 to qubits. (Right) Resulting probability distribution produced by IBM Q Composer.

Fig. 9: Symbols for Pauli X (NOT), Pauli Z, Hadamard (H), conditional not (CNOT) and measurement gates used in IBM Q Composer.

OpenQASM and Qiskit programs (see the code panel in Composer)

<table>
<tr>
<td><pre>OPENQASM 2.0;
include "qelib1.inc";

qreg q[2];
creg c[2];

h q[0];
x q[1];
h q[1];
cx q[0],q[1];
h q[0];
h q[1];
measure q[0] -> c[0];
measure q[1] -> c[1];</pre></td>
<td><pre>from qiskit import QuantumRegister,
ClassicalRegister, QuantumCircuit
from numpy import pi

qreg_q = QuantumRegister(2, 'q')
creg_c = ClassicalRegister(2, 'c')
circuit = QuantumCircuit(qreg_q, creg_c)

circuit.h(qreg_q[0])
circuit.x(qreg_q[1])
circuit.h(qreg_q[1])
circuit.cx(qreg_q[0], qreg_q[1])
circuit.h(qreg_q[0])
circuit.h(qreg_q[1])
circuit.measure(qreg_q[0], creg_c[0])
circuit.measure(qreg_q[1], creg_c[1])</pre></td>
</tr>
<tr>
<td>OpenQASM</td>
<td>Qiskit</td>
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Table I: OpenQASM and Qiskit programs for the quantum circuit in Fig. 8.

In Qiskit programming language, h() and x() are the one-qubit Hadamard and Pauli X (NOT) operators acting on the specified qubit, cx() is the two-qubit CNOT gate acting on the specified two qubits, and measure() measures the state of the specified qubit (first argument) and stores the measured value ($\in \{0,1\}$) to the specified classical bit (second argument). QuantumRegister|ClassicalRegister() creates a quantum|classical register with the specified number of bits and optional label. QuantumCircuit() creates a quantum circuit consisting of those registers.

Appendix: Tensor Product of Quantum Gates

Let the states of two qubits be

$$|x\rangle = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix};\ |y\rangle = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \tag{A1}$$

and one-qubit gates acting on respective qubits be

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix};\ B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}. \tag{A2}$$

Tensor product of the input two-qubit state is

$$|x\rangle \otimes |y\rangle = \begin{bmatrix} x_1 y_1 \\ x_1 y_2 \\ x_2 y_1 \\ x_2 y_2 \end{bmatrix} = \begin{bmatrix} x_1 \mathbf{y} \\ x_2 \mathbf{y} \end{bmatrix}, \tag{A3}$$

where boldface font was used to indicate a two-element column vector nested inside a vector. Similarly, tensor product of the output two-qubit state, after operation of both one-qubit gates on respective qubits, is

$$A|x\rangle \otimes B|y\rangle = \begin{bmatrix} (\mathbf{Ax})_1 \mathbf{By} \\ (\mathbf{Ax})_2 \mathbf{By} \end{bmatrix} = \begin{bmatrix} (a_{11}x_1 + a_{12}x_2)\mathbf{By} \\ (a_{21}x_1 + a_{22}x_2)\mathbf{By} \end{bmatrix} = \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} \end{bmatrix} \begin{bmatrix} x_1 \mathbf{y} \\ x_2 \mathbf{y} \end{bmatrix}, \tag{A4}$$

where we have used boldface font to indicate a 2×2 matrix nested inside a vector or matrix and $(\mathbf{Ax})_1$ denotes the first element of the **Ax** vector. Equation (A4) demonstrates the nested nature of one-qubit gates operating separately on two qubits. Namely, operators on the first and second qubits act on inter- and intra-2×2 blocks within 4×4 matrix.