

Quantum Computing Basics: Qubits and Quantum Gates

Basis set of a two-dimensional vector space

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}; |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (1)$$

Qubit = complex vector

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

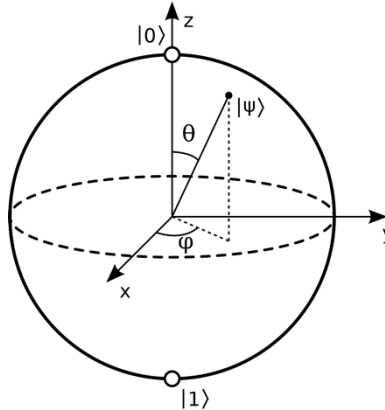


Fig. 1: Bloch sphere representation of a qubit.

(Example) Note $e^{i\phi} = \cos(\phi) + i\sin(\phi)$

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

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

Quantum gate = matrix

Pauli X (NOT) gate Spin flip

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad (3)$$

thus

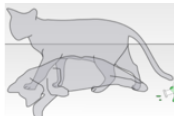
$$X|0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle; X|1\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle. \quad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

Hadamard (H) gate Important for generating superposition states for quantum parallelism

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

thus

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



Superposition!

Two-qubit state = tensor product

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

Flat vector representation of tensor product uses the following basis set

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

and thus

$$\begin{bmatrix} a \\ b \end{bmatrix} \begin{bmatrix} |0\rangle \\ |1\rangle \end{bmatrix} \otimes \begin{bmatrix} c \\ d \end{bmatrix} \begin{bmatrix} |0\rangle \\ |1\rangle \end{bmatrix} = \begin{bmatrix} ac \\ ad \\ bc \\ bd \end{bmatrix} \begin{bmatrix} |00 = 0\rangle \\ |01 = 1\rangle \\ |10 = 2\rangle \\ |11 = 3\rangle \end{bmatrix}. \quad (9)$$

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) Essential for computation

$$|x\rangle|y\rangle \xrightarrow{\text{CNOT}} \text{CNOT} \left(\begin{array}{c|c} \text{control qubit} & \text{target qubit} \\ \hline \widetilde{|x\rangle} & \widetilde{|y\rangle} \end{array} \right) = |x\rangle|x \oplus y\rangle, \quad \begin{array}{|c|c|c|c|} \hline x & y & x \oplus y & \\ \hline 0 & 0 & 0 & 0 \\ 0 & 1 & y & 1 \\ \hline 1 & 0 & \neg y & 1 \\ 1 & 1 & \neg y & 0 \\ \hline \end{array} \quad \text{Truth table} \quad (10)$$

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

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

Matrix notation of CNOT

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

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*.

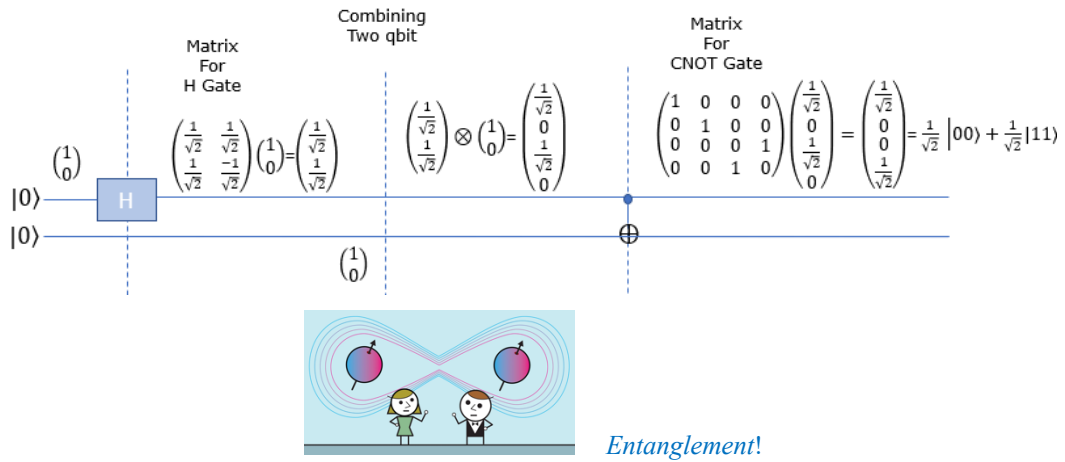


Fig. 3: Hadamard and CNOT gates example.

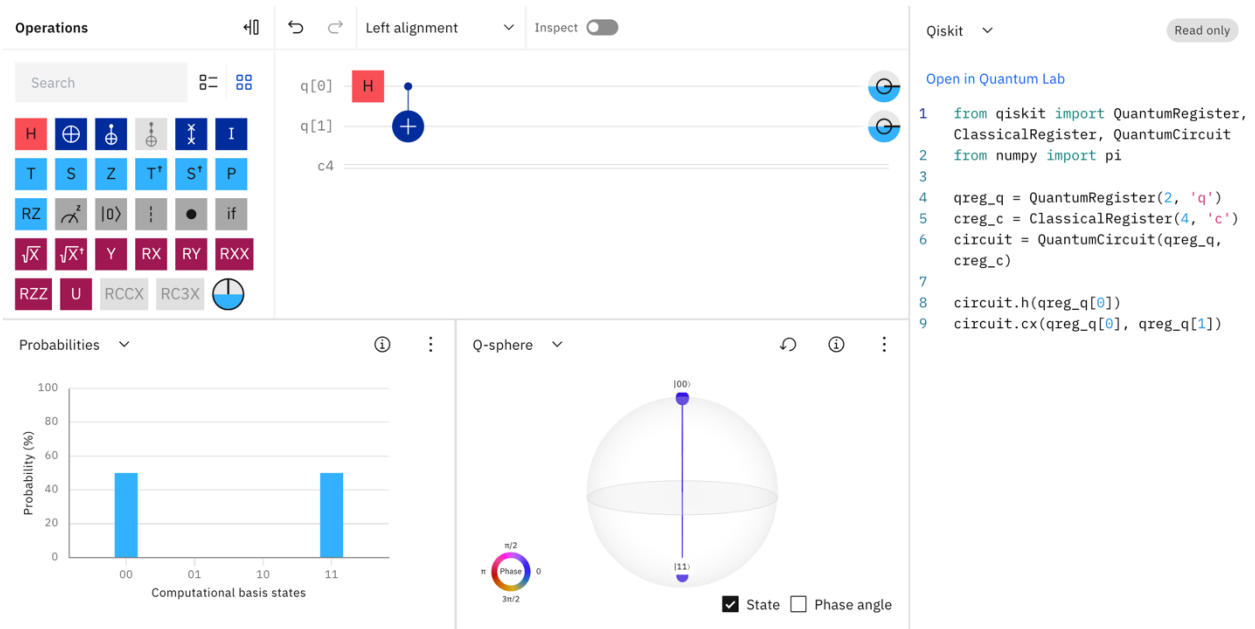


Fig. 4: Hadamard and CNOT gates example using IBM Q Composer.

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:

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

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

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

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

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

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

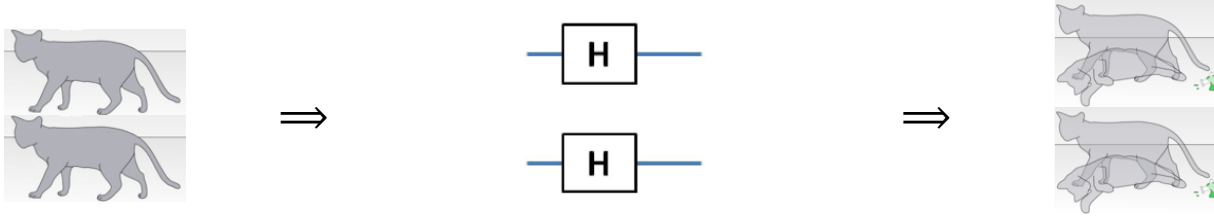


Fig. 5: An example tensor product of quantum operators.

(Application for quantum circuit reduction)

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

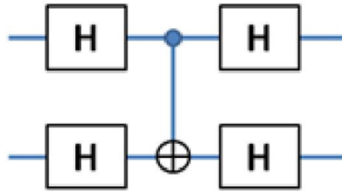


Fig. 6: Quantum circuit Λ in Eq. (15).

Here, we have used the identity,

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

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

In Eq. (15),

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

where Z denotes Pauli Z gate.

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

$$\Lambda = \frac{1}{2} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & X \end{bmatrix} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} = \frac{1}{2} \begin{bmatrix} I+Z & I-Z \\ I-Z & I+Z \end{bmatrix} = \begin{matrix} & \begin{matrix} 00 & 01 & 10 & 11 \end{matrix} & \begin{matrix} \square \\ 00 \\ 01 \\ 10 \\ 11 \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} & \end{matrix}, \quad (18)$$

where we have used the relation

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

Equation (18) states that

$$\Lambda|00\rangle = |00\rangle; \Lambda|10\rangle = |10\rangle; \Lambda|01\rangle = |11\rangle; \Lambda|11\rangle = |01\rangle \quad (20)$$

or

$$\Lambda(x, y) = x \oplus y, y \quad (21)$$

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

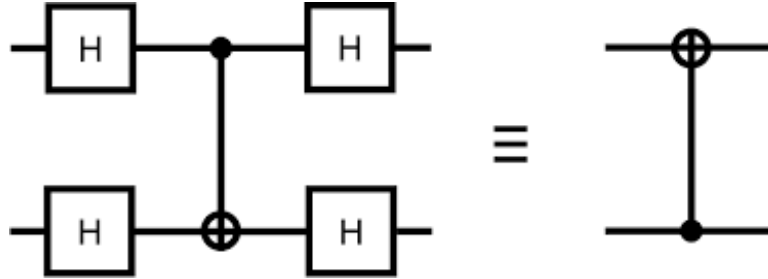


Fig. 7: Quantum-circuit equivalence.

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 .

$$M|\psi\rangle = |z\rangle\langle z|\psi\rangle = \psi(z)|z\rangle \quad (22)$$

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

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

* We need to run each circuit many times to obtain the probability.

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_0 to $|1\rangle$. The measurements thus show both qubits are 100% in $|1\rangle$, as $\Lambda|01\rangle = |11\rangle$ shown in Eq. (20).

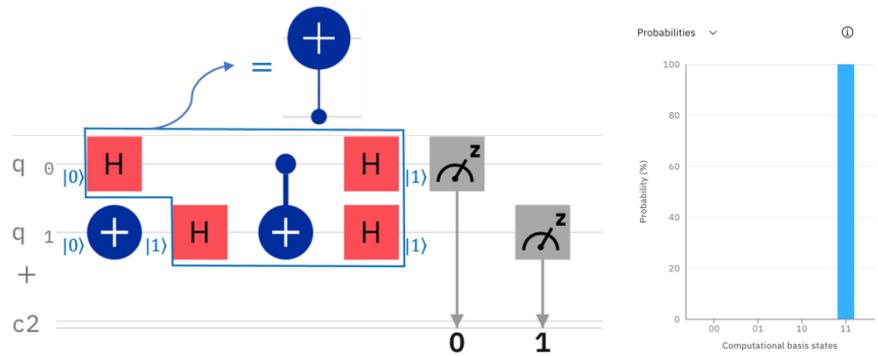


Fig. 8: (Left) Operation of the equivalent quantum circuit in Fig. 7 to qubits. (Right) Resulting probability distribution produced by IBM Q Composer.



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)

<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>	<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>
OpenQASM	Qiskit

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

$$|x\rangle = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}; |y\rangle = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad (\text{A1})$$

and one-qubit gates acting on respective qubits be

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

Tensor product of the input two-qubit state is

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

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

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

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 \mathbf{Ax} vector. Equation (A4) demonstrates the nested nature of one-qubit gates operating separably on two qubits. Namely, operators on the first and second qubits act on inter- and intra- 2×2 blocks within 4×4 matrix.