Calculating quantum gates can be done on a conceptual level or basic level. We show this with the example of a combination of Hadamard and CNOT gates.

Example

We use the following circuit:



The meter sign denotes measurement in $\{|0\rangle, |1\rangle\}$ basis.

Suppose $|\psi_i\rangle = a|0\rangle + b|1\rangle$, $a^2 + b^2 = 1$.

Conceptual level

We solve this problem by conceptual-level access.

We rewrite the initial state as:

$$|\psi_0\rangle = |0\rangle \left(\left(\frac{a+b}{\sqrt{2}} \right) |+\rangle + \left(\frac{a-b}{\sqrt{2}} \right) |-\rangle \right)$$

Note:

$$|0\rangle \left(\frac{a+b}{\sqrt{2}}\right)|+\rangle = \left(\frac{a+b}{\sqrt{2}}\right)|0\rangle|+\rangle$$

Note: $|0\rangle|+\rangle = |0+\rangle = |0\rangle \otimes +\rangle$ represents the tensor product or Kronecker product.

Note: The order of the qubits is important.

1) We apply the first Hadamard onto $|\psi_0
angle$ and get $|\psi_1
angle$:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\left(\left(\frac{a+b}{\sqrt{2}}\right)|+\rangle + \left(\frac{a-b}{\sqrt{2}}\right)|-\rangle\right)$$

Note: The Hadamard

- acts on the first qubit only
- changes $|0\rangle$ to $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ resp. to $|+\rangle$
- changes $|1\rangle$ to $\frac{1}{\sqrt{2}}(|0\rangle |1\rangle)$ resp. to $|-\rangle$.

2) We apply the CNOT onto $|\psi_1\rangle$. The CNOT swaps the second qubit if the first qubit is $|1\rangle$.

We multiply out $|\psi_1\rangle$:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\left(\left(\frac{a+b}{\sqrt{2}}\right)\Big|+\rangle + \left(\frac{a-b}{\sqrt{2}}\right)\Big|-\rangle\right) =$$

$$\frac{1}{2}((a+b)|0\rangle|+\rangle+(a-b)|0\rangle|-\rangle+(a+b)|1\rangle|+\rangle+(a-b)|1\rangle|-\rangle)$$

In case the first qubit is $|0\rangle$ the CNOT performs no action.

In case the first qubit is $|1\rangle$ the CNOT swaps the second one:

- The $|+\rangle$ qubit swapped remains the same
- The $|-\rangle$ qubit changes the sign

We get $|\psi_2\rangle$:

$$|\psi_2\rangle = \frac{1}{2} \Big(|0\rangle \big((a+b)|+\rangle + (a-b)|-\rangle \big) + |1\rangle \big((a+b)|+\rangle - (a-b)|-\rangle \big) \Big)$$

3) We apply the second Hadamard onto $|\psi_2\rangle$. The Hadamard acts on the first bit only. We get:

$$\begin{aligned} \frac{1}{2\sqrt{2}} \Big((|0\rangle + |1\rangle) \Big((a+b)|+\rangle + (a-b)|-\rangle \Big) + (|0\rangle - |1\rangle) \Big((a+b)|+\rangle - (a-b)|-\rangle \Big) \Big) &= \\ \frac{1}{2\sqrt{2}} \Big((a+b)|0\rangle|+\rangle + (a-b)|0\rangle|-\rangle + (a+b)|1\rangle|+\rangle + (a-b)|1\rangle|-\rangle + (a+b)|0\rangle|+\rangle \\ &- (a-b)|0\rangle|-\rangle - (a+b)|1\rangle|+\rangle + (a-b)|1\rangle|-\rangle \Big) &= \\ \frac{1}{2\sqrt{2}} \Big(2(a+b)|0\rangle|+\rangle + (2a-b)|1\rangle|-\rangle \Big) &= \\ \frac{1}{\sqrt{2}} \Big((a+b)|0\rangle|+\rangle + (a-b)|1\rangle|-\rangle \Big) \end{aligned}$$

The state after the second Hadamard is:

$$|\psi_3\rangle = \frac{1}{\sqrt{2}} \big((a+b)|0\rangle |+\rangle + (a-b)|1\rangle |-\rangle \big)$$

Basic level

We can do the same calculation on the basic level. We use the Kronecker product and write all states explicit.

We write the initial state as:

$$|\psi_0\rangle = (a|00\rangle + b|01\rangle) = \begin{pmatrix} a \\ b \\ 0 \\ 0 \end{pmatrix}$$

We apply the first Hadamard.

Note: In fact, we apply the Kronecker product $H \otimes I$ onto $|\psi_0\rangle$ and get $|\psi_1\rangle$.

$$H \otimes I = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$$

We apply:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} a \\ b \\ a \\ b \end{pmatrix}$$
(1)

We apply the CNOT onto $|\psi_1\rangle$.

The CNOT:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

We apply:

$$|\psi_{2}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a\\ b\\ a\\ b \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} a\\ b\\ b\\ a \end{pmatrix}$$
(2)

We apply the second Hadamard.

$$\begin{split} |\psi_{3}\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} a \\ b \\ b \\ a \end{pmatrix} = \\ \frac{1}{2} \begin{pmatrix} a+b \\ b+a \\ a-b \\ b-a \end{pmatrix} = \frac{1}{2} \begin{pmatrix} a+b \\ b+a \\ a-b \\ -(a-b) \end{pmatrix}$$
(3)

We compare with the high-level solution:

$$|\psi_3\rangle = \frac{1}{\sqrt{2}} \big((a+b)|0\rangle |+\rangle + (a-b)|1\rangle |-\rangle \big)$$

Resolving $|0\rangle|+\rangle$ and $|1\rangle|-\rangle$ gives:

$$\begin{split} |\psi_{3}\rangle &= \frac{1}{\sqrt{2}} \left((a+b) \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1\\0\\0 \end{pmatrix} + (a-b) \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\0\\1\\-1 \end{pmatrix} \right) = \\ &\frac{1}{2} \begin{pmatrix} a+b\\b+a\\a-b\\-(a-b) \end{pmatrix} \end{split}$$

Both methods yield the same result.

Result

Classically two bits are independent. Manipulating on bit doesn't change the other bits.

The qubits are not independent. The two qubits from our example build a superposition, a kind of four-dimensional entity.

The initial state ψ_i is composed from the qubit $|0\rangle$ and the state $|\psi_i\rangle = a|0\rangle + b|1\rangle$. This can be calculated via the Kronecker product:

$$|0\rangle \otimes (a|0\rangle + b|1\rangle)$$

Written as vectors:

$$\begin{pmatrix} 1\\ 0 \end{pmatrix} \otimes \begin{pmatrix} a\\ b \end{pmatrix} = \begin{pmatrix} a\\ b\\ 0\\ 0 \end{pmatrix}$$

Note: This is the superposition 4-D-representation of our 2 by 2 initial state.

Now, following the calculation in the basic level we see that the Hadamard changes the 4-D-representation (1):

$$(H \otimes I) \begin{pmatrix} a \\ b \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} a \\ b \\ a \\ b \end{pmatrix}$$

Applying the Hadamard again would reverse this effect:

$$(H \otimes I) \frac{1}{\sqrt{2}} \begin{pmatrix} a \\ b \\ a \\ b \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2a \\ 2b \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ b \\ 0 \\ 0 \end{pmatrix}$$

But the CNOT (2) interferes and reverses line three and four to:

$$\begin{pmatrix} a \\ b \\ b \\ a \end{pmatrix}$$

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The Hadamard, applied in ③ picks up the interference and does not produce

$$\begin{pmatrix} a \\ b \\ 0 \\ 0 \end{pmatrix}$$

but instead:

$$\frac{1}{2} \begin{pmatrix} a+b\\b+a\\a-b\\-(a-b) \end{pmatrix}$$

The effect: The output of the first qubit changes.

Classically, the simulation doesn't make sense because a lot of additional calculating time is needed. In a real quantum computer this happens according to the laws of physics and affects all qubits in superposition.

We examine the change of probability for measuring $|0\rangle$ at the end of the calculation.

$$|\psi_3\rangle = \frac{1}{\sqrt{2}} \big((a+b)|0\rangle |+\rangle + (a-b)|1\rangle |-\rangle \big)$$

$$P(|0\rangle) = \left(\frac{a+b}{\sqrt{2}}\right)^2 = \frac{a^2 + 2ab + b^2}{2}$$

Note: $a^2 + b^2 = 1$

$$P(|0\rangle) = \frac{1+2ab}{2} = \frac{1}{2} + a \cdot b$$

We use $a^2 + b^2 = 1$ and get:

$$P(|0\rangle) = \frac{1}{2} + \sqrt{b^2 - b^4}$$



At the two extremes b = 0 and b = 1 we have the probability $\frac{1}{2}$. If b is equal to $\sqrt{2}$ the probability is 1. Up to an ambiguity we can determine the unknown state ψ_i by measuring the first qubit.