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:

$\left|\psi_{0}\right\rangle \quad\left|\psi_{1}\right\rangle \quad\left|\psi_{2}\right\rangle \quad\left|\psi_{3}\right\rangle$

The meter sign denotes measurement in $\{|0\rangle,|1\rangle\}$ basis.
Suppose $\left|\psi_{i}\right\rangle=a|0\rangle+b|1\rangle, a^{2}+b^{2}=1$.

## Conceptual level

We solve this problem by conceptual-level access.
We rewrite the initial state as:

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

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 $\left|\psi_{0}\right\rangle$ and get $\left|\psi_{1}\right\rangle$ :

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

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 $\left|\psi_{1}\right\rangle$. The CNOT swaps the second qubit if the first qubit is $|1\rangle$.

We multiply out $\left|\psi_{1}\right\rangle$ :

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

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

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 $\left|\psi_{2}\right\rangle$ :

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

3) We apply the second Hadamard onto $\left|\psi_{2}\right\rangle$. The Hadamard acts on the first bit only. We get:

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

The state after the second Hadamard is:

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

## 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:

$$
\left|\psi_{0}\right\rangle=(a|00\rangle+b|01\rangle)=\left(\begin{array}{l}
a \\
b \\
0 \\
0
\end{array}\right)
$$

We apply the first Hadamard.
Note: In fact, we apply the Kronecker product $H \otimes I$ onto $\left|\psi_{0}\right\rangle$ and get $\left|\psi_{1}\right\rangle$.

$$
H \otimes I=\frac{1}{\sqrt{2}}\left(\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right) \otimes\left(\begin{array}{ll}
1 & 0 \\
0 & 1
\end{array}\right)=\frac{1}{\sqrt{2}}\left(\begin{array}{cc|cc}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & -1 & 0 \\
0 & 1 & 0 & -1
\end{array}\right)
$$

We apply:

$$
\left|\psi_{1}\right\rangle=\frac{1}{\sqrt{2}}\left(\begin{array}{cccc}
1 & 0 & 1 & 0  \tag{1}\\
0 & 1 & 0 & 1 \\
1 & 0 & -1 & 0 \\
0 & 1 & 0 & -1
\end{array}\right)\left(\begin{array}{l}
a \\
b \\
0 \\
0
\end{array}\right)=\frac{1}{\sqrt{2}}\left(\begin{array}{l}
a \\
b \\
a \\
b
\end{array}\right)
$$

We apply the CNOT onto $\left|\psi_{1}\right\rangle$.
The CNOT:

$$
\left(\begin{array}{llll}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{array}\right)
$$

We apply:

$$
\left|\psi_{2}\right\rangle=\frac{1}{\sqrt{2}}\left(\begin{array}{llll}
1 & 0 & 0 & 0  \tag{2}\\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{array}\right)\left(\begin{array}{l}
a \\
b \\
a \\
b
\end{array}\right)=\frac{1}{\sqrt{2}}\left(\begin{array}{l}
a \\
b \\
b \\
a
\end{array}\right)
$$

We apply the second Hadamard.

$$
\begin{align*}
\left|\psi_{3}\right\rangle=\frac{1}{\sqrt{2}}\left(\begin{array}{cccc}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & -1 & 0 \\
0 & 1 & 0 & -1
\end{array}\right) \frac{1}{\sqrt{2}}\left(\begin{array}{l}
a \\
b \\
b \\
a
\end{array}\right)= \\
\frac{1}{2}\left(\begin{array}{l}
a+b \\
b+a \\
a-b \\
b-a
\end{array}\right)=\frac{1}{2}\left(\begin{array}{c}
a+b \\
b+a \\
a-b \\
-(a-b)
\end{array}\right) \tag{3}
\end{align*}
$$

We compare with the high-level solution:

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

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

$$
\begin{gathered}
\left|\psi_{3}\right\rangle=\frac{1}{\sqrt{2}}\left((a+b) \frac{1}{\sqrt{2}}\left(\begin{array}{l}
1 \\
1 \\
0 \\
0
\end{array}\right)+(a-b) \frac{1}{\sqrt{2}}\left(\begin{array}{c}
0 \\
0 \\
1 \\
-1
\end{array}\right)\right)= \\
\frac{1}{2}\left(\begin{array}{c}
a+b \\
b+a \\
a-b \\
-(a-b)
\end{array}\right)
\end{gathered}
$$

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 $\left.\psi_{i}\right\rangle$ is composed from the qubit $|0\rangle$ and the state $\left|\psi_{i}\right\rangle=a|0\rangle+b|1\rangle$. This can be calculated via the Kronecker product:

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

Written as vectors:

$$
\binom{1}{0} \otimes\binom{a}{b}=\left(\begin{array}{l}
a \\
b \\
0 \\
0
\end{array}\right)
$$

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-Drepresentation (1):

$$
(H \otimes I)\left(\begin{array}{l}
a \\
b \\
0 \\
0
\end{array}\right)=\frac{1}{\sqrt{2}}\left(\begin{array}{l}
a \\
b \\
a \\
b
\end{array}\right)
$$

Applying the Hadamard again would reverse this effect:

$$
(H \otimes I) \frac{1}{\sqrt{2}}\left(\begin{array}{l}
a \\
b \\
a \\
b
\end{array}\right)=\frac{1}{2}\left(\begin{array}{c}
2 a \\
2 b \\
0 \\
0
\end{array}\right)=\left(\begin{array}{l}
a \\
b \\
0 \\
0
\end{array}\right)
$$

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

$$
\left(\begin{array}{l}
a \\
b \\
b \\
a
\end{array}\right)
$$

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

$$
\left(\begin{array}{l}
a \\
b \\
0 \\
0
\end{array}\right)
$$

but instead:

$$
\frac{1}{2}\left(\begin{array}{c}
a+b \\
b+a \\
a-b \\
-(a-b)
\end{array}\right)
$$

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.

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

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

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

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

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 $\left.\psi_{i}\right\rangle$ by measuring the first qubit.

