Quantum Circuit Implementing Grover's Algorithm

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Introduction

This is a tutorial on the use of Quantum`Computing` *Mathematica* add-on to implement Grover's Algorithm using Quantum Gates.
Grover's algorithm is a quantum algorithm for searching an unsorted database with N entries in O($N^{1/2}$) time and using O(log N) storage space (Grover L.K.: A fast quantum mechanical algorithm for database search, Proceedings, 28th Annual ACM Symposium on the Theory of Computing, (May 1996) p. 212).
Grover's algorithm can be generalized to "Quantum Counting" (Brassard G., P. Hoyer and Al. Tapp, arXiv:quant-ph/9805082) and "Quantum Amplitude Amplification and Estimation" (Brassard G., P. Hoyer, M. Mosca and A. Tapp, arXiv:quant-ph/0005055).
A *Mathematica* "Demonstration" implementing Grover's Algorithm can be found in this link:
Alexander Prokopenya, "Quantum Circuit Implementing Grover's Search Algorithm" from The Wolfram Demonstrations Project
http://demonstrations.wolfram.com/QuantumCircuitImplementingGroversSearchAlgorithm/

Load the Package

First load the Quantum`Computing` package. Write:
Needs["Quantum`Computing`"];
then press at the same time the keys SHIFT-ENTER to evaluate. *Mathematica* will load the package:

```
Needs["Quantum`Computing`"]
```

```
Quantum`Computing` Version 2.2.0. (July 2010)
A Mathematica package for Quantum Computing
  in Dirac bra-ket notation and plotting of quantum circuits
by José Luis Gómez-Muñoz

Execute SetComputingAliases[] in order to use
  the keyboard to enter quantum objects in Dirac's notation
SetComputingAliases[] must be executed again in each new notebook that is created
```

In order to use the keyboard to enter quantum objects write:
SetComputingAliases[ ];
then press at the same time the keys SHIFT-ENTER to evaluate. The semicolon prevents *Mathematica* from printing the help message. Remember that SetComputingAliases[ ] must be evaluated again in each new notebook:

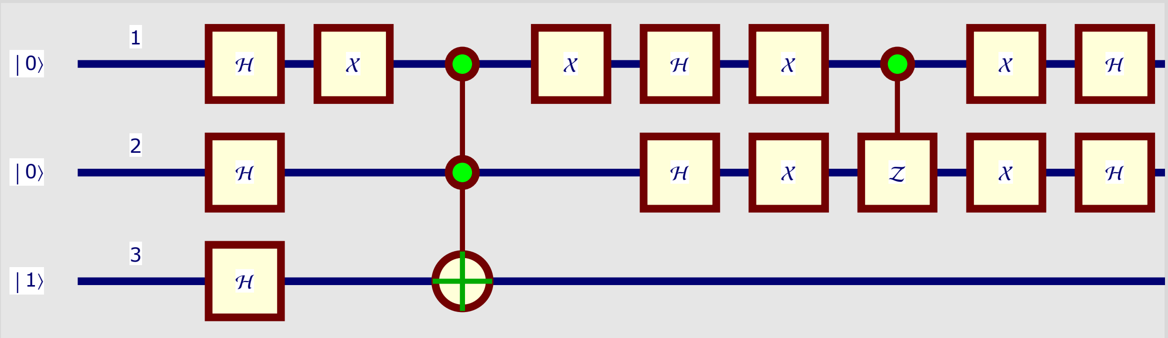
```
SetComputingAliases[];
```

Circuit implementation of Gover's Algorithm for two qubits

Following commands show and calculate the quantum circuit implementation of Grover's Algorithm for selecting the ket that represents the number k=1 as a two-qbit binary number ($0_1 \;\; 1_2$). Please continue reading below for a detailed explanation.

```
n = 2;
k = 1;
it = 1;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuit = (𝓗n · 𝓧n · 𝓒^(n-1)[𝓩n̂] · 𝓧n · 𝓗n · 𝓧mylist · 𝓒^n[𝓝𝓞𝓣(n+1)̂] · 𝓧mylist)^it ·
    𝓗n+1 · ( | 0î⟩)^⊗n · | 1(n+1)̂⟩;
Column[{
  circuit,
  QuantumPlot[
   circuit, ImageSize → {600, Automatic}],
  TraditionalForm[
   N[QuantumEvaluate[QubitMeasurement[circuit, n, FactorKet → False]]]]
   }]
```

$$\mathcal{H}_{\{\hat{1},\hat{2}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2}\}} \cdot \mathcal{C}^{\{\hat{1}\}}[\mathcal{Z}_{\hat{2}}] \cdot \mathcal{X}_{\{\hat{1},\hat{2}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2}\}} \cdot \mathcal{X}_{\{\hat{1}\}} \cdot \mathcal{C}^{\{\hat{1},\hat{2}\}}[\mathcal{NOT}_{\hat{3}}] \cdot \mathcal{X}_{\{\hat{1}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \left| 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}} \right\rangle$$

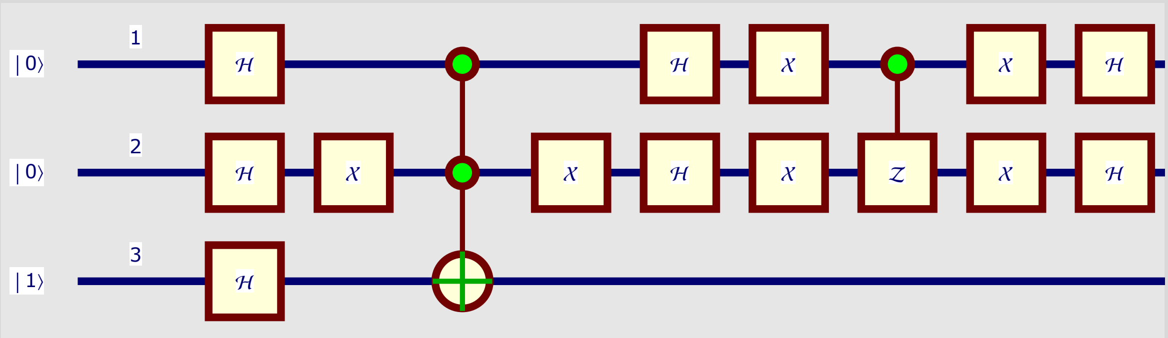


Probability	Measurement	State
1.	($0_1 \;\; 1_2$)	$0.707107\,(\,|011\rangle - 1.\;|010\rangle)$
Probability	Measurement	State

Following commands show and calculate the quantum circuit implementation of Grover's Algorithm for selecting the ket that represents the number k=2 as a binary number ($1_1 \;\; 0_2$). **See the difference with the previous circuit.** The working of this circuit is explained below in this document.

```
n = 2;
k = 2;
it = 1;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuit = (𝓗n · 𝓧n · C^(n-1)[𝓩n̂] · 𝓧n · 𝓗n · 𝓧mylist · C^n[𝓝𝓞𝓣(n+1)̂] · 𝓧mylist)^it ·
   𝓗n+1 · ( | 0_1̂⟩)^⊗n · | 1_(n+1)̂⟩;
Column[{
  circuit,
  QuantumPlot[
   circuit, ImageSize → {600, Automatic}],
  TraditionalForm[
   N[QuantumEvaluate[QubitMeasurement[circuit, n, FactorKet → False]]]]
   }]
```

$\mathcal{H}_{\{\hat{1},\hat{2}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2}\}} \cdot C^{\{\hat{1}\}}[\mathcal{Z}_{\hat{2}}] \cdot \mathcal{X}_{\{\hat{1},\hat{2}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2}\}} \cdot \mathcal{X}_{\{\hat{2}\}} \cdot C^{\{\hat{1},\hat{2}\}}[\mathcal{NOT}_{\hat{3}}] \cdot \mathcal{X}_{\{\hat{2}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot |0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}\rangle$



Probability	Measurement	State
1.	$(1_1 \ \ 0_2)$	$0.707107\,(\,|101\rangle - 1.\ |100\rangle)$
Probability	Measurement	State

Step-by-step explanation of the circuit implementing Grover's Algorithm for two qubits

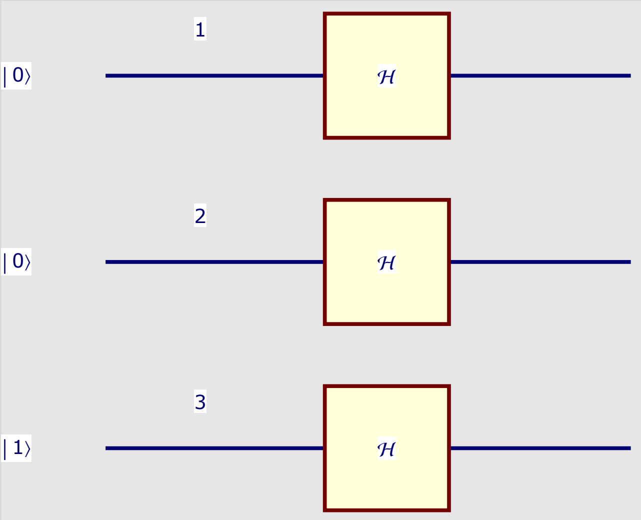
Initial State

An equally weighted superposition of all basis-states is generated using three Hadamard gates.
Notice that at this stage all the kets having a positive sign have the ancillary qubit set to $0_{\hat{3}}$, and all the kets having a negative sign have the ancillary qubit set to $1_{\hat{3}}$

The state of the system is stored in $|g1\rangle$

```
n = 2;
circuitpart = 𝓗n+1 · ( | 0_1̂⟩)^⊗n · | 1_(n+1)̂⟩;
Column[{
  circuitpart,
  QuantumPlot[circuitpart],
  | g1⟩ = QuantumEvaluate[circuitpart]}]
```

$\mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mid 0_{\hat{1}},\, 0_{\hat{2}},\, 1_{\hat{3}}\rangle$



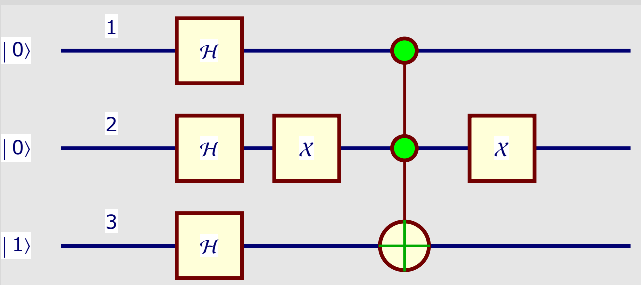
$$\frac{|0_{\hat{1}},0_{\hat{2}},0_{\hat{3}}\rangle}{2\sqrt{2}} - \frac{|0_{\hat{1}},0_{\hat{2}},1_{\hat{3}}\rangle}{2\sqrt{2}} + \frac{|0_{\hat{1}},1_{\hat{2}},0_{\hat{3}}\rangle}{2\sqrt{2}} - \frac{|0_{\hat{1}},1_{\hat{2}},1_{\hat{3}}\rangle}{2\sqrt{2}} + \frac{|1_{\hat{1}},0_{\hat{2}},0_{\hat{3}}\rangle}{2\sqrt{2}} - \frac{|1_{\hat{1}},0_{\hat{2}},1_{\hat{3}}\rangle}{2\sqrt{2}} + \frac{|1_{\hat{1}},1_{\hat{2}},0_{\hat{3}}\rangle}{2\sqrt{2}} - \frac{|1_{\hat{1}},1_{\hat{2}},1_{\hat{3}}\rangle}{2\sqrt{2}}$$

Changing the phase of those kets that meet the search criteria

The search criteria in this example is to represent the number 2 in binary digits: ($1_{\hat{1}}$,$0_{\hat{2}}$), those kets that meet the criteria get their phase changed (the signs plus and minus are exchanged). The conditional negation of the ancillary qubit gives this change of sign.
The state of the system is stored in $\mid g2\rangle$

```
n = 2;
k = 2;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuitpart = 𝒳mylist · Cⁿ[𝒩𝒪𝒯 n+1^] · 𝒳mylist · ℋn+1 · ( | 0 1^⟩)⊗n · | 1 n+1^⟩;
Column[{
   circuitpart,
   QuantumPlot[circuitpart],
    | g2⟩ = QuantumEvaluate[circuitpart]}]
```

$\mathcal{X}_{\{\hat{2}\}} \cdot C^{\{\hat{1},\hat{2}\}}[\mathcal{NOT}_{\hat{3}}] \cdot \mathcal{X}_{\{\hat{2}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mid 0_{\hat{1}},\, 0_{\hat{2}},\, 1_{\hat{3}}\rangle$



$$\frac{|0_{\hat{1}},0_{\hat{2}},0_{\hat{3}}\rangle}{2\sqrt{2}} - \frac{|0_{\hat{1}},0_{\hat{2}},1_{\hat{3}}\rangle}{2\sqrt{2}} + \frac{|0_{\hat{1}},1_{\hat{2}},0_{\hat{3}}\rangle}{2\sqrt{2}} - \frac{|0_{\hat{1}},1_{\hat{2}},1_{\hat{3}}\rangle}{2\sqrt{2}} - \frac{|1_{\hat{1}},0_{\hat{2}},0_{\hat{3}}\rangle}{2\sqrt{2}} + \frac{|1_{\hat{1}},0_{\hat{2}},1_{\hat{3}}\rangle}{2\sqrt{2}} + \frac{|1_{\hat{1}},1_{\hat{2}},0_{\hat{3}}\rangle}{2\sqrt{2}} - \frac{|1_{\hat{1}},1_{\hat{2}},1_{\hat{3}}\rangle}{2\sqrt{2}}$$

It is very important to understand the **difference** between the states just after the Hadamard gates ($\mid g1\rangle$), and the state after the conditional change of sign (phase) for those kets that meet the criteria ($\mid g2\rangle$):

```
TraditionalForm[
 Column[{"The sign was changed (+↔-) only on those kets that meet the
     search criteria", | g1⟩, | g2⟩}, Dividers → All]]
```

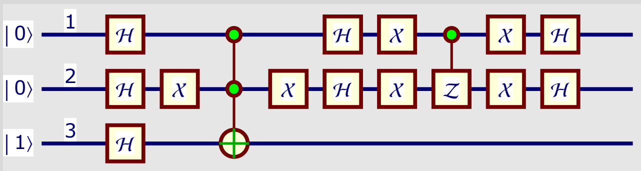
The sign was changed (+↔−) only on those kets that meet the search criteria
$\frac{\lvert 000\rangle}{2\sqrt{2}}-\frac{\lvert 001\rangle}{2\sqrt{2}}+\frac{\lvert 010\rangle}{2\sqrt{2}}-\frac{\lvert 011\rangle}{2\sqrt{2}}+\frac{\lvert 100\rangle}{2\sqrt{2}}-\frac{\lvert 101\rangle}{2\sqrt{2}}+\frac{\lvert 110\rangle}{2\sqrt{2}}-\frac{\lvert 111\rangle}{2\sqrt{2}}$
$\frac{\lvert 000\rangle}{2\sqrt{2}}-\frac{\lvert 001\rangle}{2\sqrt{2}}+\frac{\lvert 010\rangle}{2\sqrt{2}}-\frac{\lvert 011\rangle}{2\sqrt{2}}-\frac{\lvert 100\rangle}{2\sqrt{2}}+\frac{\lvert 101\rangle}{2\sqrt{2}}+\frac{\lvert 110\rangle}{2\sqrt{2}}-\frac{\lvert 111\rangle}{2\sqrt{2}}$

Increasing the amplitude of those kets that had their phase changed

The rest of the circuit increases the amplitude of those kets that had their phase changed.
In the case of two qubits, the other kets get their amplitude reduced to zero.

```
n = 2;
k = 2;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuitpart =
  ℋn · 𝒳n · C^(n-1)[𝒵n̂] · 𝒳n · ℋn · 𝒳mylist · C^n[𝒩𝒪𝒯(n+1)̂] · 𝒳mylist · ℋn+1 · ( | 0î⟩)^⊗n · | 1(n+1)̂⟩;
Column[{
  circuitpart,
  QuantumPlot[circuitpart],
  QuantumEvaluate[circuitpart]}]
```

$\mathcal{H}_{\{\hat{1},\hat{2}\}}\cdot\mathcal{X}_{\{\hat{1},\hat{2}\}}\cdot C^{\{\hat{1}\}}[\mathcal{Z}_{\hat{2}}]\cdot\mathcal{X}_{\{\hat{1},\hat{2}\}}\cdot\mathcal{H}_{\{\hat{1},\hat{2}\}}\cdot\mathcal{X}_{\{\hat{2}\}}\cdot C^{\{\hat{1},\hat{2}\}}[\mathcal{NOT}_{\hat{3}}]\cdot\mathcal{X}_{\{\hat{2}\}}\cdot\mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}}\cdot\lvert 0_{\hat{1}},0_{\hat{2}},1_{\hat{3}}\rangle$



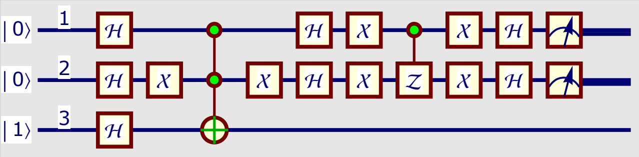
$-\frac{\lvert 1_{\hat{1}},0_{\hat{2}},0_{\hat{3}}\rangle}{\sqrt{2}}+\frac{\lvert 1_{\hat{1}},0_{\hat{2}},1_{\hat{3}}\rangle}{\sqrt{2}}$

Measurement gives with those kets that had their amplitude increased

In the case of **two qubits**, measurment will give those values that satisfy the search criteria with a 100% of probability

```
n = 2;
k = 2;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuitpart = QubitMeasurement[ℋn · 𝒳n · C^(n-1)[𝒵n̂] · 𝒳n · ℋn · 𝒳mylist ·
    C^n[𝒩𝒪𝒯(n+1)̂] · 𝒳mylist · ℋn+1 · ( | 0î⟩)^⊗n · | 1(n+1)̂⟩, n, FactorKet → False];
Column[{
  circuitpart,
  QuantumPlot[circuitpart],
  QuantumEvaluate[circuitpart]}]
```

$$\text{QubitMeasurement}\left[\mathcal{H}_{\{\hat{1},\hat{2}\}}\cdot \mathcal{X}_{\{\hat{1},\hat{2}\}}\cdot \mathcal{C}^{\{\hat{1}\}}\left[\mathcal{Z}_{\hat{2}}\right]\cdot \mathcal{X}_{\{\hat{1},\hat{2}\}}\cdot \mathcal{H}_{\{\hat{1},\hat{2}\}}\cdot \mathcal{X}_{\{\hat{2}\}}\cdot \mathcal{C}^{\{\hat{1},\hat{2}\}}\left[\mathcal{NOT}_{\hat{3}}\right]\cdot \mathcal{X}_{\{\hat{2}\}}\cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}}\cdot \left|0_{\hat{1}},0_{\hat{2}},1_{\hat{3}}\right\rangle, \left\{\hat{1},\hat{2}\right\}, \text{FactorKet}\to\text{False}\right]$$



Probability	Measurement	State
1	$\{\{1_{\hat{1}}, 0_{\hat{2}}\}\}$	$\frac{-\left\|1_{\hat{1}},0_{\hat{2}},0_{\hat{3}}\right\rangle+\left\|1_{\hat{1}},0_{\hat{2}},1_{\hat{3}}\right\rangle}{\sqrt{2}}$
Probability	Measurement	State

Circuit implementation of Gover's Algorithm for three qubits

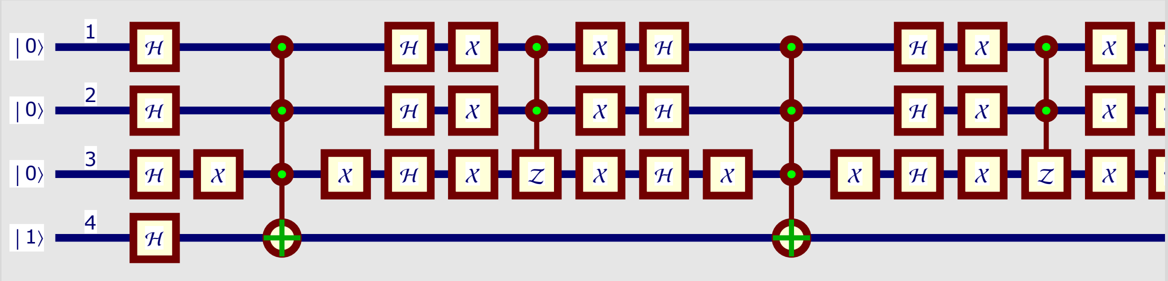
Following commands show and calculate the quantum circuit implementation of Grover's Algorithm for selecting the ket that represents the number k=6 as a three-qubit binary number (1_1 1_2 0_3). Please continue reading below for a detailed explanation. The use of the standard *Mathematica* command **Expand[]** makes the calculation faster because it expands the power of the operators:

```
n = 3;
k = 6;
it = 2;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
```

$$\textbf{circuit} = \textbf{Expand}\left[\left(\mathcal{H}_{n}\cdot \mathcal{X}_{n}\cdot \mathcal{C}^{n-1}\left[\mathcal{Z}_{\hat{n}}\right]\cdot \mathcal{X}_{n}\cdot \mathcal{H}_{n}\cdot \mathcal{X}_{mylist}\cdot \mathcal{C}^{n}\left[\mathcal{NOT}_{\widehat{n+1}}\right]\cdot \mathcal{X}_{mylist}\right)^{it}\cdot \mathcal{H}_{n+1}\cdot \left(\left|0_{\hat{1}}\right\rangle\right)^{\otimes n}\cdot \left|1_{\widehat{n+1}}\right\rangle\right];$$

```
Column[{
  circuit,
  QuantumPlot[
   circuit, ImageSize → {600, Automatic}],
  TraditionalForm[
   N[QuantumEvaluate[QubitMeasurement[circuit, n, FactorKet → False]]]]
   }]
```

$$\mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2}\}}\left[\mathcal{Z}_{\hat{3}}\right] \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{3}\}} \cdot C^{\{\hat{1},\hat{2},\hat{3}\}}\left[\mathcal{NOT}_{\hat{4}}\right] \cdot \mathcal{X}_{\{\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2}\}}\left[\mathcal{Z}_{\hat{3}}\right] \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{3}\}} \cdot C^{\{\hat{1},\hat{2},\hat{3}\}}\left[\mathcal{NOT}_{\hat{4}}\right] \cdot \mathcal{X}_{\{\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3},\hat{4}\}} \cdot \left|0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}\right\rangle$$

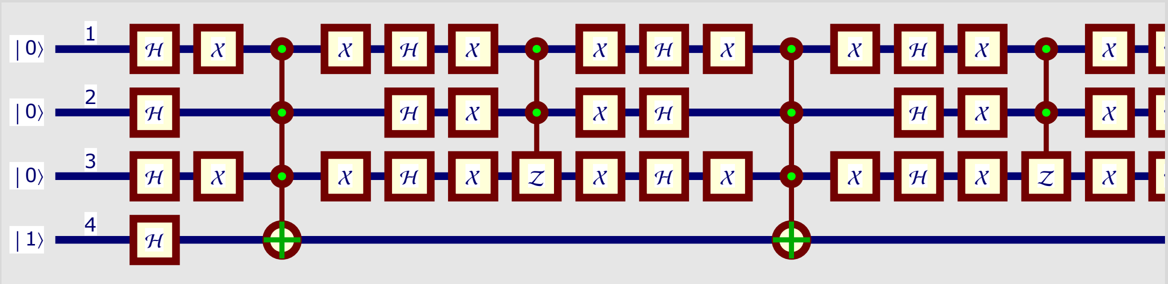


Probability	Measurement	State
0.0078125	$(0_1\ 0_2\ 0_3)$	$0.707107\,(\mid 0001\rangle - 1.\ \mid 0000\rangle)$
0.0078125	$(0_1\ 0_2\ 1_3)$	$0.707107\,(\mid 0011\rangle - 1.\ \mid 0010\rangle)$
0.0078125	$(0_1\ 1_2\ 0_3)$	$0.707107\,(\mid 0101\rangle - 1.\ \mid 0100\rangle)$
0.0078125	$(0_1\ 1_2\ 1_3)$	$0.707107\,(\mid 0111\rangle - 1.\ \mid 0110\rangle)$
0.0078125	$(1_1\ 0_2\ 0_3)$	$0.707107\,(\mid 1001\rangle - 1.\ \mid 1000\rangle)$
0.0078125	$(1_1\ 0_2\ 1_3)$	$0.707107\,(\mid 1011\rangle - 1.\ \mid 1010\rangle)$
0.945313	$(1_1\ 1_2\ 0_3)$	$0.707107\,(\mid 1100\rangle - 1.\ \mid 1101\rangle)$
0.0078125	$(1_1\ 1_2\ 1_3)$	$0.707107\,(\mid 1111\rangle - 1.\ \mid 1110\rangle)$
Probability	Measurement	State

Following commands show and calculate the quantum circuit implementation of Grover's Algorithm for selecting the ket that represents the number k=2 as a three-qubit binary number ($0_1\ \ 1_2\ \ 0_3$). **Compare it with the previous circuit**. This circuit is explained below in this document. The use of the standard *Mathematica* command **Expand[]** makes the calculation faster because it expands the power of the operators:

```
n = 3;
k = 2;
it = 2;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuit = Expand[(ℋn · 𝒳n · C^(n-1)[𝒵n̂] · 𝒳n · ℋn · 𝒳mylist · C^n[𝒩𝒪𝒯(n+1)̂] · 𝒳mylist)^it ·
    ℋn+1 · ( | 0 1̂⟩)^⊗n · | 1 (n+1)̂⟩];
Column[{
  circuit,
  QuantumPlot[
   circuit, ImageSize → {600, Automatic}],
  TraditionalForm[
   N[QuantumEvaluate[QubitMeasurement[circuit, n, FactorKet → False]]]]
  }]
```

$\mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2}\}}[\mathcal{Z}_{\hat{3}}] \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2},\hat{3}\}}[\mathcal{NOT}_{\hat{4}}] \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot$
$C^{\{\hat{1},\hat{2}\}}[\mathcal{Z}_{\hat{3}}] \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2},\hat{3}\}}[\mathcal{NOT}_{\hat{4}}] \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3},\hat{4}\}} \cdot |0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}\rangle$



Probability	Measurement	State
0.0078125	$(0_1\ 0_2\ 0_3)$	0.707107 (| 0001〉 − 1. | 0000〉)
0.0078125	$(0_1\ 0_2\ 1_3)$	0.707107 (| 0011〉 − 1. | 0010〉)
0.945313	$(0_1\ 1_2\ 0_3)$	0.707107 (| 0100〉 − 1. | 0101〉)
0.0078125	$(0_1\ 1_2\ 1_3)$	0.707107 (| 0111〉 − 1. | 0110〉)
0.0078125	$(1_1\ 0_2\ 0_3)$	0.707107 (| 1001〉 − 1. | 1000〉)
0.0078125	$(1_1\ 0_2\ 1_3)$	0.707107 (| 1011〉 − 1. | 1010〉)
0.0078125	$(1_1\ 1_2\ 0_3)$	0.707107 (| 1101〉 − 1. | 1100〉)
0.0078125	$(1_1\ 1_2\ 1_3)$	0.707107 (| 1111〉 − 1. | 1110〉)
Probability	Measurement	State

Step-by-step explanation of the circuit implementing Grover's Algorithm for three qubits

Initial State

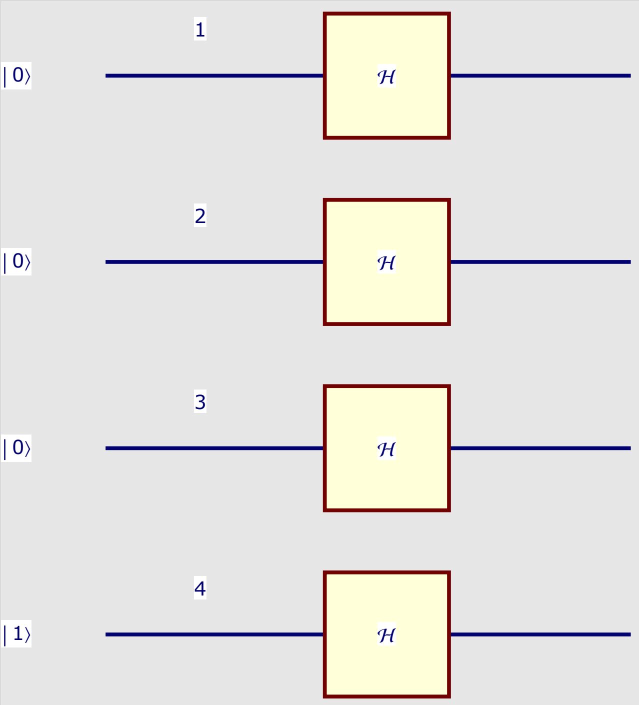
An equally weighted superposition of all basis-states is generated using four Hadamard gates.

Notice that at this stage all the kets having a positive sign have the ancillary qubit set to $0_{\hat{4}}$, and all the kets having a negative sign have the ancillary qubit set to $1_{\hat{4}}$

The state of the system is stored in | h1〉

```
n = 3;
circuitpart = ℋ_{n+1} · ( | 0_1̂〉)^⊗n · | 1_{n̂+1}〉;
Column[{
   circuitpart,
   QuantumPlot[circuitpart],
    | h1〉 = QuantumEvaluate[circuitpart]}]
```

$\mathcal{H}_{\{\hat{1},\hat{2},\hat{3},\hat{4}\}} \cdot \left| 0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle$



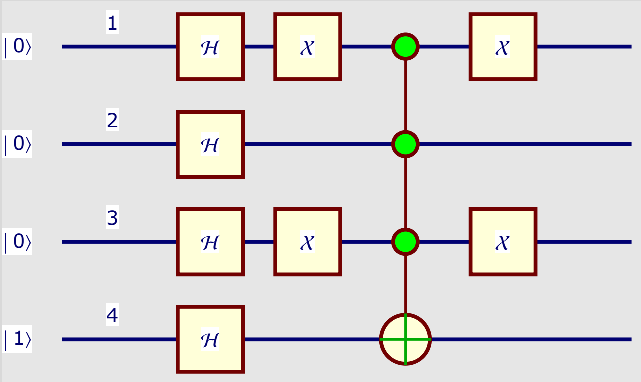
$$\tfrac{1}{4} \left| 0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \right\rangle - \tfrac{1}{4} \left| 0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle + \tfrac{1}{4} \left| 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \right\rangle - \tfrac{1}{4} \left| 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \right\rangle +$$
$$\tfrac{1}{4} \left| 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \right\rangle - \tfrac{1}{4} \left| 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle + \tfrac{1}{4} \left| 0_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \right\rangle - \tfrac{1}{4} \left| 0_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \right\rangle +$$
$$\tfrac{1}{4} \left| 1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \right\rangle - \tfrac{1}{4} \left| 1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle + \tfrac{1}{4} \left| 1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \right\rangle - \tfrac{1}{4} \left| 1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \right\rangle +$$
$$\tfrac{1}{4} \left| 1_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \right\rangle - \tfrac{1}{4} \left| 1_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle + \tfrac{1}{4} \left| 1_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \right\rangle - \tfrac{1}{4} \left| 1_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \right\rangle$$

Changing the phase of those kets that meet the search criteria

The search criteria in this example is to represent the number 2 in three binary digits: (0_1 1_2 0_3), those kets that meet the criteria get their phase changed (the signs plus and minus are exchanged). The conditional negation of the ancillary qubit gives this change of sign.
The state of the system is stored in $| \mathrm{h2} \rangle$

```
n = 3;
k = 2;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuitpart = X_mylist · C^n[NOT_(n+1^)] · X_mylist · H_(n+1) · ( | 0_1^⟩)^⊗n · | 1_(n+1^)⟩;
Column[{
  circuitpart,
  QuantumPlot[circuitpart],
  | h2⟩ = QuantumEvaluate[circuitpart]}]
```

$$\mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot \mathcal{C}^{\{\hat{1},\hat{2},\hat{3}\}}[\mathcal{NOT}_{\hat{4}}] \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3},\hat{4}\}} \cdot |0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}\rangle$$



$$\tfrac{1}{4}|0_{\hat{1}},0_{\hat{2}},0_{\hat{3}},0_{\hat{4}}\rangle - \tfrac{1}{4}|0_{\hat{1}},0_{\hat{2}},0_{\hat{3}},1_{\hat{4}}\rangle + \tfrac{1}{4}|0_{\hat{1}},0_{\hat{2}},1_{\hat{3}},0_{\hat{4}}\rangle - \tfrac{1}{4}|0_{\hat{1}},0_{\hat{2}},1_{\hat{3}},1_{\hat{4}}\rangle -$$
$$\tfrac{1}{4}|0_{\hat{1}},1_{\hat{2}},0_{\hat{3}},0_{\hat{4}}\rangle + \tfrac{1}{4}|0_{\hat{1}},1_{\hat{2}},0_{\hat{3}},1_{\hat{4}}\rangle + \tfrac{1}{4}|0_{\hat{1}},1_{\hat{2}},1_{\hat{3}},0_{\hat{4}}\rangle - \tfrac{1}{4}|0_{\hat{1}},1_{\hat{2}},1_{\hat{3}},1_{\hat{4}}\rangle +$$
$$\tfrac{1}{4}|1_{\hat{1}},0_{\hat{2}},0_{\hat{3}},0_{\hat{4}}\rangle - \tfrac{1}{4}|1_{\hat{1}},0_{\hat{2}},0_{\hat{3}},1_{\hat{4}}\rangle + \tfrac{1}{4}|1_{\hat{1}},0_{\hat{2}},1_{\hat{3}},0_{\hat{4}}\rangle - \tfrac{1}{4}|1_{\hat{1}},0_{\hat{2}},1_{\hat{3}},1_{\hat{4}}\rangle +$$
$$\tfrac{1}{4}|1_{\hat{1}},1_{\hat{2}},0_{\hat{3}},0_{\hat{4}}\rangle - \tfrac{1}{4}|1_{\hat{1}},1_{\hat{2}},0_{\hat{3}},1_{\hat{4}}\rangle + \tfrac{1}{4}|1_{\hat{1}},1_{\hat{2}},1_{\hat{3}},0_{\hat{4}}\rangle - \tfrac{1}{4}|1_{\hat{1}},1_{\hat{2}},1_{\hat{3}},1_{\hat{4}}\rangle$$

It is very important to understand the **difference** between the states just after the Hadamard gates ($|h1\rangle$), and the state after the conditional change of sign (phase) for those kets that meet the criteria ($|h2\rangle$):

```
TraditionalForm[
 Column[{"The sign was changed (+↔-) only on those kets that meet the
     search criteria", | h1⟩, | h2⟩}, Dividers → All]]
```

The sign was changed (+↔−) only on those kets that meet the search criteria
$\tfrac{1}{4}|0000\rangle - \tfrac{1}{4}|0001\rangle + \tfrac{1}{4}|0010\rangle - \tfrac{1}{4}|0011\rangle + \tfrac{1}{4}|0100\rangle - \tfrac{1}{4}|0101\rangle + \tfrac{1}{4}|0110\rangle - \tfrac{1}{4}|0111\rangle + \tfrac{1}{4}|1000\rangle - \tfrac{1}{4}|1001\rangle + \tfrac{1}{4}|1010\rangle - \tfrac{1}{4}|1011\rangle + \tfrac{1}{4}|1100\rangle - \tfrac{1}{4}|1101\rangle + \tfrac{1}{4}|1110\rangle - \tfrac{1}{4}|1111\rangle$
$\tfrac{1}{4}|0000\rangle - \tfrac{1}{4}|0001\rangle + \tfrac{1}{4}|0010\rangle - \tfrac{1}{4}|0011\rangle - \tfrac{1}{4}|0100\rangle + \tfrac{1}{4}|0101\rangle + \tfrac{1}{4}|0110\rangle - \tfrac{1}{4}|0111\rangle + \tfrac{1}{4}|1000\rangle - \tfrac{1}{4}|1001\rangle + \tfrac{1}{4}|1010\rangle - \tfrac{1}{4}|1011\rangle + \tfrac{1}{4}|1100\rangle - \tfrac{1}{4}|1101\rangle + \tfrac{1}{4}|1110\rangle - \tfrac{1}{4}|1111\rangle$

Increasing the amplitude of those kets that had their phase changed

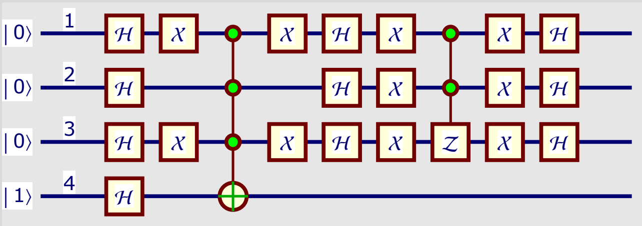
The rest of the circuit increases the amplitude of those kets that had their phase changed.
The state of the system is stored in $|h3\rangle$

```
n = 3;
k = 2;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuitpart =
```

$$\mathcal{H}_n \cdot \mathcal{X}_n \cdot \mathcal{C}^{n-1}[\mathcal{Z}_{\hat{n}}] \cdot \mathcal{X}_n \cdot \mathcal{H}_n \cdot \mathcal{X}_{mylist} \cdot \mathcal{C}^n[\mathcal{NOT}_{\widehat{n+1}}] \cdot \mathcal{X}_{mylist} \cdot \mathcal{H}_{n+1} \cdot (|0_{\hat{1}}\rangle)^{\otimes n} \cdot |1_{\widehat{n+1}}\rangle;$$

```
Column[{
  circuitpart,
  QuantumPlot[circuitpart],
  | h3⟩ = QuantumEvaluate[circuitpart]}]
```

$$\mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2}\}}\left[\mathcal{Z}_{\hat{3}}\right] \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2},\hat{3}\}}\left[\mathcal{NOT}_{\hat{4}}\right] \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3},\hat{4}\}} \cdot \left| 0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle$$



$$-\frac{1}{8} \left| 0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \right\rangle + \frac{1}{8} \left| 0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle - \frac{1}{8} \left| 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \right\rangle + \frac{1}{8} \left| 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \right\rangle -$$
$$\frac{5}{8} \left| 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \right\rangle + \frac{5}{8} \left| 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle - \frac{1}{8} \left| 0_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \right\rangle + \frac{1}{8} \left| 0_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \right\rangle -$$
$$\frac{1}{8} \left| 1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \right\rangle + \frac{1}{8} \left| 1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle - \frac{1}{8} \left| 1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \right\rangle + \frac{1}{8} \left| 1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \right\rangle -$$
$$\frac{1}{8} \left| 1_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \right\rangle + \frac{1}{8} \left| 1_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}} \right\rangle - \frac{1}{8} \left| 1_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \right\rangle + \frac{1}{8} \left| 1_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \right\rangle$$

Measurement gives with those kets that had their amplitude increased

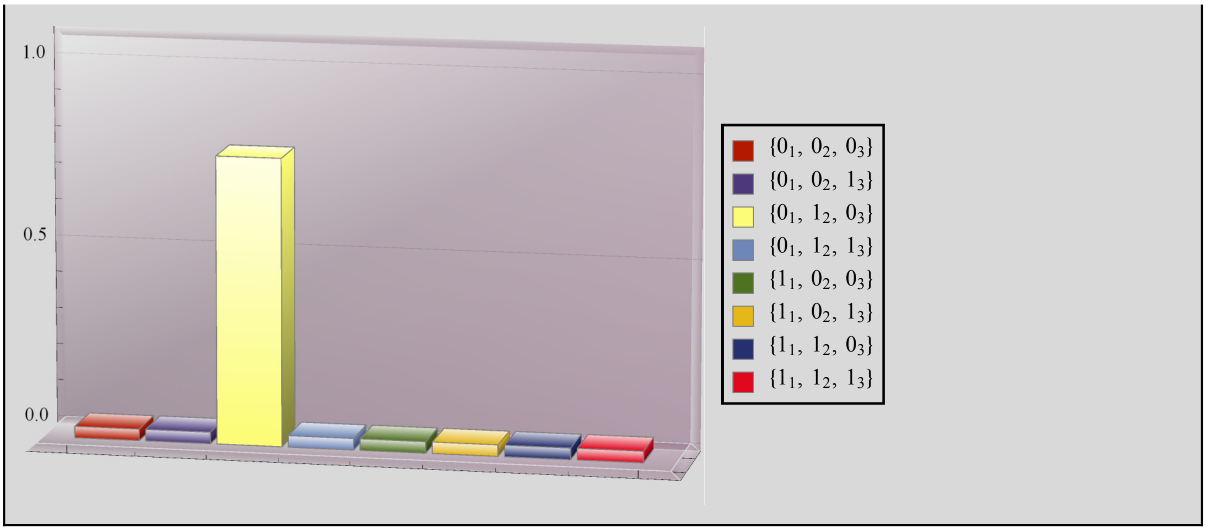
The result of a measurement on the state $|\,\mathrm{h3}\rangle$ has a high probability of giving the state that meets the search criteria:

```
TraditionalForm[
 N[QuantumEvaluate[QubitMeasurement[ | h3〉, {1̂, 2̂, 3̂}, FactorKet → False]]]]
```

Probability	Measurement	State
0.03125	$(0_1\ 0_2\ 0_3)$	$0.707107\,(\,\lvert 0001\rangle - 1.\ \lvert 0000\rangle)$
0.03125	$(0_1\ 0_2\ 1_3)$	$0.707107\,(\,\lvert 0011\rangle - 1.\ \lvert 0010\rangle)$
0.78125	$(0_1\ 1_2\ 0_3)$	$0.707107\,(\,\lvert 0101\rangle - 1.\ \lvert 0100\rangle)$
0.03125	$(0_1\ 1_2\ 1_3)$	$0.707107\,(\,\lvert 0111\rangle - 1.\ \lvert 0110\rangle)$
0.03125	$(1_1\ 0_2\ 0_3)$	$0.707107\,(\,\lvert 1001\rangle - 1.\ \lvert 1000\rangle)$
0.03125	$(1_1\ 0_2\ 1_3)$	$0.707107\,(\,\lvert 1011\rangle - 1.\ \lvert 1010\rangle)$
0.03125	$(1_1\ 1_2\ 0_3)$	$0.707107\,(\,\lvert 1101\rangle - 1.\ \lvert 1100\rangle)$
0.03125	$(1_1\ 1_2\ 1_3)$	$0.707107\,(\,\lvert 1111\rangle - 1.\ \lvert 1110\rangle)$
Probability	Measurement	State

The result of a measurement on the state $|\,\mathrm{h3}\rangle$ has a high probability of giving the state that meets the search criteria:

```
QuantumPlot3D[QuantumEvaluate[QubitMeasurement[ | h3〉, {1̂, 2̂, 3̂}, FactorKet → False]]]
```



A second iteration gives the optimal increase of probability for three qubits

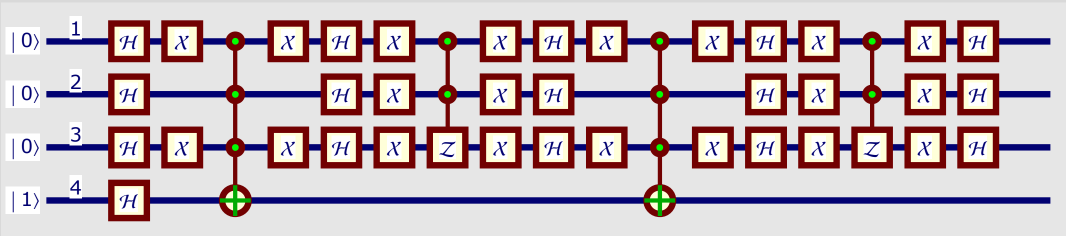
A second iteration further increments the amplitude of the kets that meets the criteria.

The optimal number of iterations is given by IntegerPart$\left[\pi \middle/ \left(4\, \text{ArcSin}\left(\frac{1}{\sqrt{2^n}}\right)\right)\right]$. For three qubits, this optimal is two; further iterations would decrease (instead of increase) the desired amplitude.

The state of the system is stored in | h4〉

```
n = 3;
k = 2;
it = 2;
mylist = Flatten[Position[IntegerDigits[k, 2, n], 0]];
circuitpart = Expand[
    (ℋn · 𝒳n · C^(n-1)[𝒵n̂] · 𝒳n · ℋn · 𝒳mylist · C^n[𝒩𝒪𝒯(n+1)̂] · 𝒳mylist)^it · ℋn+1 · ( | 0 1̂〉)^⊗n · | 1 (n+1)̂〉];
Column[{
  circuitpart,
  QuantumPlot[circuitpart, ImageSize → 500],
  | h4〉 = QuantumEvaluate[circuitpart]}]
```

$$\mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2}\}}\left[\mathcal{Z}_{\hat{3}}\right] \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2},\hat{3}\}}\left[\mathcal{NOT}_{\hat{4}}\right] \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2}\}}\left[\mathcal{Z}_{\hat{3}}\right] \cdot \mathcal{X}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3}\}} \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot C^{\{\hat{1},\hat{2},\hat{3}\}}\left[\mathcal{NOT}_{\hat{4}}\right] \cdot \mathcal{X}_{\{\hat{1},\hat{3}\}} \cdot \mathcal{H}_{\{\hat{1},\hat{2},\hat{3},\hat{4}\}} \cdot \left|0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}\right\rangle$$



$$-\frac{1}{16}\left|0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}}\right\rangle + \frac{1}{16}\left|0_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}\right\rangle - \frac{1}{16}\left|0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}}\right\rangle + \frac{1}{16}\left|0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}}\right\rangle + \frac{11}{16}\left|0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}}\right\rangle - \frac{11}{16}\left|0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}\right\rangle - \frac{1}{16}\left|0_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}}\right\rangle + \frac{1}{16}\left|0_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}}\right\rangle - \frac{1}{16}\left|1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}}\right\rangle + \frac{1}{16}\left|1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}\right\rangle - \frac{1}{16}\left|1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}}\right\rangle + \frac{1}{16}\left|1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}}\right\rangle - \frac{1}{16}\left|1_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}}\right\rangle + \frac{1}{16}\left|1_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}\right\rangle - \frac{1}{16}\left|1_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}}\right\rangle + \frac{1}{16}\left|1_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}}\right\rangle$$

Measurement gives with those kets that had their amplitude increased

The result of a measurement on the state $|\,h4\rangle$ has the highest probability of giving the state that meets the search criteria:

```
TraditionalForm[
 N[QuantumEvaluate[QubitMeasurement[ | h4〉, {1̂, 2̂, 3̂}, FactorKet → False]]]]
```

Probability	Measurement	State
0.0078125	$(0_1\ 0_2\ 0_3)$	$0.707107\,(\lvert 0001\rangle - 1.\ \lvert 0000\rangle)$
0.0078125	$(0_1\ 0_2\ 1_3)$	$0.707107\,(\lvert 0011\rangle - 1.\ \lvert 0010\rangle)$
0.945313	$(0_1\ 1_2\ 0_3)$	$0.707107\,(\lvert 0100\rangle - 1.\ \lvert 0101\rangle)$
0.0078125	$(0_1\ 1_2\ 1_3)$	$0.707107\,(\lvert 0111\rangle - 1.\ \lvert 0110\rangle)$
0.0078125	$(1_1\ 0_2\ 0_3)$	$0.707107\,(\lvert 1001\rangle - 1.\ \lvert 1000\rangle)$
0.0078125	$(1_1\ 0_2\ 1_3)$	$0.707107\,(\lvert 1011\rangle - 1.\ \lvert 1010\rangle)$
0.0078125	$(1_1\ 1_2\ 0_3)$	$0.707107\,(\lvert 1101\rangle - 1.\ \lvert 1100\rangle)$
0.0078125	$(1_1\ 1_2\ 1_3)$	$0.707107\,(\lvert 1111\rangle - 1.\ \lvert 1110\rangle)$
Probability	Measurement	State

A *Mathematica* "Demonstration" implementing Grover's Algorithm can be found in this link:
Alexander Prokopenya, "Quantum Circuit Implementing Grover's Search Algorithm" from The Wolfram Demonstrations Project
http://demonstrations.wolfram.com/QuantumCircuitImplementingGroversSearchAlgorithm/

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