# Superposition States, Bell States and Change of Basis Using QuantumReplace

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#### Introduction

This is a tutorial on the use of Quantum Computing Mathematica add-on to work with superposition states  $\Big| +_{\hat{1}} \Big\rangle = \frac{\Big| 0_{\hat{1}} \Big\rangle + \Big| 1_{\hat{1}} \Big\rangle}{\sqrt{2}}, \quad \Big| -_{\hat{1}} \Big\rangle = \frac{\Big| 0_{\hat{1}} \Big\rangle - \Big| 1_{\hat{1}} \Big\rangle}{\sqrt{2}};$  Bell states  $\Big| \mathcal{B}_{00,\hat{1},\hat{2}} \Big\rangle = \Big| \Phi_{\hat{1},\hat{2}}^{+} \Big\rangle = \frac{\Big| 0_{\hat{1}}, 0_{\hat{2}} \Big\rangle + \Big| 1_{\hat{1}}, 1_{\hat{2}} \Big\rangle}{\sqrt{2}},$  etc; and the use of the command QuantumReplace in order to change from the computational basis to another basis

#### Load the Package

First load the Quantum' Computing' package. Write:

Needs["Quantum'Computing'"]

then press at the same time the keys [SHIT]-[INTER 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 sufficient to evaluate. The semicolon prevents *Mathematica* from printing the help message. Remember that SetComputingAliases[] must be evaluated again in each new notebook:

```
SetComputingAliases[];
```

# Superposition States $|+_{\hat{1}}\rangle$ and $|-_{\hat{1}}\rangle$

Superposition kets can be easily entered. For example, press:

[ESC]k+[ESC][TAB]3

then press at the same time the keys SHIFT-ENTER to evaluate:

The command QuantumEvaluate gives the representation of this ket in terms of the computational basis:

QuantumEvaluate  $[ | +_{\hat{3}} \rangle ]$ 

$$\frac{\left|\begin{array}{c}0_{\hat{3}}\right\rangle}{\sqrt{2}}+\frac{\left|\begin{array}{c}1_{\hat{3}}\right\rangle}{\sqrt{2}}\end{array}$$

Quantum Mathematica knows that the superposition states are orthonormal

[ESC]b+[ESC][ESC]on[ESC][ESC]k-[ESC]

Press the [TAB] key one or two times in order to select the first place-holder (empty square) and press he keys:

1[TAB]1[TAB]

then press at the same time the keys SHFT-ENTER to evaluate:

$$\langle +_{\hat{1}} \mid \cdot \mid -_{\hat{1}} \rangle$$

0

[ESC]b-[ESC][ESC]on[ESC][ESC]k-[ESC]

Press the [TAB] key one or two times in order to select the first place-holder (empty square) and press he keys: 1[TAB]1[TAB]

then press at the same time the keys SHIFT-ENTER to evaluate:

$$\langle -_{\hat{1}} \mid \cdot \mid -_{\hat{1}} \rangle$$

1

This is a tensor product:

$$| +_{\hat{1}} \rangle \cdot | -_{\hat{2}} \rangle \cdot | +_{\hat{3}} \rangle$$

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

Tensor products can include some qubits in the computational basis and other qubits in the superposition basis. Notice that the labels are not organized by qubit, they are organized by the type of state (-, + or computational basis)

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

The command QuantumEvaluate gives the representation of this ket in terms of the computational basis:

QuantumEvaluate 
$$\begin{bmatrix} & -\frac{1}{2}, & +\frac{1}{3}, & 1_{\hat{1}}, & 0_{\hat{4}} \end{bmatrix}$$

$$\frac{1}{2} \mid 1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \rangle + \frac{1}{2} \mid 1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \rangle - \frac{1}{2} \mid 1_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \rangle - \frac{1}{2} \mid 1_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \rangle$$

This is a factorized version of the same state

 $\texttt{FactorKet}\left[\texttt{QuantumEvaluate}\left[ \ \left| \ -_{\hat{2}} \,, \ +_{\hat{3}} \,, \ \mathbf{1}_{\hat{1}} , \ \mathbf{0}_{\hat{4}} \right\rangle \right] \right]$ 

$$\operatorname{Hold} \left[ \ \left| \ \mathbf{1}_{\hat{1}} \right\rangle \otimes \left( \ \left| \ \mathbf{0}_{\hat{2}} \right\rangle - \ \left| \ \mathbf{1}_{\hat{2}} \right\rangle \right) \otimes \left( \ \left| \ \mathbf{0}_{\hat{3}} \right\rangle + \ \left| \ \mathbf{1}_{\hat{3}} \right\rangle \right) \otimes \left( \frac{1}{2} \ \left| \ \mathbf{0}_{\hat{4}} \right\rangle \right) \right] \right]$$

Copy-paste the previous output without the Hold[] wrapper and the result is an expanded version:

$$\frac{1}{2} \mid 1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \rangle + \frac{1}{2} \mid 1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \rangle - \frac{1}{2} \mid 1_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \rangle - \frac{1}{2} \mid 1_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}} \rangle$$

We can get a list of the factors, ready to be used with the standard *Mathematica* commands for list manipulation, like Part, Length, Select, Cases, GatherBy, etc.

 $\texttt{FactorKetList} \big[ \texttt{QuantumEvaluate} \big[ \ \big| \ -_{\hat{2}} \,, \ +_{\hat{3}} \,, \ \mathbf{1}_{\hat{1}} \,, \ \mathbf{0}_{\hat{4}} \big\rangle \big] \, \big]$ 

Dirac notation can be used to create an operator that works on superposition kets

$$op1 = \frac{1}{\sqrt{2}} \left( \begin{array}{c|c|c|c} -\hat{1} & \cdot & -\hat{1} \end{array} \right) \cdot \left\langle -\hat{1} & + & +\hat{1} \end{array} \right) \cdot \left\langle -\hat{1} & + & -\hat{1} \end{array} \right) \cdot \left\langle +\hat{1} & - & +\hat{1} \end{array} \right) \cdot \left\langle +\hat{1} & + & +\hat{1} \end{array}$$

The operator created before applies to a ket:s

op1 · 
$$\left| -\frac{1}{1} \right\rangle$$

$$\frac{\left|\begin{array}{c|c} -_{\hat{1}} \end{array}\right\rangle + \left|\begin{array}{c|c} +_{\hat{1}} \end{array}\right\rangle}{\sqrt{2}}$$

#### Use of Solve and QuantumReplace in order to change basis of superposition states

The standard Mathematica command Solve can be used to obtain the replacement rules to transform from the computational basis to the superposition basis

```
 \left\{ \begin{array}{l} \left| \begin{array}{l} +_{\hat{1}} \right\rangle == \text{QuantumEvaluate} \left[ \begin{array}{l} +_{\hat{1}} \right\rangle \right], \\ \left| \begin{array}{l} -_{\hat{1}} \right\rangle == \text{QuantumEvaluate} \left[ \begin{array}{l} -_{\hat{1}} \right\rangle \right] \right\}, \\ \left\{ \begin{array}{l} \left| \begin{array}{l} 0_{\hat{1}} \right\rangle, & \left| \begin{array}{l} 1_{\hat{1}} \right\rangle \right\} \end{array} \right\}
```

$$\left\{ \left\{ \begin{array}{c} \left| \begin{array}{c} 0_{\hat{1}} \right\rangle \rightarrow \frac{\left| \begin{array}{c} -_{\hat{1}} \right\rangle}{\sqrt{2}} + \frac{\left| \begin{array}{c} +_{\hat{1}} \right\rangle}{\sqrt{2}}, & \left| \begin{array}{c} 1_{\hat{1}} \right\rangle \rightarrow - \frac{\left| \begin{array}{c} -_{\hat{1}} \right\rangle}{\sqrt{2}} + \frac{\left| \begin{array}{c} +_{\hat{1}} \right\rangle}{\sqrt{2}} \end{array} \right\} \right\}$$

Copy the inner list of the previous output (without the outer curly braces {} ) and paste it as the second argument of QuantumReplace in order to change an expression from the computational basis to the superposition basis in the first qubit. The first argument of QuantumReplace,  $|1_{\hat{1}}, 1_{\hat{2}}\rangle \cdot \langle 0_{\hat{1}}, 1_{\hat{2}}|$ , is the original expression that we want to express in another basis

$$\begin{split} & \texttt{Expand} \Big[ \texttt{QuantumReplace} \Big[ \\ & & \left| \ \mathbf{1}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \right\rangle \cdot \left\langle \mathbf{0}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \right|, \\ & \left\{ \ \left| \ \mathbf{0}_{\hat{1}} \right\rangle \rightarrow \frac{\left| \ -_{\hat{1}} \right\rangle}{\sqrt{2}} + \frac{\left| \ +_{\hat{1}} \right\rangle}{\sqrt{2}}, \ \ \left| \ \mathbf{1}_{\hat{1}} \right\rangle \rightarrow - \frac{\left| \ -_{\hat{1}} \right\rangle}{\sqrt{2}} + \frac{\left| \ +_{\hat{1}} \right\rangle}{\sqrt{2}} \Big\} \\ & \ \left] \Big] \Big] \end{split}$$

$$\begin{vmatrix} -\frac{1}{2} & | & -_{\hat{1}}, & 1_{\hat{2}} \rangle \cdot \langle -_{\hat{1}}, & 1_{\hat{2}} & | & +_{\hat{1}}, & 1_{\hat{2}} \rangle \cdot \langle -_{\hat{1}}, & 1_{\hat{2}} & | & - \\ \frac{1}{2} & | & -_{\hat{1}}, & 1_{\hat{2}} \rangle \cdot \langle +_{\hat{1}}, & 1_{\hat{2}} & | & +_{\hat{1}}, & 1_{\hat{2}} \rangle \cdot \langle +_{\hat{1}}, & 1_{\hat{2}} & | & + \\ \end{vmatrix}$$

Copy the result of the previous calculation and paste it as argument to QuantumEvaluate, in order to verify that we recover the original expression  $|1_{\hat{1}}, 1_{\hat{2}}\rangle \cdot \langle 0_{\hat{1}}, 1_{\hat{2}}|$ :

$$\mid$$
 1 $_{\hat{1}}$ , 1 $_{\hat{2}}$  $\rangle$  ·  $\langle$  0 $_{\hat{1}}$ , 1 $_{\hat{2}}$   $\mid$ 

This time both qubits become expressed in the superposition basis:

$$\begin{split} & \text{Expand} \left[ \text{QuantumReplace} \right[ \\ & \left| \ \mathbf{1}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \right\rangle \cdot \left\langle \mathbf{0}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \right|, \\ & \left\{ \ \left| \ \mathbf{0}_{\hat{1}} \right\rangle \rightarrow \frac{\left| \ -_{\hat{1}} \right\rangle}{\sqrt{2}} + \frac{\left| \ +_{\hat{1}} \right\rangle}{\sqrt{2}}, \quad \left| \ \mathbf{1}_{\hat{1}} \right\rangle \rightarrow - \frac{\left| \ -_{\hat{1}} \right\rangle}{\sqrt{2}} + \frac{\left| \ +_{\hat{1}} \right\rangle}{\sqrt{2}}, \\ & \left| \ \mathbf{0}_{\hat{2}} \right\rangle \rightarrow \frac{\left| \ -_{\hat{2}} \right\rangle}{\sqrt{2}} + \frac{\left| \ +_{\hat{2}} \right\rangle}{\sqrt{2}}, \quad \left| \ \mathbf{1}_{\hat{2}} \right\rangle \rightarrow - \frac{\left| \ -_{\hat{2}} \right\rangle}{\sqrt{2}} + \frac{\left| \ +_{\hat{2}} \right\rangle}{\sqrt{2}} \right\} \\ & \left| \ \right] \right] \end{split}$$

Copy the result of the previous calculation and paste it as argument to QuantumEvaluate, in order to verify that we recover the original expression in the computational basis:

$$\begin{aligned} & \frac{1}{4} \, \left| \, -_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle -_{\hat{1}} \,, \, \, -_{\hat{2}} \right\rangle \cdot \left\langle -_{\hat{1}} \,, \, \, -_{\hat{2}} \right| \, + \\ & \frac{1}{4} \, \left| \, -_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle -_{\hat{1}} \,, \, \, -_{\hat{2}} \, \right| + \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, -_{\hat{2}} \right\rangle \cdot \left\langle -_{\hat{1}} \,, \, \, -_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle -_{\hat{1}} \,, \, \, +_{\hat{2}} \right| + \\ & \frac{1}{4} \, \left| \, -_{\hat{1}} \,, \, \, -_{\hat{2}} \right\rangle \cdot \left\langle -_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, -_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle -_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, -_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, -_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, -_{\hat{2}} \right| + \\ & \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, -_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, -_{\hat{2}} \, \right| + \frac{1}{4} \, \left| \, -_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \\ & \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, -_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, -_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, -_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \\ & \frac{1}{4} \, \left| \, -_{\hat{1}} \,, \, \, +_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, -_{\hat{2}} \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \\ & \frac{1}{4} \, \left| \, -_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, -_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \\ & \frac{1}{4} \, \left| \, -_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, -_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \\ & \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right| - \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, +_{\hat{2}} \, \right| - \\ & \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, \, +_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, +_{\hat{2}} \, \right| - \\ & \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, +_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, +_{\hat{2}} \, \right| - \\ & \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, +_{\hat{2}} \, \right\rangle \cdot \left\langle +_{\hat{1}} \,, \, +_{\hat{1}} \, \right| - \\ & \frac{1}{4} \, \left| \, +_{\hat{1}} \,, \, +_{\hat{2}} \, \right\rangle \cdot \left\langle +_{$$

QuantumEvaluate must be included in order to represent gates in the computational basis as operators in Dirac notation in the superposition basis

 $| 1_{\hat{1}}, 1_{\hat{2}} \rangle \cdot \langle 0_{\hat{1}}, 1_{\hat{2}} |$ 

$$\begin{split} & \texttt{Expand} \left[ \texttt{QuantumReplace} \left[ \\ & \texttt{QuantumEvaluate} \left[ C^{\left( \hat{1} \right)} \left[ \texttt{NOT}_{\hat{2}} \right] \cdot \mathcal{H}_{\hat{1}} \right], \\ & \left\{ \begin{array}{c} \left| \right. 0_{\hat{1}} \right\rangle \rightarrow \frac{\left| \right. -_{\hat{1}} \right\rangle}{\sqrt{2}} + \frac{\left| \right. +_{\hat{1}} \right\rangle}{\sqrt{2}}, \quad \left| \right. 1_{\hat{1}} \right\rangle \rightarrow -\frac{\left| \right. -_{\hat{1}} \right\rangle}{\sqrt{2}} + \frac{\left| \right. +_{\hat{1}} \right\rangle}{\sqrt{2}}, \\ & \left| \right. 0_{\hat{2}} \right\rangle \rightarrow \frac{\left| \right. -_{\hat{2}} \right\rangle}{\sqrt{2}} + \frac{\left| \right. +_{\hat{2}} \right\rangle}{\sqrt{2}}, \quad \left| \right. 1_{\hat{2}} \right\rangle \rightarrow -\frac{\left| \right. -_{\hat{2}} \right\rangle}{\sqrt{2}} + \frac{\left| \right. +_{\hat{2}} \right\rangle}{\sqrt{2}} \right\} \\ & \left. \left. \right] \right] \right] \end{split}$$

#### Warning: QuantumReplace is Not Forced to Obey Algebraic Rules

QuantumReplace is not an algebraic command. It does not check if the replacement gives a new expression that is equivalent to the new one. This behavior is inherited from the standard Mathematica commands Replace and ReplaceAll. The replacement is structural, it is not algebraic, therefore, in other uses of QuantumReplace, the result might be different and not equivalent to the input (in the examples of this document all the results are algebraically correct, but Mathematica does not check if this is the case).

#### **Bell States**

Bell State kets can be easily entered. For example, press:

[ESC]k00[ESC][TAB]4[TAB]7

then press at the same time the keys SHIFT-ENTER to evaluate:

$$\left|\begin{array}{c} \mathcal{B}_{oo,\hat{\mathbf{4}},\hat{\mathbf{7}}} \rangle \\ \\ \left|\begin{array}{c} \mathcal{B}_{oo,\hat{\mathbf{4}},\hat{\mathbf{7}}} \rangle \end{array}\right.$$

The command QuantumEvaluate gives the representation of this ket in terms of the computational basis:

QuantumEvaluate 
$$\left[ \begin{array}{c} \left| \mathcal{B}_{oo,\hat{4},\hat{7}} \right\rangle \right]$$

$$\frac{\left| \begin{array}{c} 0_{\hat{4}}, \ 0_{\hat{7}} \right\rangle}{\sqrt{2}} + \frac{\left| \begin{array}{c} 1_{\hat{4}}, \ 1_{\hat{7}} \right\rangle}{\sqrt{2}} \end{array} \right.$$

Here is another notation for Bell sates:

[ESC]kphi+[ESC][TAB]4[TAB]7

then press at the same time the keys SHIFT - ENTER to evaluate:

$$\left|\begin{array}{c} \Phi_{\hat{4},\hat{7}}^{+} \end{array}\right\rangle$$

$$\left| \Phi_{\hat{4},\hat{7}}^{+} \right\rangle$$

The command QuantumEvaluate gives the representation of this ket in terms of the computational basis:

QuantumEvaluate  $\left[\begin{array}{c|c} \Phi_{\hat{4},\hat{7}}^{+} \end{array}\right]$ 

$$\frac{\mid 0_{\hat{4}}, \ 0_{\hat{\gamma}} \rangle}{\sqrt{2}} + \frac{\mid 1_{\hat{4}}, \ 1_{\hat{\gamma}} \rangle}{\sqrt{2}}$$

Quantum Mathematica knows that the superposition states are orthonormal

[ESC]b11[ESC][ESC]on[ESC][ESC]k01[ESC]

Press the [TAB] key one or two times in order to select the first place-holder (empty square) and press he keys:

1[TAB]2[TAB]1[TAB]2

then press at the same time the keys SHFT-ENTER to evaluate:

$$\left\langle \mathcal{B}_{11,\hat{1},\hat{2}} \mid \cdot \mid \mathcal{B}_{01,\hat{1},\hat{2}} \right\rangle$$

0

[ESC]b10[ESC][ESC]on[ESC][ESC]k10[ESC]

Press the [TAB] key one or two times in order to select the first place-holder (empty square) and press he keys: 1[TAB]2[TAB]1[TAB]2

then press at the same time the keys SHFT-ENTER to evaluate:

$$\left\langle \mathcal{B}_{_{10},\hat{1},\hat{2}} \mid \cdot \mid \mathcal{B}_{_{10},\hat{1},\hat{2}} \right\rangle$$

[ESC]bpsi+[ESC][ESC]on[ESC][ESC]kphi-[ESC]

Press the [TAB] key one or two times in order to select the first place-holder (empty square) and press he keys: 1[TAB]2[TAB]1[TAB]2

then press at the same time the keys SHFT-ENTER to evaluate:

$$\left\langle \Psi_{\hat{1},\,\hat{2}}^{\star} \mid \cdot \mid \Phi_{\hat{1},\,\hat{2}}^{\star} 
ight
angle$$

[ESC]bpsi+[ESC][ESC]on[ESC][ESC]kpsi+[ESC]

Press the [TAB] key one or two times in order to select the first place-holder (empty square) and press he keys: 1[TAB]2[TAB]1[TAB]2

then press at the same time the keys SHFT-ENTER to evaluate:

$$\left\langle \Psi_{\hat{1},\hat{2}}^{\star} \mid \cdot \mid \Psi_{\hat{1},\hat{2}}^{\star} \right\rangle$$
1

This is a tensor product:

The command QuantumEvaluate gives the representation of this ket in terms of the computational basis:

QuantumEvaluate 
$$\left[ \mid \Psi_{\hat{1},\hat{2}}^{\star}, \Psi_{\hat{3},\hat{4}}^{\star} \right]$$
   
  $\frac{1}{2} \mid 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \rangle - \frac{1}{2} \mid 0_{\hat{1}}, 1_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \rangle + \frac{1}{2} \mid 1_{\hat{1}}, 0_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}} \rangle - \frac{1}{2} \mid 1_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}} \rangle$ 

This is a factorized version of the same state:

$$\begin{aligned} & \mathbf{FactorKet} \Big[ \mathbf{QuantumEvaluate} \Big[ \ \big| \ \underline{\Psi}_{\hat{1},\hat{2}}^{+}, \ \underline{\Psi}_{\hat{3},\hat{4}}^{+} \Big\rangle \Big] \Big] \\ & \\ & \mathbf{Hold} \Big[ \big( \ \big| \ \mathbf{1}_{\hat{1}} \big) \otimes \ \big| \ \mathbf{0}_{\hat{2}} \big\rangle + \ \big| \ \mathbf{0}_{\hat{1}} \big\rangle \otimes \ \big| \ \mathbf{1}_{\hat{2}} \big\rangle \big) \otimes \left( \frac{1}{2} \ \big( \ \big| \ \mathbf{0}_{\hat{3}} \big\rangle \otimes \ \big| \ \mathbf{0}_{\hat{4}} \big\rangle + \ \big| \ \mathbf{1}_{\hat{3}} \big\rangle \otimes - \ \big| \ \mathbf{1}_{\hat{4}} \big\rangle \big) \Big) \Big] \end{aligned}$$

Copy-paste the previous output without the Hold[] wrapper and the result is an expanded version:

We can get a list of the factors, ready to be used with the standard *Mathematica* commands for list manipulation, like Part, Length, Select, Cases, GatherBy, etc.

FactorKetList [QuantumEvaluate [ 
$$|\Psi_{\hat{1},\hat{2}}^{+}, \Phi_{\hat{3},\hat{4}}^{-}\rangle$$
]] 
$$\left\{ |0_{\hat{1}}, 1_{\hat{2}}\rangle + |1_{\hat{1}}, 0_{\hat{2}}\rangle, \frac{1}{2} |0_{\hat{3}}, 0_{\hat{4}}\rangle - \frac{1}{2} |1_{\hat{3}}, 1_{\hat{4}}\rangle \right\}$$

Tensor products can include some qubits in the computational basis, other qubits in the superposition basis and other qubits in Bell states. Notice that in the result the labels are not organized by qubit, they are organized by the type of state (Bell states, -, + or computational basis)

$$\begin{vmatrix} \mathbf{0}_{\hat{\mathbf{1}}} \rangle \cdot & | \mathbf{\mathcal{B}}_{11,\hat{\mathbf{2}},\hat{\mathbf{3}}} \rangle \cdot & | +_{\hat{\mathbf{4}}} \rangle \cdot & | \mathbf{0}_{\hat{\mathbf{5}}} \rangle \cdot & | \mathbf{\mathcal{B}}_{oo,\hat{\mathbf{6}},\hat{\mathbf{7}}} \rangle$$

$$\begin{vmatrix} \mathcal{B}_{oo,\hat{\mathbf{6}},\hat{\mathbf{7}}}, & \mathcal{B}_{11,\hat{\mathbf{2}},\hat{\mathbf{3}}}, & +_{\hat{\mathbf{4}}}, & \mathbf{0}_{\hat{\mathbf{1}}}, & \mathbf{0}_{\hat{\mathbf{5}}} \rangle \end{vmatrix}$$

The command QuantumEvaluate gives the representation of this ket in terms of the computational basis:

$$\begin{array}{l} \text{QuantumEvaluate} \Big[ \hspace{0.1cm} \big| \hspace{0.1cm} \mathcal{B}_{00,\hat{\mathbf{6}},\hat{\mathbf{7}}}, \hspace{0.1cm} \mathcal{B}_{11,\hat{\mathbf{2}},\hat{\mathbf{3}}}, \hspace{0.1cm} +_{\hat{\mathbf{4}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}} \hspace{0.1cm} \big) \Big] \\ \\ & \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{1}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{2}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{3}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{6}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{7}}} \big)}{2 \sqrt{2}} \hspace{0.1cm} + \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{1}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{2}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{3}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{6}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{7}}} \big)}{2 \sqrt{2}} \hspace{0.1cm} + \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{1}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{2}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{3}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{6}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{7}}} \big)}{2 \sqrt{2}} \hspace{0.1cm} + \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{1}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{6}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{7}}} \big)}{2 \sqrt{2}} \hspace{0.1cm} - \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{1}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{2}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{3}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{4}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{6}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{7}}} \big)}{2 \sqrt{2}} \hspace{0.1cm} - \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{1}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{6}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{7}}} \big)}{2 \sqrt{2}} \hspace{0.1cm} - \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{1}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{6}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{7}}} \big)}{2 \sqrt{2}} \hspace{0.1cm} - \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{1}}}, \hspace{0.1cm} \mathbf{1}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}} \big)}{2 \sqrt{2}} \hspace{0.1cm} - \hspace{0.1cm} \frac{ \hspace{0.1cm} \big| \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}, \hspace{0.1cm} \mathbf{0}_{\hat{\mathbf{5}}}$$

This is a factorized version of the same state. Notice that the result shows that qubits  $\hat{2}$  and  $\hat{3}$  are entangled, and qubits  $\hat{6}$  and  $\hat{7}$  are also entangled:

$$\begin{split} & \textbf{FactorKet} \big[ \textbf{QuantumEvaluate} \big[ \hspace{0.1cm} \Big| \hspace{0.1cm} \boldsymbol{\mathcal{B}}_{00,\,\hat{6},\,\hat{7}}, \hspace{0.1cm} \boldsymbol{\mathcal{B}}_{11,\,\hat{2},\,\hat{3}}, \hspace{0.1cm} +_{\hat{4}}, \hspace{0.1cm} \boldsymbol{0}_{\hat{5}} \big\rangle \big] \big] \\ & \\ & \text{Hold} \big[ \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{0}_{\hat{1}} \big\rangle \otimes \big( \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{1}_{\hat{2}} \big\rangle \otimes \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{0}_{\hat{3}} \big\rangle + \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{0}_{\hat{2}} \big\rangle \otimes - \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{1}_{\hat{3}} \big\rangle \big) \otimes \\ & \\ & \hspace{0.1cm} \big( \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{0}_{\hat{4}} \big\rangle + \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{1}_{\hat{4}} \big\rangle \big) \otimes \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{0}_{\hat{5}} \big\rangle \otimes - \hspace{0.1cm} \frac{\hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{0}_{\hat{6}} \big\rangle \otimes \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{1}_{\hat{6}} \big\rangle \otimes \hspace{0.1cm} \big| \hspace{0.1cm} \boldsymbol{1}_{\hat{7}} \big\rangle}{\hspace{0.1cm} 2 \hspace{0.1cm} \sqrt{2}} \big] \end{split}$$

Copy-paste the previous output without the Hold[] wrapper and the result is a expanded version:

$$\frac{\mid 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}}, 0_{\hat{5}}, 0_{\hat{6}}, 0_{\hat{7}}\rangle + \mid 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 0_{\hat{4}}, 0_{\hat{5}}, 1_{\hat{6}}, 1_{\hat{7}}\rangle}{2\sqrt{2}} + \frac{2\sqrt{2}}{2\sqrt{2}}$$

$$\frac{\mid 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}}, 0_{\hat{5}}, 0_{\hat{6}}, 0_{\hat{7}}\rangle + \mid 0_{\hat{1}}, 0_{\hat{2}}, 1_{\hat{3}}, 1_{\hat{4}}, 0_{\hat{5}}, 1_{\hat{6}}, 1_{\hat{7}}\rangle}{2\sqrt{2}} - \frac{\mid 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}}, 0_{\hat{5}}, 0_{\hat{6}}, 0_{\hat{7}}\rangle + \mid 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 0_{\hat{4}}, 0_{\hat{5}}, 1_{\hat{6}}, 1_{\hat{7}}\rangle}{2\sqrt{2}} - \frac{\mid 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}, 0_{\hat{5}}, 0_{\hat{6}}, 0_{\hat{7}}\rangle + \mid 0_{\hat{1}}, 1_{\hat{2}}, 0_{\hat{3}}, 1_{\hat{4}}, 0_{\hat{5}}, 1_{\hat{6}}, 1_{\hat{7}}\rangle}{2\sqrt{2}} - \frac{2\sqrt{2}}{2\sqrt{2}}$$

We can get a list of the factors, ready to be used with the standard *Mathematica* commands for list manipulation, like Part, Length, Select, Cases, GatherBy, etc.

```
\texttt{FactorKetList} \big[ \texttt{QuantumEvaluate} \big[ \ \big| \ \textit{$\mathcal{B}$}_{\textit{00},\,\hat{6},\,\hat{7}}, \ \textit{$\mathcal{B}$}_{\textit{11},\,\hat{2},\,\hat{3}}, \ \textit{$+_{\hat{4}}$}, \ \textit{$0$}_{\hat{1}}, \ \textit{$0$}_{\hat{5}} \big\rangle \big] \big]
 \left\{ | 0_{\hat{1}} \rangle, - | 0_{\hat{2}}, 1_{\hat{3}} \rangle + | 1_{\hat{2}}, 0_{\hat{3}} \rangle, | 0_{\hat{4}} \rangle + | 1_{\hat{4}} \rangle, | 0_{\hat{5}} \rangle, - \frac{| 0_{\hat{6}}, 0_{\hat{7}} \rangle}{| 0_{\hat{6}} \rangle | 0_{\hat{7}} \rangle} - \frac{| 1_{\hat{6}}, 1_{\hat{7}} \rangle}{| 0_{\hat{6}} \rangle | 0_{\hat{7}} \rangle} \right\}
```

Dirac notation can be used to create an operator that works on superposition kets

```
op2 = c0 \mid \mathcal{B}_{00,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{00,\hat{1},\hat{2}} \mid + c1 \mid \mathcal{B}_{10,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{10,\hat{1},\hat{2}} \mid +
     c2 \mid \mathcal{B}_{01,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{10,\hat{1},\hat{2}} \mid + c3 \mid \mathcal{B}_{11,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{11,\hat{1},\hat{2}} \mid
```

The operator created before can be applied to kets:

```
op2 · \left( \mid \mathcal{B}_{10,\hat{1},\hat{2}} \right) + \mid \mathcal{B}_{11,\hat{1},\hat{2}} \right)
c2 \left| \mathcal{B}_{01,\hat{1},\hat{2}} \right\rangle + c1 \left| \mathcal{B}_{10,\hat{1},\hat{2}} \right\rangle + c3 \left| \mathcal{B}_{11,\hat{1},\hat{2}} \right\rangle
```

### Use of Solve and QuantumReplace in order to change basis of Bell states

The standard Mathematica command Solve can be used to obtain the replacement rules to transform from the computational basis to Bell state basis

```
 \left\{ \begin{array}{l} \left\{ \begin{array}{l} \mathcal{B}_{oo,\hat{1},\hat{2}} \right\rangle == \text{QuantumEvaluate} \left[ \begin{array}{l} \mathcal{B}_{oo,\hat{1},\hat{2}} \right\rangle \right], \\ \left| \begin{array}{l} \mathcal{B}_{oi,\hat{1},\hat{2}} \right\rangle == \text{QuantumEvaluate} \left[ \begin{array}{l} \mathcal{B}_{oo,\hat{1},\hat{2}} \right\rangle \right], \\ \left| \begin{array}{l} \mathcal{B}_{10,\hat{1},\hat{2}} \right\rangle == \text{QuantumEvaluate} \left[ \begin{array}{l} \mathcal{B}_{10,\hat{1},\hat{2}} \right\rangle \right], \\ \left| \begin{array}{l} \mathcal{B}_{11,\hat{1},\hat{2}} \right\rangle == \text{QuantumEvaluate} \left[ \begin{array}{l} \mathcal{B}_{11,\hat{1},\hat{2}} \right\rangle \right], \\ \left| \begin{array}{l} \left| \begin{array}{l} 0_{\hat{1}}, \\ 0_{\hat{2}} \right\rangle, \\ \end{array} \right| \left| \begin{array}{l} 0_{\hat{1}}, \\ 0_{\hat{2}} \right\rangle, \\ \end{array} \right| \left| \begin{array}{l} 0_{\hat{1}}, \\ 1_{\hat{2}} \right\rangle, \\ \end{array} \right| \left| \begin{array}{l} 1_{\hat{1}}, \\ 1_{\hat{2}} \right\rangle, \\ \end{array} \right| \left| \begin{array}{l} 1_{\hat{1}}, \\ 1_{\hat{2}} \right\rangle, \\ \end{array} \right| \left| \begin{array}{l} 1_{\hat{1}}, \\ 1_{\hat{2}} \\ \end{array} \right| \left| \begin{array}{l} 1_{\hat{1}}, \\ \end{array} \right
```

$$\begin{split} \Big\{ \Big\{ & \mid \mathbf{1}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \big\rangle \rightarrow \frac{ \mid \mathcal{B}_{oo,\hat{1},\hat{2}} \big\rangle}{\sqrt{2}} - \frac{ \mid \mathcal{B}_{1o,\hat{1},\hat{2}} \big\rangle}{\sqrt{2}}, \quad \mid \mathbf{0}_{\hat{1}}, \ \mathbf{0}_{\hat{2}} \big\rangle \rightarrow \frac{ \mid \mathcal{B}_{oo,\hat{1},\hat{2}} \big\rangle}{\sqrt{2}} + \frac{ \mid \mathcal{B}_{1o,\hat{1},\hat{2}} \big\rangle}{\sqrt{2}}, \quad \mid \mathbf{0}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \big\rangle \rightarrow \\ & \frac{ \mid \mathcal{B}_{o1,\hat{1},\hat{2}} \big\rangle}{\sqrt{2}} + \frac{ \mid \mathcal{B}_{11,\hat{1},\hat{2}} \big\rangle}{\sqrt{2}}, \quad \mid \mathbf{1}_{\hat{1}}, \ \mathbf{0}_{\hat{2}} \big\rangle \rightarrow \frac{ \mid \mathcal{B}_{o1,\hat{1},\hat{2}} \big\rangle}{\sqrt{2}} - \frac{ \mid \mathcal{B}_{11,\hat{1},\hat{2}} \big\rangle}{\sqrt{2}} \Big\} \Big\} \end{split}$$

Copy the inner list of the previous output (without the outer curly braces \{\}) and paste it as the second argument of QuantumReplace in order to change an expression from the computational basis to Bell state basis. The first argument of QuantumReplace,  $|1_{\hat{1}}, 1_{\hat{2}}\rangle \cdot \langle 0_{\hat{1}}, 1_{\hat{2}}|$ , is the original expression that we want to express in another basis:

$$\begin{split} & \texttt{Expand} \Big[ \texttt{QuantumReplace} \Big[ \\ & \mid \mathbf{1}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \big\rangle \cdot \left\langle \mathbf{0}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \right|, \\ & \Big\{ \mid \mathbf{1}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \big\rangle \rightarrow \frac{\left| \ \mathcal{B}_{oo, \hat{1}, \hat{2}} \right\rangle}{\sqrt{2}} - \frac{\left| \ \mathcal{B}_{1o, \hat{1}, \hat{2}} \right\rangle}{\sqrt{2}}, \\ & \mid \mathbf{0}_{\hat{1}}, \ \mathbf{0}_{\hat{2}} \big\rangle \rightarrow \frac{\left| \ \mathcal{B}_{oo, \hat{1}, \hat{2}} \right\rangle}{\sqrt{2}} + \frac{\left| \ \mathcal{B}_{1o, \hat{1}, \hat{2}} \right\rangle}{\sqrt{2}}, \\ & \mid \mathbf{0}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \big\rangle \rightarrow \frac{\left| \ \mathcal{B}_{oi, \hat{1}, \hat{2}} \right\rangle}{\sqrt{2}} + \frac{\left| \ \mathcal{B}_{1i, \hat{1}, \hat{2}} \right\rangle}{\sqrt{2}}, \\ & \mid \mathbf{1}_{\hat{1}}, \ \mathbf{0}_{\hat{2}} \big\rangle \rightarrow \frac{\left| \ \mathcal{B}_{oi, \hat{1}, \hat{2}} \right\rangle}{\sqrt{2}} - \frac{\left| \ \mathcal{B}_{1i, \hat{1}, \hat{2}} \right\rangle}{\sqrt{2}} \Big\} \\ & \Big] \Big] \Big] \end{split}$$

$$\begin{array}{c|c} \frac{1}{2} & \mid \mathcal{B}_{oo,\hat{1},\hat{2}} \rangle \cdot \left\langle \mathcal{B}_{o1,\hat{1},\hat{2}} \mid -\frac{1}{2} \mid \mathcal{B}_{1o,\hat{1},\hat{2}} \right\rangle \cdot \left\langle \mathcal{B}_{o1,\hat{1},\hat{2}} \mid + \right. \\ \\ \frac{1}{2} & \mid \mathcal{B}_{oo,\hat{1},\hat{2}} \rangle \cdot \left\langle \mathcal{B}_{11,\hat{1},\hat{2}} \mid -\frac{1}{2} \mid \mathcal{B}_{1o,\hat{1},\hat{2}} \right\rangle \cdot \left\langle \mathcal{B}_{11,\hat{1},\hat{2}} \mid \right. \end{array}$$

Copy the result of the previous calculation and paste it as argument to QuantumEvaluate, in order to verify that we recover the original expression in the computational basis  $\mid 1_{\hat{1}}, 1_{\hat{2}} \rangle \cdot \langle 0_{\hat{1}}, 1_{\hat{2}} \mid$ :

$$\begin{aligned} & \text{QuantumEvaluate} \Big[ \frac{1}{2} \; \Big| \; \boldsymbol{\mathcal{B}}_{oo,\hat{1},\hat{2}} \Big\rangle \cdot \left\langle \boldsymbol{\mathcal{B}}_{o1,\hat{1},\hat{2}} \; \Big| \; - \\ & \frac{1}{2} \; \Big| \; \boldsymbol{\mathcal{B}}_{1o,\hat{1},\hat{2}} \Big\rangle \cdot \left\langle \boldsymbol{\mathcal{B}}_{o1,\hat{1},\hat{2}} \; \Big| \; + \; \frac{1}{2} \; \Big| \; \boldsymbol{\mathcal{B}}_{oo,\hat{1},\hat{2}} \Big\rangle \cdot \left\langle \boldsymbol{\mathcal{B}}_{11,\hat{1},\hat{2}} \; \Big| \; - \; \frac{1}{2} \; \Big| \; \boldsymbol{\mathcal{B}}_{1o,\hat{1},\hat{2}} \Big\rangle \cdot \left\langle \boldsymbol{\mathcal{B}}_{11,\hat{1},\hat{2}} \; \Big| \; \Big] \\ & \Big| \; \boldsymbol{1}_{\hat{1}}, \; \boldsymbol{1}_{\hat{2}} \Big\rangle \cdot \left\langle \boldsymbol{0}_{\hat{1}}, \; \boldsymbol{1}_{\hat{2}} \; \Big| \end{aligned}$$

QuantumEvaluate must be used in order to represent gates in the computational basis as operators in Dirac notation in the Bell state basis

$$\begin{split} & \text{Expand} \Big[ \text{QuantumReplace} \Big[ \\ & \text{QuantumEvaluate} \Big[ C^{(\hat{1})} \left[ \text{NOT}_{\hat{2}} \right] \Big], \\ & \Big\{ \mid \mathbf{1}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \Big\rangle \rightarrow \frac{ \mid \mathcal{B}_{oo, \hat{1}, \hat{2}} \Big\rangle }{\sqrt{2}} - \frac{ \mid \mathcal{B}_{1o, \hat{1}, \hat{2}} \Big\rangle }{\sqrt{2}}, \\ & \mid \mathbf{0}_{\hat{1}}, \ \mathbf{0}_{\hat{2}} \Big\rangle \rightarrow \frac{ \mid \mathcal{B}_{oo, \hat{1}, \hat{2}} \Big\rangle }{\sqrt{2}} + \frac{ \mid \mathcal{B}_{1o, \hat{1}, \hat{2}} \Big\rangle }{\sqrt{2}}, \\ & \mid \mathbf{0}_{\hat{1}}, \ \mathbf{1}_{\hat{2}} \Big\rangle \rightarrow \frac{ \mid \mathcal{B}_{ol, \hat{1}, \hat{2}} \Big\rangle }{\sqrt{2}} + \frac{ \mid \mathcal{B}_{1l, \hat{1}, \hat{2}} \Big\rangle }{\sqrt{2}}, \\ & \mid \mathbf{1}_{\hat{1}}, \ \mathbf{0}_{\hat{2}} \Big\rangle \rightarrow \frac{ \mid \mathcal{B}_{ol, \hat{1}, \hat{2}} \Big\rangle }{\sqrt{2}} - \frac{ \mid \mathcal{B}_{1l, \hat{1}, \hat{2}} \Big\rangle }{\sqrt{2}} \Big\} \\ & \Big\} \Big] \Big] \end{split}$$

$$\begin{vmatrix} \frac{1}{2} & | \mathcal{B}_{oo,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{oo,\hat{1},\hat{2}} & | + \frac{1}{2} & | \mathcal{B}_{o1,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{oo,\hat{1},\hat{2}} & | + \\ \frac{1}{2} & | \mathcal{B}_{10,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{oo,\hat{1},\hat{2}} & | - \frac{1}{2} & | \mathcal{B}_{11,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{oo,\hat{1},\hat{2}} & | + \\ \frac{1}{2} & | \mathcal{B}_{10,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{01,\hat{1},\hat{2}} & | + \frac{1}{2} & | \mathcal{B}_{01,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{01,\hat{1},\hat{2}} & | - \frac{1}{2} & | \mathcal{B}_{10,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{01,\hat{1},\hat{2}} & | + \\ \frac{1}{2} & | \mathcal{B}_{11,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{01,\hat{1},\hat{2}} & | + \frac{1}{2} & | \mathcal{B}_{00,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{10,\hat{1},\hat{2}} & | - \frac{1}{2} & | \mathcal{B}_{01,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{10,\hat{1},\hat{2}} & | + \\ \frac{1}{2} & | \mathcal{B}_{10,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{10,\hat{1},\hat{2}} & | + \frac{1}{2} & | \mathcal{B}_{11,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{10,\hat{1},\hat{2}} & | - \frac{1}{2} & | \mathcal{B}_{00,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{11,\hat{1},\hat{2}} & | + \\ \frac{1}{2} & | \mathcal{B}_{01,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{11,\hat{1},\hat{2}} & | + \frac{1}{2} & | \mathcal{B}_{11,\hat{1},\hat{2}} \rangle \cdot \langle \mathcal{B}_{11,\hat{1},\hat{2}} & | + \frac{1}{2} & | \mathcal{B}_{11,\hat{1},\hat{2}} & | + \frac{1}{2}$$

Copy the result of the previous calculation and paste it as argument to QuantumEvaluate, in order to verify that we recover the original expression in the computational basis:

$$\begin{aligned} & \text{QuantumEvaluate} \Big[ \frac{1}{2} \ \Big| \ \mathcal{B}_{oo,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{oo,\hat{1},\hat{2}} \ \Big| \ + \\ & \frac{1}{2} \ \Big| \ \mathcal{B}_{o1,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{oo,\hat{1},\hat{2}} \ \Big| \ + \frac{1}{2} \ \Big| \ \mathcal{B}_{1o,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{oo,\hat{1},\hat{2}} \ \Big| \ - \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{oo,\hat{1},\hat{2}} \ \Big| \ + \\ & \frac{1}{2} \ \Big| \ \mathcal{B}_{oo,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{o1,\hat{1},\hat{2}} \Big\rangle + \frac{1}{2} \ \Big| \ \mathcal{B}_{o1,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{o1,\hat{1},\hat{2}} \Big\rangle + \\ & \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{10,\hat{1},\hat{2}} \Big\rangle + \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{10,\hat{1},\hat{2}} \Big\rangle - \frac{1}{2} \ \Big| \ \mathcal{B}_{o0,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle + \\ & \frac{1}{2} \ \Big| \ \mathcal{B}_{01,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle + \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle + \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle + \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle \cdot \Big\langle \ \mathcal{B}_{11,\hat{1},\hat{2}} \Big\rangle + \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{1},\hat{2}} \Big\rangle + \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{1},\hat{1},\hat{1},\hat{1} \Big\rangle + \frac{1}{2} \ \Big| \ \mathcal{B}_{11,\hat{1},\hat{1},\hat{1$$

 $| 0_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 0_{\hat{1}}, 0_{\hat{2}} | + | 0_{\hat{1}}, 1_{\hat{2}} \rangle \cdot \langle 0_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 1_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 1_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}} | + | 1_{\hat{1}}, 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, 0_{\hat{2}$ 

Here we verify the answer was correct:

$${\tt QuantumEvaluate} \Big[ {\tt C}^{\{\hat{1}\}} \left[ {\tt NOT}_{\hat{2}} \right] \Big]$$

$$\mid 0_{\hat{1}}, \ 0_{\hat{2}} \rangle \cdot \langle 0_{\hat{1}}, \ 0_{\hat{2}} \mid + \ \mid 0_{\hat{1}}, \ 1_{\hat{2}} \rangle \cdot \langle 0_{\hat{1}}, \ 1_{\hat{2}} \mid + \ \mid 1_{\hat{1}}, \ 1_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, \ 0_{\hat{2}} \mid + \ \mid 1_{\hat{1}}, \ 0_{\hat{2}} \rangle \cdot \langle 1_{\hat{1}}, \ 1_{\hat{2}} \mid$$

## Warning: QuantumReplace is Not Forced to Obey Algebraic Rules

QuantumReplace is not an algebraic command. It does not check if the replacement gives a new expression that is equivalent to the new one. This behavior is inherited from the standard Mathematica commands Replace and ReplaceAll. The replacement is structural, it is not algebraic, therefore, in other uses of QuantumReplace, the result might be different and not equivalent to the input (in the examples of this document all the results are algebraically correct, but Mathematica does not check if this is the case).

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