Operator Diagonalization, Partial Trace and Partial Transpose

by José Luis Gómez-Muñoz
http://homepage.cem.itesm.mx/lgomez/quantum/
jose.luis.gomez@itesm.mx
This document is based on suggestions by Anirban Das

Introduction

This is a tutorial on the use of Quantum *Mathematica* add-on to calculate partial traces and partial transposes of operators in Dirac Notation

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[];
```

Operator Diagonalization

QuantumEigensystem gives a list of eigenvalues and eigenvectors of an operator, in the same format as the standard *Mathematica* command Eigensystem:

```
QuantumEigensystem[C^{1̂}[NOT_2̂]]
```

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

QuantumEigensystemForm gives a nicer formating:

```
QuantumEigensystemForm[C^{1̂}[NOT_2̂]]
```

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

TraditionalForm gives a format closer to the format used in papers:

```
TraditionalForm[QuantumEigensystemForm[C^{1̂}[NOT_2̂]]]
```

Eigenvalue	Eigenvector
−1	$\frac{\lvert 11\rangle}{\sqrt{2}} - \frac{\lvert 10\rangle}{\sqrt{2}}$
1	$\frac{\lvert 10\rangle}{\sqrt{2}} + \frac{\lvert 11\rangle}{\sqrt{2}}$
1	$\lvert 01\rangle$
1	$\lvert 00\rangle$

One simple way to force numerical evaluation is to multiply the operator times 1.0 (with a decimal point!)

```
TraditionalForm[QuantumEigensystemForm[1.0 * C^{1̂}[NOT_2̂]]]
```

Eigenvalue	Eigenvector
1.	$1.\ \lvert 01\rangle$
1.	$1.\ \lvert 00\rangle$
1.	$0.707107\ \lvert 10\rangle + 0.707107\ \lvert 11\rangle$
−1.	$0.707107\ \lvert 10\rangle - 0.707107\ \lvert 11\rangle$

A more interesting example:

```
TraditionalForm[QuantumEigensystemForm[C^{1̂}[NOT_2̂] · H_1̂]]
```

Eigenvalue	Eigenvector
-1	$\left(\frac{1}{2\sqrt{2-\sqrt{2}}}-\frac{1}{\sqrt{2\left(2-\sqrt{2}\right)}}\right)\mid 00\rangle+\left(\frac{1}{2\sqrt{2-\sqrt{2}}}-\frac{1}{\sqrt{2\left(2-\sqrt{2}\right)}}\right)\mid 01\rangle+\frac{\mid 10\rangle}{2\sqrt{2-\sqrt{2}}}+\frac{\mid 11\rangle}{2\sqrt{2-\sqrt{2}}}$
1	$\left(\frac{1}{2\sqrt{2+\sqrt{2}}}+\frac{1}{\sqrt{2\left(2+\sqrt{2}\right)}}\right)\mid 00\rangle+\left(\frac{1}{2\sqrt{2+\sqrt{2}}}+\frac{1}{\sqrt{2\left(2+\sqrt{2}\right)}}\right)\mid 01\rangle+\frac{\mid 10\rangle}{2\sqrt{2+\sqrt{2}}}+\frac{\mid 11\rangle}{2\sqrt{2+\sqrt{2}}}$
$\frac{1+i}{\sqrt{2}}$	$\frac{1}{2}\,i\mid 00\rangle-\frac{1}{2}\,i\mid 01\rangle-\frac{1}{2}\mid 10\rangle+\frac{1}{2}\mid 11\rangle$
$\frac{1-i}{\sqrt{2}}$	$-\frac{1}{2}\,i\mid 00\rangle+\frac{1}{2}\,i\mid 01\rangle-\frac{1}{2}\mid 10\rangle+\frac{1}{2}\mid 11\rangle$

One simple way to force numerical evaluation is to multiply the operator times 1.0 (with a decimal point!)

```
TraditionalForm[QuantumEigensystemForm[1.0 * C^{1̂}[NOT_2̂] · H_1̂]]
```

Eigenvalue	Eigenvector
$-1.$	$0.270598\mid 00\rangle+0.270598\mid 01\rangle-0.653281\mid 10\rangle-0.653281\mid 11\rangle$
$0.707107+0.707107\,i$	$-0.5\,i\mid 00\rangle+0.5\,i\mid 01\rangle+0.5\mid 10\rangle-0.5\mid 11\rangle$
$0.707107-0.707107\,i$	$0.5\,i\mid 00\rangle-0.5\,i\mid 01\rangle+0.5\mid 10\rangle-0.5\mid 11\rangle$
$1.$	$-0.653281\mid 00\rangle-0.653281\mid 01\rangle-0.270598\mid 10\rangle-0.270598\mid 11\rangle$

Here we obtain only the first eigenvalue, together with its eigenvector:

```
QuantumEigensystem[1.0 * C^{1̂}[NOT_2̂] · H_1̂, 1]
```

$\{\{-1.\},\ \{0.270598\ \mid 0_{\hat{1}},\,0_{\hat{2}}\rangle+0.270598\ \mid 0_{\hat{1}},\,1_{\hat{2}}\rangle-0.653281\ \mid 1_{\hat{1}},\,0_{\hat{2}}\rangle-0.653281\ \mid 1_{\hat{1}},\,1_{\hat{2}}\rangle\}\}$

Here we obtain only the last eigenvalue, together with its eigenvector:

```
QuantumEigensystem[1.0 * C^{1̂}[NOT_2̂] · H_1̂, -1]
```

$\{\{1.\},\ \{-0.653281\ \mid 0_{\hat{1}},\,0_{\hat{2}}\rangle-0.653281\ \mid 0_{\hat{1}},\,1_{\hat{2}}\rangle-0.270598\ \mid 1_{\hat{1}},\,0_{\hat{2}}\rangle-0.270598\ \mid 1_{\hat{1}},\,1_{\hat{2}}\rangle\}\}$

Here we extract the eigenvector corresponding to the last eigenvalue using standard *Mathematica* notation to access elements of lists:

```
QuantumEigensystem[1.0 * C^{1̂}[NOT_2̂] · H_1̂, -1][[2, 1]]
```

$-0.653281\ \mid 0_{\hat{1}},\,0_{\hat{2}}\rangle-0.653281\ \mid 0_{\hat{1}},\,1_{\hat{2}}\rangle-0.270598\ \mid 1_{\hat{1}},\,0_{\hat{2}}\rangle-0.270598\ \mid 1_{\hat{1}},\,1_{\hat{2}}\rangle$

You can use the operator in Dirac bra-ket notation:

```
TraditionalForm[QuantumEigensystemForm[ⅈ |0₁̂, 1₂̂⟩ · ⟨0₁̂, 0₂̂| +
    ⅈ |1₁̂, 1₂̂⟩ · ⟨0₁̂, 1₂̂| - ⅈ |0₁̂, 0₂̂⟩ · ⟨1₁̂, 0₂̂| - ⅈ |1₁̂, 0₂̂⟩ · ⟨1₁̂, 1₂̂|]]
```

Eigenvalue	Eigenvector
-1	$-\frac{1}{2}\,\vert 00\rangle+\frac{1}{2}\,i\,\vert 01\rangle+\frac{1}{2}\,i\,\vert 10\rangle+\frac{1}{2}\,\vert 11\rangle$
i	$\frac{1}{2}\,\vert 00\rangle+\frac{1}{2}\,\vert 01\rangle-\frac{1}{2}\,\vert 10\rangle+\frac{1}{2}\,\vert 11\rangle$
$-i$	$\frac{1}{2}\,\vert 00\rangle-\frac{1}{2}\,\vert 01\rangle+\frac{1}{2}\,\vert 10\rangle+\frac{1}{2}\,\vert 11\rangle$
1	$-\frac{1}{2}\,\vert 00\rangle-\frac{1}{2}\,i\,\vert 01\rangle-\frac{1}{2}\,i\,\vert 10\rangle+\frac{1}{2}\,\vert 11\rangle$

Partial Traces

Here we define a ket as a linear combination of two qubits:

```
|ψ⟩ = α |0₁̂, 0₂̂⟩ + β |0₁̂, 1₂̂⟩ + γ |1₁̂, 0₂̂⟩ + δ |1₁̂, 1₂̂⟩
```

$$\alpha\,\lvert 0_{\hat 1},0_{\hat 2}\rangle+\beta\,\lvert 0_{\hat 1},1_{\hat 2}\rangle+\gamma\,\lvert 1_{\hat 1},0_{\hat 2}\rangle+\delta\,\lvert 1_{\hat 1},1_{\hat 2}\rangle$$

An operator can be obtained from the external product of the ket with its corresponding dual:

```
mydensityop = Expand[ |ψ⟩ · ⟨ψ| ]
```

$$\begin{aligned}&\alpha\alpha^*\,\lvert 0_{\hat 1},0_{\hat 2}\rangle\cdot\langle 0_{\hat 1},0_{\hat 2}\rvert+\beta\alpha^*\,\lvert 0_{\hat 1},1_{\hat 2}\rangle\cdot\langle 0_{\hat 1},0_{\hat 2}\rvert+\\&\gamma\alpha^*\,\lvert 1_{\hat 1},0_{\hat 2}\rangle\cdot\langle 0_{\hat 1},0_{\hat 2}\rvert+\delta\alpha^*\,\lvert 1_{\hat 1},1_{\hat 2}\rangle\cdot\langle 0_{\hat 1},0_{\hat 2}\rvert+\\&\alpha\beta^*\,\lvert 0_{\hat 1},0_{\hat 2}\rangle\cdot\langle 0_{\hat 1},1_{\hat 2}\rvert+\beta\beta^*\,\lvert 0_{\hat 1},1_{\hat 2}\rangle\cdot\langle 0_{\hat 1},1_{\hat 2}\rvert+\gamma\beta^*\,\lvert 1_{\hat 1},0_{\hat 2}\rangle\cdot\langle 0_{\hat 1},1_{\hat 2}\rvert+\\&\delta\beta^*\,\lvert 1_{\hat 1},1_{\hat 2}\rangle\cdot\langle 0_{\hat 1},1_{\hat 2}\rvert+\alpha\gamma^*\,\lvert 0_{\hat 1},0_{\hat 2}\rangle\cdot\langle 1_{\hat 1},0_{\hat 2}\rvert+\beta\gamma^*\,\lvert 0_{\hat 1},1_{\hat 2}\rangle\cdot\langle 1_{\hat 1},0_{\hat 2}\rvert+\\&\gamma\gamma^*\,\lvert 1_{\hat 1},0_{\hat 2}\rangle\cdot\langle 1_{\hat 1},0_{\hat 2}\rvert+\delta\gamma^*\,\lvert 1_{\hat 1},1_{\hat 2}\rangle\cdot\langle 1_{\hat 1},0_{\hat 2}\rvert+\alpha\delta^*\,\lvert 0_{\hat 1},0_{\hat 2}\rangle\cdot\langle 1_{\hat 1},1_{\hat 2}\rvert+\\&\beta\delta^*\,\lvert 0_{\hat 1},1_{\hat 2}\rangle\cdot\langle 1_{\hat 1},1_{\hat 2}\rvert+\gamma\delta^*\,\lvert 1_{\hat 1},0_{\hat 2}\rangle\cdot\langle 1_{\hat 1},1_{\hat 2}\rvert+\delta\delta^*\,\lvert 1_{\hat 1},1_{\hat 2}\rangle\cdot\langle 1_{\hat 1},1_{\hat 2}\rvert\end{aligned}$$

TraditionalForm gives a format closer to the format used in papers and textbooks:

```
TraditionalForm[mydensityop]
```

$$\begin{aligned}&\beta\alpha^*\,\lvert 01\rangle\langle 00\rvert+\alpha\beta^*\,\lvert 00\rangle\langle 01\rvert+\gamma\alpha^*\,\lvert 10\rangle\langle 00\rvert+\alpha\gamma^*\,\lvert 00\rangle\langle 10\rvert+\delta\alpha^*\,\lvert 11\rangle\langle 00\rvert+\\&\alpha\delta^*\,\lvert 00\rangle\langle 11\rvert+\alpha\alpha^*\,\lvert 00\rangle\langle 00\rvert+\gamma\beta^*\,\lvert 10\rangle\langle 01\rvert+\beta\gamma^*\,\lvert 01\rangle\langle 10\rvert+\delta\beta^*\,\lvert 11\rangle\langle 01\rvert+\\&\beta\delta^*\,\lvert 01\rangle\langle 11\rvert+\beta\beta^*\,\lvert 01\rangle\langle 01\rvert+\delta\gamma^*\,\lvert 11\rangle\langle 10\rvert+\gamma\delta^*\,\lvert 10\rangle\langle 11\rvert+\gamma\gamma^*\,\lvert 10\rangle\langle 10\rvert+\delta\delta^*\,\lvert 11\rangle\langle 11\rvert\end{aligned}$$

Here is the partial trace of the operator, with respect to qubit $\hat{1}$

```
mypartialtrace1 = QuantumPartialTrace[mydensityop, 1̂]
```

$$\begin{aligned}&\alpha\alpha^*\,\lvert 0_{\hat 2}\rangle\cdot\langle 0_{\hat 2}\rvert+\gamma\gamma^*\,\lvert 0_{\hat 2}\rangle\cdot\langle 0_{\hat 2}\rvert+\beta\alpha^*\,\lvert 1_{\hat 2}\rangle\cdot\langle 0_{\hat 2}\rvert+\delta\gamma^*\,\lvert 1_{\hat 2}\rangle\cdot\langle 0_{\hat 2}\rvert+\\&\alpha\beta^*\,\lvert 0_{\hat 2}\rangle\cdot\langle 1_{\hat 2}\rvert+\gamma\delta^*\,\lvert 0_{\hat 2}\rangle\cdot\langle 1_{\hat 2}\rvert+\beta\beta^*\,\lvert 1_{\hat 2}\rangle\cdot\langle 1_{\hat 2}\rvert+\delta\delta^*\,\lvert 1_{\hat 2}\rangle\cdot\langle 1_{\hat 2}\rvert\end{aligned}$$

Here is the partial trace of the operator, with respect to qubit $\hat{2}$

```
mypartialtrace2 = QuantumPartialTrace[mydensityop, 2̂]
```

$$\alpha\,\alpha^{*}\ \vert 0_{\hat{1}}\rangle\cdot\langle 0_{\hat{1}}\vert + \beta\,\beta^{*}\ \vert 0_{\hat{1}}\rangle\cdot\langle 0_{\hat{1}}\vert + \gamma\,\alpha^{*}\ \vert 1_{\hat{1}}\rangle\cdot\langle 0_{\hat{1}}\vert + \delta\,\beta^{*}\ \vert 1_{\hat{1}}\rangle\cdot\langle 0_{\hat{1}}\vert + \alpha\,\gamma^{*}\ \vert 0_{\hat{1}}\rangle\cdot\langle 1_{\hat{1}}\vert + \beta\,\delta^{*}\ \vert 0_{\hat{1}}\rangle\cdot\langle 1_{\hat{1}}\vert + \gamma\,\gamma^{*}\ \vert 1_{\hat{1}}\rangle\cdot\langle 1_{\hat{1}}\vert + \delta\,\delta^{*}\ \vert 1_{\hat{1}}\rangle\cdot\langle 1_{\hat{1}}\vert$$

Here is the trace of the operator. It is stored in the variable **mytrace**, in order to use it later in this document:

```
mytrace = QuantumPartialTrace[mydensityop, {1̂, 2̂}]
```

$$\alpha\,\alpha^{*} + \beta\,\beta^{*} + \gamma\,\gamma^{*} + \delta\,\delta^{*}$$

Partial Transposes

Here is the partial transpose of the operator defined above, with respect to qubit $\hat{1}$. Partial Transpose is used as a witness of entanglement in Quantum Computing.

```
mypartialtranspose1 = QuantumPartialTranspose[mydensityop, 1̂]
```

$$\begin{aligned}
&\alpha\,\alpha^{*}\ \vert 0_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 0_{\hat{2}}\vert + \beta\,\alpha^{*}\ \vert 0_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 0_{\hat{2}}\vert +\\
&\alpha\,\gamma^{*}\ \vert 1_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 0_{\hat{2}}\vert + \beta\,\gamma^{*}\ \vert 1_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 0_{\hat{2}}\vert +\\
&\alpha\,\beta^{*}\ \vert 0_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 1_{\hat{2}}\vert + \beta\,\beta^{*}\ \vert 0_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 1_{\hat{2}}\vert + \alpha\,\delta^{*}\ \vert 1_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 1_{\hat{2}}\vert +\\
&\beta\,\delta^{*}\ \vert 1_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 1_{\hat{2}}\vert + \gamma\,\alpha^{*}\ \vert 0_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 0_{\hat{2}}\vert + \delta\,\alpha^{*}\ \vert 0_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 0_{\hat{2}}\vert +\\
&\gamma\,\gamma^{*}\ \vert 1_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 0_{\hat{2}}\vert + \delta\,\gamma^{*}\ \vert 1_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 0_{\hat{2}}\vert + \gamma\,\beta^{*}\ \vert 0_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 1_{\hat{2}}\vert +\\
&\delta\,\beta^{*}\ \vert 0_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 1_{\hat{2}}\vert + \gamma\,\delta^{*}\ \vert 1_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 1_{\hat{2}}\vert + \delta\,\delta^{*}\ \vert 1_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 1_{\hat{2}}\vert
\end{aligned}$$

Here is the partial transpose of the operator, with respect to the qubit $\hat{2}$. Partial Transpose is used as a witness of entanglement in Quantum Computing.

```
mypartialtranspose2 = QuantumPartialTranspose[mydensityop, 2̂]
```

$$\begin{aligned}
&\alpha\,\alpha^{*}\ \vert 0_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 0_{\hat{2}}\vert + \alpha\,\beta^{*}\ \vert 0_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 0_{\hat{2}}\vert +\\
&\gamma\,\alpha^{*}\ \vert 1_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 0_{\hat{2}}\vert + \gamma\,\beta^{*}\ \vert 1_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 0_{\hat{2}}\vert +\\
&\beta\,\alpha^{*}\ \vert 0_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 1_{\hat{2}}\vert + \beta\,\beta^{*}\ \vert 0_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 1_{\hat{2}}\vert + \delta\,\alpha^{*}\ \vert 1_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 1_{\hat{2}}\vert +\\
&\delta\,\beta^{*}\ \vert 1_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}}, 1_{\hat{2}}\vert + \alpha\,\gamma^{*}\ \vert 0_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 0_{\hat{2}}\vert + \alpha\,\delta^{*}\ \vert 0_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 0_{\hat{2}}\vert +\\
&\gamma\,\gamma^{*}\ \vert 1_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 0_{\hat{2}}\vert + \gamma\,\delta^{*}\ \vert 1_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 0_{\hat{2}}\vert + \beta\,\gamma^{*}\ \vert 0_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 1_{\hat{2}}\vert +\\
&\beta\,\delta^{*}\ \vert 0_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 1_{\hat{2}}\vert + \delta\,\gamma^{*}\ \vert 1_{\hat{1}}, 0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 1_{\hat{2}}\vert + \delta\,\delta^{*}\ \vert 1_{\hat{1}}, 1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}}, 1_{\hat{2}}\vert
\end{aligned}$$

Here is the transpose of the operator. Notice that it is stored in the variable "mytranspose", so that we can use it later in this document:

```
mytranspose = QuantumPartialTranspose[mydensityop, {1̂, 2̂}]
```

$\alpha\,\alpha^{*}\ |0_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},0_{\hat{2}}| + \alpha\,\beta^{*}\ |0_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},0_{\hat{2}}| +$
$\alpha\,\gamma^{*}\ |1_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},0_{\hat{2}}| + \alpha\,\delta^{*}\ |1_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},0_{\hat{2}}| +$
$\beta\,\alpha^{*}\ |0_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},1_{\hat{2}}| + \beta\,\beta^{*}\ |0_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},1_{\hat{2}}| + \beta\,\gamma^{*}\ |1_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},1_{\hat{2}}| +$
$\beta\,\delta^{*}\ |1_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},1_{\hat{2}}| + \gamma\,\alpha^{*}\ |0_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},0_{\hat{2}}| + \gamma\,\beta^{*}\ |0_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},0_{\hat{2}}| +$
$\gamma\,\gamma^{*}\ |1_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},0_{\hat{2}}| + \gamma\,\delta^{*}\ |1_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},0_{\hat{2}}| + \delta\,\alpha^{*}\ |0_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},1_{\hat{2}}| +$
$\delta\,\beta^{*}\ |0_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},1_{\hat{2}}| + \delta\,\gamma^{*}\ |1_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},1_{\hat{2}}| + \delta\,\delta^{*}\ |1_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},1_{\hat{2}}|$

Verifying traces and transposes with Matrix Notation

We can transform the operator, which was defined above, from Dirac Notation to standard *Mathematica* Matrix Notation (list of lists). Therefore, we can take advantage of the built-in *Mathematica* commands for matrices:

```
mymatrix = QuantumMatrix[mydensityop]
```

$\{\{\alpha\,\alpha^{*}, \alpha\,\beta^{*}, \alpha\,\gamma^{*}, \alpha\,\delta^{*}\}, \{\beta\,\alpha^{*}, \beta\,\beta^{*}, \beta\,\gamma^{*}, \beta\,\delta^{*}\},$
$\{\gamma\,\alpha^{*}, \gamma\,\beta^{*}, \gamma\,\gamma^{*}, \gamma\,\delta^{*}\}, \{\delta\,\alpha^{*}, \delta\,\beta^{*}, \delta\,\gamma^{*}, \delta\,\delta^{*}\}\}$

Here we can visualizar the Matrix in a textbook-like format:

```
MatrixForm[mymatrix]
```

$$\begin{pmatrix} \alpha\,\alpha^{*} & \alpha\,\beta^{*} & \alpha\,\gamma^{*} & \alpha\,\delta^{*} \\ \beta\,\alpha^{*} & \beta\,\beta^{*} & \beta\,\gamma^{*} & \beta\,\delta^{*} \\ \gamma\,\alpha^{*} & \gamma\,\beta^{*} & \gamma\,\gamma^{*} & \gamma\,\delta^{*} \\ \delta\,\alpha^{*} & \delta\,\beta^{*} & \delta\,\gamma^{*} & \delta\,\delta^{*} \end{pmatrix}$$

This is the trace of the matrix. We store the result in the variable matrixtrace

```
matrixtrace = Tr[mymatrix]
```

$\alpha\,\alpha^{*} + \beta\,\beta^{*} + \gamma\,\gamma^{*} + \delta\,\delta^{*}$

The trace "matrixtrace" was obtained by transforming the original Dirac expression to a Matrix, then calculating the trace of the matrix. On the other hand, the trace "mytrace" was obtained by direct application of the command QuantumPartialTrace to the original Dirac expression.
As expected, both "matrixtrace" and "mytrace" are the same (notice the use of two equal symbols == in order to make the comparison)

```
matrixtrace == mytrace
```

```
True
```

This is the transpose of the matrix:

```
matrixtranspose = Transpose[mymatrix]
```

$\{\{\alpha\,\alpha^*, \beta\,\alpha^*, \gamma\,\alpha^*, \delta\,\alpha^*\}, \{\alpha\,\beta^*, \beta\,\beta^*, \gamma\,\beta^*, \delta\,\beta^*\}, \{\alpha\,\gamma^*, \beta\,\gamma^*, \gamma\,\gamma^*, \delta\,\gamma^*\}, \{\alpha\,\delta^*, \beta\,\delta^*, \gamma\,\delta^*, \delta\,\delta^*\}\}$

The transpose is transformed to Dirac notation

```
secondtranspose = MatrixQuantum[matrixtranspose]
```

$$\begin{aligned}
&\alpha\,\alpha^* \left|0_{\hat{1}}, 0_{\hat{2}}\right\rangle\cdot\left\langle 0_{\hat{1}}, 0_{\hat{2}}\right| + \alpha\,\beta^* \left|0_{\hat{1}}, 1_{\hat{2}}\right\rangle\cdot\left\langle 0_{\hat{1}}, 0_{\hat{2}}\right| + \\
&\alpha\,\gamma^* \left|1_{\hat{1}}, 0_{\hat{2}}\right\rangle\cdot\left\langle 0_{\hat{1}}, 0_{\hat{2}}\right| + \alpha\,\delta^* \left|1_{\hat{1}}, 1_{\hat{2}}\right\rangle\cdot\left\langle 0_{\hat{1}}, 0_{\hat{2}}\right| + \\
&\beta\,\alpha^* \left|0_{\hat{1}}, 0_{\hat{2}}\right\rangle\cdot\left\langle 0_{\hat{1}}, 1_{\hat{2}}\right| + \beta\,\beta^* \left|0_{\hat{1}}, 1_{\hat{2}}\right\rangle\cdot\left\langle 0_{\hat{1}}, 1_{\hat{2}}\right| + \beta\,\gamma^* \left|1_{\hat{1}}, 0_{\hat{2}}\right\rangle\cdot\left\langle 0_{\hat{1}}, 1_{\hat{2}}\right| + \\
&\beta\,\delta^* \left|1_{\hat{1}}, 1_{\hat{2}}\right\rangle\cdot\left\langle 0_{\hat{1}}, 1_{\hat{2}}\right| + \gamma\,\alpha^* \left|0_{\hat{1}}, 0_{\hat{2}}\right\rangle\cdot\left\langle 1_{\hat{1}}, 0_{\hat{2}}\right| + \gamma\,\beta^* \left|0_{\hat{1}}, 1_{\hat{2}}\right\rangle\cdot\left\langle 1_{\hat{1}}, 0_{\hat{2}}\right| + \\
&\gamma\,\gamma^* \left|1_{\hat{1}}, 0_{\hat{2}}\right\rangle\cdot\left\langle 1_{\hat{1}}, 0_{\hat{2}}\right| + \gamma\,\delta^* \left|1_{\hat{1}}, 1_{\hat{2}}\right\rangle\cdot\left\langle 1_{\hat{1}}, 0_{\hat{2}}\right| + \delta\,\alpha^* \left|0_{\hat{1}}, 0_{\hat{2}}\right\rangle\cdot\left\langle 1_{\hat{1}}, 1_{\hat{2}}\right| + \\
&\delta\,\beta^* \left|0_{\hat{1}}, 1_{\hat{2}}\right\rangle\cdot\left\langle 1_{\hat{1}}, 1_{\hat{2}}\right| + \delta\,\gamma^* \left|1_{\hat{1}}, 0_{\hat{2}}\right\rangle\cdot\left\langle 1_{\hat{1}}, 1_{\hat{2}}\right| + \delta\,\delta^* \left|1_{\hat{1}}, 1_{\hat{2}}\right\rangle\cdot\left\langle 1_{\hat{1}}, 1_{\hat{2}}\right|
\end{aligned}$$

The operator "secondtranspose" was obtained by transforming the original Dirac expression to a Matrix, then calculating the transpose of the matrix, and finally transforming back to Dirac notation.
On the other hand, the operartor "mytranspose" was obtained by direct application of the command QuantumPartialTranspose to the original Dirac expression.
As expected, both "secondtranspose" and "mytranspose" are the same:

```
secondtranspose == mytranspose
```

```
True
```

by José Luis Gómez-Muñoz
http://homepage.cem.itesm.mx/lgomez/quantum/
jose.luis.gomez@itesm.mx