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# Partial Trace and Partial Transpose

by José Luis Gómez-Muñoz

<http://homepage.cem.itesm.mx/lgomez/quantum/>

[jose.luis.gomez@itesm.mx](mailto:jose.luis.gomez@itesm.mx)

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## 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

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## Load the Package

First load the Quantum`Notation` package. Write:

`Needs["Quantum`Notation`"]`

then press at the same time the keys `SHIFT-ENTER` to evaluate. *Mathematica* will load the package:

```
Needs["Quantum`Notation`"]
```

```
Quantum`Notation` Version 2.2.0. (July 2010)
A Mathematica package for Quantum calculations in Dirac bra-ket notation
by José Luis Gómez-Muñoz
```

```
Execute SetQuantumAliases[] in order to use
the keyboard to enter quantum objects in Dirac's notation
SetQuantumAliases[] must be executed again in each new
notebook that is created, only one time per notebook.
```

In order to use the keyboard to enter quantum objects write:

`SetQuantumAliases[];`

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

```
SetQuantumAliases[];
```

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## Partial Traces

Here we define a ket as a linear combination of eigenkets of two base operators. The base operators are named  $\hat{1}$  and  $\hat{2}$ .

$$|\psi\rangle = \alpha |0_1, 0_2\rangle + \beta |0_1, 1_2\rangle + \gamma |1_1, 0_2\rangle + \delta |1_1, 1_2\rangle$$

$$\alpha |0_1, 0_2\rangle + \beta |0_1, 1_2\rangle + \gamma |1_1, 0_2\rangle + \delta |1_1, 1_2\rangle$$

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

```
mydensityop = Expand[ |  $\psi$   $\rangle \cdot \langle \psi$  | ]
```

$$\begin{aligned} & \alpha \alpha^* | 0_1, 0_2 \rangle \cdot \langle 0_1, 0_2 | + \beta \alpha^* | 0_1, 1_2 \rangle \cdot \langle 0_1, 0_2 | + \\ & \gamma \alpha^* | 1_1, 0_2 \rangle \cdot \langle 0_1, 0_2 | + \delta \alpha^* | 1_1, 1_2 \rangle \cdot \langle 0_1, 0_2 | + \\ & \alpha \beta^* | 0_1, 0_2 \rangle \cdot \langle 0_1, 1_2 | + \beta \beta^* | 0_1, 1_2 \rangle \cdot \langle 0_1, 1_2 | + \gamma \beta^* | 1_1, 0_2 \rangle \cdot \langle 0_1, 1_2 | + \\ & \delta \beta^* | 1_1, 1_2 \rangle \cdot \langle 0_1, 1_2 | + \alpha \gamma^* | 0_1, 0_2 \rangle \cdot \langle 1_1, 0_2 | + \beta \gamma^* | 0_1, 1_2 \rangle \cdot \langle 1_1, 0_2 | + \\ & \gamma \gamma^* | 1_1, 0_2 \rangle \cdot \langle 1_1, 0_2 | + \delta \gamma^* | 1_1, 1_2 \rangle \cdot \langle 1_1, 0_2 | + \alpha \delta^* | 0_1, 0_2 \rangle \cdot \langle 1_1, 1_2 | + \\ & \beta \delta^* | 0_1, 1_2 \rangle \cdot \langle 1_1, 1_2 | + \gamma \delta^* | 1_1, 0_2 \rangle \cdot \langle 1_1, 1_2 | + \delta \delta^* | 1_1, 1_2 \rangle \cdot \langle 1_1, 1_2 | \end{aligned}$$

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

```
mypartialtrace1 = QuantumPartialTrace[mydensityop,  $\hat{1}$ ]
```

$$\begin{aligned} & \alpha \alpha^* | 0_2 \rangle \cdot \langle 0_2 | + \gamma \gamma^* | 0_2 \rangle \cdot \langle 0_2 | + \beta \alpha^* | 1_2 \rangle \cdot \langle 0_2 | + \delta \gamma^* | 1_2 \rangle \cdot \langle 0_2 | + \\ & \alpha \beta^* | 0_2 \rangle \cdot \langle 1_2 | + \gamma \delta^* | 0_2 \rangle \cdot \langle 1_2 | + \beta \beta^* | 1_2 \rangle \cdot \langle 1_2 | + \delta \delta^* | 1_2 \rangle \cdot \langle 1_2 | \end{aligned}$$

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

```
mypartialtrace2 = QuantumPartialTrace[mydensityop,  $\hat{2}$ ]
```

$$\begin{aligned} & \alpha \alpha^* | 0_1 \rangle \cdot \langle 0_1 | + \beta \beta^* | 0_1 \rangle \cdot \langle 0_1 | + \gamma \alpha^* | 1_1 \rangle \cdot \langle 0_1 | + \delta \beta^* | 1_1 \rangle \cdot \langle 0_1 | + \\ & \alpha \gamma^* | 0_1 \rangle \cdot \langle 1_1 | + \beta \delta^* | 0_1 \rangle \cdot \langle 1_1 | + \gamma \gamma^* | 1_1 \rangle \cdot \langle 1_1 | + \delta \delta^* | 1_1 \rangle \cdot \langle 1_1 | \end{aligned}$$

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, { $\hat{1}$ ,  $\hat{2}$ }]
```

$$\alpha \alpha^* + \beta \beta^* + \gamma \gamma^* + \delta \delta^*$$

## Partial Transposes

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

```
mypartialtranspose1 = QuantumPartialTranspose[mydensityop,  $\hat{1}$ ]
```

$$\begin{aligned} & \alpha \alpha^* | 0_1, 0_2 \rangle \cdot \langle 0_1, 0_2 | + \beta \alpha^* | 0_1, 1_2 \rangle \cdot \langle 0_1, 0_2 | + \\ & \alpha \gamma^* | 1_1, 0_2 \rangle \cdot \langle 0_1, 0_2 | + \beta \gamma^* | 1_1, 1_2 \rangle \cdot \langle 0_1, 0_2 | + \\ & \alpha \beta^* | 0_1, 0_2 \rangle \cdot \langle 0_1, 1_2 | + \beta \beta^* | 0_1, 1_2 \rangle \cdot \langle 0_1, 1_2 | + \alpha \delta^* | 1_1, 0_2 \rangle \cdot \langle 0_1, 1_2 | + \\ & \beta \delta^* | 1_1, 1_2 \rangle \cdot \langle 0_1, 1_2 | + \gamma \alpha^* | 0_1, 0_2 \rangle \cdot \langle 1_1, 0_2 | + \delta \alpha^* | 0_1, 1_2 \rangle \cdot \langle 1_1, 0_2 | + \\ & \gamma \gamma^* | 1_1, 0_2 \rangle \cdot \langle 1_1, 0_2 | + \delta \gamma^* | 1_1, 1_2 \rangle \cdot \langle 1_1, 0_2 | + \gamma \beta^* | 0_1, 0_2 \rangle \cdot \langle 1_1, 1_2 | + \\ & \delta \beta^* | 0_1, 1_2 \rangle \cdot \langle 1_1, 1_2 | + \gamma \delta^* | 1_1, 0_2 \rangle \cdot \langle 1_1, 1_2 | + \delta \delta^* | 1_1, 1_2 \rangle \cdot \langle 1_1, 1_2 | \end{aligned}$$

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

```
mypartialtranspose2 = QuantumPartialTranspose[mydensityop,  $\hat{2}$ ]
```

$$\begin{aligned} & \alpha \alpha^* |0_1, 0_2\rangle \cdot \langle 0_1, 0_2| + \alpha \beta^* |0_1, 1_2\rangle \cdot \langle 0_1, 0_2| + \\ & \gamma \alpha^* |1_1, 0_2\rangle \cdot \langle 0_1, 0_2| + \gamma \beta^* |1_1, 1_2\rangle \cdot \langle 0_1, 0_2| + \\ & \beta \alpha^* |0_1, 0_2\rangle \cdot \langle 0_1, 1_2| + \beta \beta^* |0_1, 1_2\rangle \cdot \langle 0_1, 1_2| + \delta \alpha^* |1_1, 0_2\rangle \cdot \langle 0_1, 1_2| + \\ & \delta \beta^* |1_1, 1_2\rangle \cdot \langle 0_1, 1_2| + \alpha \gamma^* |0_1, 0_2\rangle \cdot \langle 1_1, 0_2| + \alpha \delta^* |0_1, 1_2\rangle \cdot \langle 1_1, 0_2| + \\ & \gamma \gamma^* |1_1, 0_2\rangle \cdot \langle 1_1, 0_2| + \gamma \delta^* |1_1, 1_2\rangle \cdot \langle 1_1, 0_2| + \beta \gamma^* |0_1, 0_2\rangle \cdot \langle 1_1, 1_2| + \\ & \beta \delta^* |0_1, 1_2\rangle \cdot \langle 1_1, 1_2| + \delta \gamma^* |1_1, 0_2\rangle \cdot \langle 1_1, 1_2| + \delta \delta^* |1_1, 1_2\rangle \cdot \langle 1_1, 1_2| \end{aligned}$$

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, { $\hat{1}$ ,  $\hat{2}$ }]
```

$$\begin{aligned} & \alpha \alpha^* |0_1, 0_2\rangle \cdot \langle 0_1, 0_2| + \alpha \beta^* |0_1, 1_2\rangle \cdot \langle 0_1, 0_2| + \\ & \alpha \gamma^* |1_1, 0_2\rangle \cdot \langle 0_1, 0_2| + \alpha \delta^* |1_1, 1_2\rangle \cdot \langle 0_1, 0_2| + \\ & \beta \alpha^* |0_1, 0_2\rangle \cdot \langle 0_1, 1_2| + \beta \beta^* |0_1, 1_2\rangle \cdot \langle 0_1, 1_2| + \beta \gamma^* |1_1, 0_2\rangle \cdot \langle 0_1, 1_2| + \\ & \beta \delta^* |1_1, 1_2\rangle \cdot \langle 0_1, 1_2| + \gamma \alpha^* |0_1, 0_2\rangle \cdot \langle 1_1, 0_2| + \gamma \beta^* |0_1, 1_2\rangle \cdot \langle 1_1, 0_2| + \\ & \gamma \gamma^* |1_1, 0_2\rangle \cdot \langle 1_1, 0_2| + \gamma \delta^* |1_1, 1_2\rangle \cdot \langle 1_1, 0_2| + \delta \alpha^* |0_1, 0_2\rangle \cdot \langle 1_1, 1_2| + \\ & \delta \beta^* |0_1, 1_2\rangle \cdot \langle 1_1, 1_2| + \delta \gamma^* |1_1, 0_2\rangle \cdot \langle 1_1, 1_2| + \delta \delta^* |1_1, 1_2\rangle \cdot \langle 1_1, 1_2| \end{aligned}$$

## 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 = DiracToMatrix[mydensityop, {{01, 11}, {02, 12}}]
```

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

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 = MatrixToDirac[matrixtranspose, {2, 2}]
```

$$\begin{aligned} & \alpha \alpha^* |0_1, 0_2\rangle \cdot \langle 0_1, 0_2| + \alpha \beta^* |0_1, 1_2\rangle \cdot \langle 0_1, 0_2| + \\ & \alpha \gamma^* |1_1, 0_2\rangle \cdot \langle 0_1, 0_2| + \alpha \delta^* |1_1, 1_2\rangle \cdot \langle 0_1, 0_2| + \\ & \beta \alpha^* |0_1, 0_2\rangle \cdot \langle 0_1, 1_2| + \beta \beta^* |0_1, 1_2\rangle \cdot \langle 0_1, 1_2| + \beta \gamma^* |1_1, 0_2\rangle \cdot \langle 0_1, 1_2| + \\ & \beta \delta^* |1_1, 1_2\rangle \cdot \langle 0_1, 1_2| + \gamma \alpha^* |0_1, 0_2\rangle \cdot \langle 1_1, 0_2| + \gamma \beta^* |0_1, 1_2\rangle \cdot \langle 1_1, 0_2| + \\ & \gamma \gamma^* |1_1, 0_2\rangle \cdot \langle 1_1, 0_2| + \gamma \delta^* |1_1, 1_2\rangle \cdot \langle 1_1, 0_2| + \delta \alpha^* |0_1, 0_2\rangle \cdot \langle 1_1, 1_2| + \\ & \delta \beta^* |0_1, 1_2\rangle \cdot \langle 1_1, 1_2| + \delta \gamma^* |1_1, 0_2\rangle \cdot \langle 1_1, 1_2| + \delta \delta^* |1_1, 1_2\rangle \cdot \langle 1_1, 1_2| \end{aligned}$$

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 operator "mytranspose" was obtained by direct application of the command QuantumPartialTranspose to the original Dirac expression.

As expected, both "secondtranspose" and "mytranspose" are the same (notice the use of two equal symbols == in order to make the comparison):

```
secondtranspose == mytranspose
```

```
True
```

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by José Luis Gómez-Muñoz  
<http://homepage.cem.itesm.mx/lgoomez/quantum/>  
[jose.luis.gomez@itesm.mx](mailto:jose.luis.gomez@itesm.mx)