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# Dirac Notation, Matrix Notation and Operator Diagonalization.

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## Introduction

This is a tutorial on the use of Quantum *Mathematica* add-on to transform expressions in Dirac Notation to Matrix Notation and viceversa.

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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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## From Matrix Notation to Dirac Notation

A matrix can be generated with the standard *Mathematica* command `Table`.

```
mymatrix = Table[k[i, j], {i, 0, 3}, {j, 0, 3}]
```

```
{ {k[0, 0], k[0, 1], k[0, 2], k[0, 3]}, {k[1, 0], k[1, 1], k[1, 2], k[1, 3]},
  {k[2, 0], k[2, 1], k[2, 2], k[2, 3]}, {k[3, 0], k[3, 1], k[3, 2], k[3, 3]} }
```

The matrix can be visualized with the standard *Mathematica* command `MatrixForm`:

```
MatrixForm[mymatrix]
```

$$\begin{pmatrix} k[0, 0] & k[0, 1] & k[0, 2] & k[0, 3] \\ k[1, 0] & k[1, 1] & k[1, 2] & k[1, 3] \\ k[2, 0] & k[2, 1] & k[2, 2] & k[2, 3] \\ k[3, 0] & k[3, 1] & k[3, 2] & k[3, 3] \end{pmatrix}$$

The matrix can be transformed to Dirac Notation using the Quantum *Mathematica* command `MatrixToDirac`. Here it is specified that there is only one quantum number with 4 possible values (0,1,2,3):

```
MatrixToDirac[mymatrix, {4}]
```

$$\begin{aligned} & k[0, 0] \mid 0_1 \rangle \cdot \langle 0_1 \mid + k[1, 0] \mid 1_1 \rangle \cdot \langle 0_1 \mid + k[2, 0] \mid 2_1 \rangle \cdot \langle 0_1 \mid + k[3, 0] \mid 3_1 \rangle \cdot \langle 0_1 \mid + \\ & k[0, 1] \mid 0_1 \rangle \cdot \langle 1_1 \mid + k[1, 1] \mid 1_1 \rangle \cdot \langle 1_1 \mid + k[2, 1] \mid 2_1 \rangle \cdot \langle 1_1 \mid + k[3, 1] \mid 3_1 \rangle \cdot \langle 1_1 \mid + \\ & k[0, 2] \mid 0_1 \rangle \cdot \langle 2_1 \mid + k[1, 2] \mid 1_1 \rangle \cdot \langle 2_1 \mid + k[2, 2] \mid 2_1 \rangle \cdot \langle 2_1 \mid + k[3, 2] \mid 3_1 \rangle \cdot \langle 2_1 \mid + \\ & k[0, 3] \mid 0_1 \rangle \cdot \langle 3_1 \mid + k[1, 3] \mid 1_1 \rangle \cdot \langle 3_1 \mid + k[2, 3] \mid 2_1 \rangle \cdot \langle 3_1 \mid + k[3, 3] \mid 3_1 \rangle \cdot \langle 3_1 \mid \end{aligned}$$

Here it is specified that there are two quantum numbers, with 2 possible values each one (0,1):

```
MatrixToDirac[mymatrix, {2, 2}]
```

$$\begin{aligned} & k[0, 0] \mid 0_1, 0_2 \rangle \cdot \langle 0_1, 0_2 \mid + k[1, 0] \mid 0_1, 1_2 \rangle \cdot \langle 0_1, 0_2 \mid + \\ & k[2, 0] \mid 1_1, 0_2 \rangle \cdot \langle 0_1, 0_2 \mid + k[3, 0] \mid 1_1, 1_2 \rangle \cdot \langle 0_1, 0_2 \mid + \\ & k[0, 1] \mid 0_1, 0_2 \rangle \cdot \langle 0_1, 1_2 \mid + k[1, 1] \mid 0_1, 1_2 \rangle \cdot \langle 0_1, 1_2 \mid + k[2, 1] \mid 1_1, 0_2 \rangle \cdot \langle 0_1, 1_2 \mid + \\ & k[3, 1] \mid 1_1, 1_2 \rangle \cdot \langle 0_1, 1_2 \mid + k[0, 2] \mid 0_1, 0_2 \rangle \cdot \langle 1_1, 0_2 \mid + k[1, 2] \mid 0_1, 1_2 \rangle \cdot \langle 1_1, 0_2 \mid + \\ & k[2, 2] \mid 1_1, 0_2 \rangle \cdot \langle 1_1, 0_2 \mid + k[3, 2] \mid 1_1, 1_2 \rangle \cdot \langle 1_1, 0_2 \mid + k[0, 3] \mid 0_1, 0_2 \rangle \cdot \langle 1_1, 1_2 \mid + \\ & k[1, 3] \mid 0_1, 1_2 \rangle \cdot \langle 1_1, 1_2 \mid + k[2, 3] \mid 1_1, 0_2 \rangle \cdot \langle 1_1, 1_2 \mid + k[3, 3] \mid 1_1, 1_2 \rangle \cdot \langle 1_1, 1_2 \mid \end{aligned}$$

Here it is specified that there are two quantum numbers, with 2 possible values each one, and explicit labels for each eigenvalue and each operator are given:

```
MatrixToDirac[mymatrix, {2, 2}, {0_1 -> a1_a, 1_1 -> a2_a, 0_2 -> b1_b, 1_2 -> b2_b}]
```

$$\begin{aligned} & k[0, 0] \mid a1_a, b1_b \rangle \cdot \langle a1_a, b1_b \mid + k[1, 0] \mid a1_a, b2_b \rangle \cdot \langle a1_a, b1_b \mid + \\ & k[2, 0] \mid a2_a, b1_b \rangle \cdot \langle a1_a, b1_b \mid + k[3, 0] \mid a2_a, b2_b \rangle \cdot \langle a1_a, b1_b \mid + \\ & k[0, 1] \mid a1_a, b1_b \rangle \cdot \langle a1_a, b2_b \mid + k[1, 1] \mid a1_a, b2_b \rangle \cdot \langle a1_a, b2_b \mid + \\ & k[2, 1] \mid a2_a, b1_b \rangle \cdot \langle a1_a, b2_b \mid + k[3, 1] \mid a2_a, b2_b \rangle \cdot \langle a1_a, b2_b \mid + \\ & k[0, 2] \mid a1_a, b1_b \rangle \cdot \langle a2_a, b1_b \mid + k[1, 2] \mid a1_a, b2_b \rangle \cdot \langle a2_a, b1_b \mid + \\ & k[2, 2] \mid a2_a, b1_b \rangle \cdot \langle a2_a, b1_b \mid + k[3, 2] \mid a2_a, b2_b \rangle \cdot \langle a2_a, b1_b \mid + \\ & k[0, 3] \mid a1_a, b1_b \rangle \cdot \langle a2_a, b2_b \mid + k[1, 3] \mid a1_a, b2_b \rangle \cdot \langle a2_a, b2_b \mid + \\ & k[2, 3] \mid a2_a, b1_b \rangle \cdot \langle a2_a, b2_b \mid + k[3, 3] \mid a2_a, b2_b \rangle \cdot \langle a2_a, b2_b \mid \end{aligned}$$

The command `Table` is used to generate a larger matrix:

```
mymatrix2 = Table[k[i, j], {i, 0, 5}, {j, 0, 5}]
```

```
{ {k[0, 0], k[0, 1], k[0, 2], k[0, 3], k[0, 4], k[0, 5]},  
  {k[1, 0], k[1, 1], k[1, 2], k[1, 3], k[1, 4], k[1, 5]},  
  {k[2, 0], k[2, 1], k[2, 2], k[2, 3], k[2, 4], k[2, 5]},  
  {k[3, 0], k[3, 1], k[3, 2], k[3, 3], k[3, 4], k[3, 5]},  
  {k[4, 0], k[4, 1], k[4, 2], k[4, 3], k[4, 4], k[4, 5]},  
  {k[5, 0], k[5, 1], k[5, 2], k[5, 3], k[5, 4], k[5, 5]} }
```

The larger matrix can be visualized with the standard *Mathematica* command `MatrixForm`:

```
MatrixForm[mymatrix2]
```

$$\begin{pmatrix} k[0, 0] & k[0, 1] & k[0, 2] & k[0, 3] & k[0, 4] & k[0, 5] \\ k[1, 0] & k[1, 1] & k[1, 2] & k[1, 3] & k[1, 4] & k[1, 5] \\ k[2, 0] & k[2, 1] & k[2, 2] & k[2, 3] & k[2, 4] & k[2, 5] \\ k[3, 0] & k[3, 1] & k[3, 2] & k[3, 3] & k[3, 4] & k[3, 5] \\ k[4, 0] & k[4, 1] & k[4, 2] & k[4, 3] & k[4, 4] & k[4, 5] \\ k[5, 0] & k[5, 1] & k[5, 2] & k[5, 3] & k[5, 4] & k[5, 5] \end{pmatrix}$$

The matrix can be transformed to Dirac Notation using the Quantum *Mathematica* command `MatrixToDirac`. Here it is specified that there are two quantum numbers, the first one with 3 possible values (0,1,2) and the second one with 2 possible eigenvalues (0,1):

```
MatrixToDirac[mymatrix2, {3, 2}]
```

$$\begin{aligned} & k[0, 0] \mid 0_1, 0_2 \rangle \cdot \langle 0_1, 0_2 \mid + k[1, 0] \mid 0_1, 1_2 \rangle \cdot \langle 0_1, 0_2 \mid + k[2, 0] \mid 1_1, 0_2 \rangle \cdot \langle 0_1, 0_2 \mid + \\ & k[3, 0] \mid 1_1, 1_2 \rangle \cdot \langle 0_1, 0_2 \mid + k[4, 0] \mid 2_1, 0_2 \rangle \cdot \langle 0_1, 0_2 \mid + k[5, 0] \mid 2_1, 1_2 \rangle \cdot \langle 0_1, 0_2 \mid + \\ & k[0, 1] \mid 0_1, 0_2 \rangle \cdot \langle 0_1, 1_2 \mid + k[1, 1] \mid 0_1, 1_2 \rangle \cdot \langle 0_1, 1_2 \mid + k[2, 1] \mid 1_1, 0_2 \rangle \cdot \langle 0_1, 1_2 \mid + \\ & k[3, 1] \mid 1_1, 1_2 \rangle \cdot \langle 0_1, 1_2 \mid + k[4, 1] \mid 2_1, 0_2 \rangle \cdot \langle 0_1, 1_2 \mid + k[5, 1] \mid 2_1, 1_2 \rangle \cdot \langle 0_1, 1_2 \mid + \\ & k[0, 2] \mid 0_1, 0_2 \rangle \cdot \langle 1_1, 0_2 \mid + k[1, 2] \mid 0_1, 1_2 \rangle \cdot \langle 1_1, 0_2 \mid + k[2, 2] \mid 1_1, 0_2 \rangle \cdot \langle 1_1, 0_2 \mid + \\ & k[3, 2] \mid 1_1, 1_2 \rangle \cdot \langle 1_1, 0_2 \mid + k[4, 2] \mid 2_1, 0_2 \rangle \cdot \langle 1_1, 0_2 \mid + k[5, 2] \mid 2_1, 1_2 \rangle \cdot \langle 1_1, 0_2 \mid + \\ & k[0, 3] \mid 0_1, 0_2 \rangle \cdot \langle 1_1, 1_2 \mid + k[1, 3] \mid 0_1, 1_2 \rangle \cdot \langle 1_1, 1_2 \mid + k[2, 3] \mid 1_1, 0_2 \rangle \cdot \langle 1_1, 1_2 \mid + \\ & k[3, 3] \mid 1_1, 1_2 \rangle \cdot \langle 1_1, 1_2 \mid + k[4, 3] \mid 2_1, 0_2 \rangle \cdot \langle 1_1, 1_2 \mid + k[5, 3] \mid 2_1, 1_2 \rangle \cdot \langle 1_1, 1_2 \mid + \\ & k[0, 4] \mid 0_1, 0_2 \rangle \cdot \langle 2_1, 0_2 \mid + k[1, 4] \mid 0_1, 1_2 \rangle \cdot \langle 2_1, 0_2 \mid + k[2, 4] \mid 1_1, 0_2 \rangle \cdot \langle 2_1, 0_2 \mid + \\ & k[3, 4] \mid 1_1, 1_2 \rangle \cdot \langle 2_1, 0_2 \mid + k[4, 4] \mid 2_1, 0_2 \rangle \cdot \langle 2_1, 0_2 \mid + k[5, 4] \mid 2_1, 1_2 \rangle \cdot \langle 2_1, 0_2 \mid + \\ & k[0, 5] \mid 0_1, 0_2 \rangle \cdot \langle 2_1, 1_2 \mid + k[1, 5] \mid 0_1, 1_2 \rangle \cdot \langle 2_1, 1_2 \mid + k[2, 5] \mid 1_1, 0_2 \rangle \cdot \langle 2_1, 1_2 \mid + \\ & k[3, 5] \mid 1_1, 1_2 \rangle \cdot \langle 2_1, 1_2 \mid + k[4, 5] \mid 2_1, 0_2 \rangle \cdot \langle 2_1, 1_2 \mid + k[5, 5] \mid 2_1, 1_2 \rangle \cdot \langle 2_1, 1_2 \mid \end{aligned}$$

## From Dirac Notation to Matrix Notation

Here is a simple Dirac expression which will be used to illustrate the opposite procedure:

```
mydirac = k1 \mid a1_a, b2_b \rangle \cdot \langle a1_a, b1_b \mid + k2 \mid a1_a, b1_b \rangle \cdot \langle a2_a, b1_b \mid
```

```
k1 \mid a1_a, b2_b \rangle \cdot \langle a1_a, b1_b \mid + k2 \mid a1_a, b1_b \rangle \cdot \langle a2_a, b1_b \mid
```

The Dirac expression can be transformed to a matrix using the Quantum *Mathematica* command `DiracToMatrix`. It is specified that each operator has two possible eigenvalues:

```
m1 = DiracToMatrix[mydirac, {{a1â, a2â}, {b1ĥ, b2ĥ}}]
{{0, 0, k2, 0}, {k1, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

The calculated matrix can be visualized with the standard *Mathematica* command `MatrixForm`:

```
MatrixForm[m1]
```

$$\begin{pmatrix} 0 & 0 & k2 & 0 \\ k1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The Dirac expression can be transformed to a tensor (matrix of matrices) using the Quantum *Mathematica* command `DiracToTensor`. It is specified that each operator has two possible eigenvalues:

```
t1 = DiracToTensor[mydirac, {{a1â, a2â}, {b1ĥ, b2ĥ}}]
{{{0, 0}, {k1, 0}}, {{k2, 0}, {0, 0}}, {{{0, 0}, {0, 0}}, {{0, 0}, {0, 0}}}}
```

The calculated tensor can be visualized with the standard *Mathematica* command `MatrixForm`:

```
MatrixForm[t1]
```

$$\begin{pmatrix} \begin{pmatrix} 0 & 0 \\ k1 & 0 \end{pmatrix} & \begin{pmatrix} k2 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix}$$


---

## Operator Diagonalization

The command `DiracEigensystem` gives eigenvalues and eigenstates of operators. The input syntax is the same as the syntax of `DiracToMatrix` and `DiracToTensor`, and the output has the same format as the output of the standard *Mathematica* command `Eigensystem`: first the list of eigenvalues, then the list of the corresponding eigenvectors:

```
DiracEigensystem[
  | 0â ⟩ · ⟨ 0â | + ĩ | 1â ⟩ · ⟨ 1â | + | 3â ⟩ · ⟨ 2â | + | 2â ⟩ · ⟨ 3â | ,
  {{0â, 1â, 2â, 3â}}]
{{-1, ĩ, 1, 1}, {- (| 2â ⟩ / √2 + | 3â ⟩ / √2, | 1â ⟩, | 2â ⟩ / √2 + | 3â ⟩ / √2, | 0â ⟩}}}
```

Here we use `Transpose` and `Grid` to give a nicer formatting for the output:

```
Grid[Transpose[
  DiracEigensystem[
    | 0a⟩ · ⟨0a | + i | 1a⟩ · ⟨1a | + | 3a⟩ · ⟨2a | + | 2a⟩ · ⟨3a | ,
    {{0a, 1a, 2a, 3a}}]
], Dividers → All]
```

-1	$-\frac{ 2_a\rangle}{\sqrt{2}} + \frac{ 3_a\rangle}{\sqrt{2}}$
i	$ 1_a\rangle$
1	$\frac{ 2_a\rangle}{\sqrt{2}} + \frac{ 3_a\rangle}{\sqrt{2}}$
1	$ 0_a\rangle$

## From Symbolic Operators to Matrix Notation

Here is the definition of a simple operator (named "myop") which will be used to illustrate the procedure in the operators created with the Quantum *Mathematica* command DefineOperatorOnKets:

```
DefineOperatorOnKets[myop, { | 0i⟩ → a | 0i⟩ + b | 1i⟩, | 1i⟩ → c | 0i⟩ + d | 1i⟩ }]
```

```
| 0i⟩ → a | 0i⟩ + b | 1i⟩
| 1i⟩ → c | 0i⟩ + d | 1i⟩
```

Here is the simple operator applied to a linear combination of kets:

```
myop · (e | 0i⟩ + g | 1i⟩)
```

```
e (a | 0i⟩ + b | 1i⟩) + g (c | 0i⟩ + d | 1i⟩)
```

Here is the simple operator applied to a linear combination of kets and expanded:

```
Expand[myop · (e | 0i⟩ + g | 1i⟩)]
```

```
a e | 0i⟩ + c g | 0i⟩ + b e | 1i⟩ + d g | 1i⟩
```

Here is the simple operator applied to a linear combination of kets and kets are "collected":

```
CollectKet[myop · (e | 0i⟩ + g | 1i⟩)]
```

```
(a e + c g) | 0i⟩ + (b e + d g) | 1i⟩
```

The operator can be transformed to a matrix using the Quantum *Mathematica* command DiracToMatrix. It is specified that the operator has two possible eigenvalues:

```
matrixop = DiracToMatrix[myop, {{0i, 1i}}
```

```
{a, c}, {b, d}}
```

The calculated matrix can be visualized with the standard *Mathematica* command `MatrixForm`:

```
MatrixForm[matrixop]
```

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

We can also diagonalize this operator. Notice that *Mathematica* manipulates  $a, b, c, d$  as **complex numbers**:

```
DiracEigensystem[myop, {{0i, 1i}}
```

$$\left\{ \left\{ \frac{1}{2} \left( a + d - \sqrt{a^2 + 4bc - 2ad + d^2} \right), \frac{1}{2} \left( a + d + \sqrt{a^2 + 4bc - 2ad + d^2} \right) \right\}, \right. \\ \left. \left\{ \frac{\left( a - d - \sqrt{a^2 + 4bc - 2ad + d^2} \right) | 0_i \rangle}{b \sqrt{4 + \text{Abs} \left[ \frac{-a + d + \sqrt{a^2 + 4bc - 2ad + d^2}}{b} \right]^2}} + \frac{2 | 1_i \rangle}{\sqrt{4 + \text{Abs} \left[ \frac{-a + d + \sqrt{a^2 + 4bc - 2ad + d^2}}{b} \right]^2}}, \right. \right. \\ \left. \left. \frac{\left( a - d + \sqrt{a^2 + 4bc - 2ad + d^2} \right) | 0_i \rangle}{b \sqrt{4 + \text{Abs} \left[ \frac{-a + d + \sqrt{a^2 + 4bc - 2ad + d^2}}{b} \right]^2}} + \frac{2 | 1_i \rangle}{\sqrt{4 + \text{Abs} \left[ \frac{-a + d + \sqrt{a^2 + 4bc - 2ad + d^2}}{b} \right]^2}} \right\} \right\}$$

Here we use `Transpose` and `Grid` to give a nicer formatting for the output:

```
Grid[Transpose[
  DiracEigensystem[myop, {{0i, 1i}}]
], Dividers -> All]
```

$\frac{1}{2} \left( a + d - \sqrt{a^2 + 4bc - 2ad + d^2} \right)$	$\frac{\left( a - d - \sqrt{a^2 + 4bc - 2ad + d^2} \right)   0_i \rangle}{b \sqrt{4 + \text{Abs} \left[ \frac{-a + d + \sqrt{a^2 + 4bc - 2ad + d^2}}{b} \right]^2}} + \frac{2   1_i \rangle}{\sqrt{4 + \text{Abs} \left[ \frac{-a + d + \sqrt{a^2 + 4bc - 2ad + d^2}}{b} \right]^2}}$
$\frac{1}{2} \left( a + d + \sqrt{a^2 + 4bc - 2ad + d^2} \right)$	$\frac{\left( a - d + \sqrt{a^2 + 4bc - 2ad + d^2} \right)   0_i \rangle}{b \sqrt{4 + \text{Abs} \left[ \frac{-a + d + \sqrt{a^2 + 4bc - 2ad + d^2}}{b} \right]^2}} + \frac{2   1_i \rangle}{\sqrt{4 + \text{Abs} \left[ \frac{-a + d + \sqrt{a^2 + 4bc - 2ad + d^2}}{b} \right]^2}}$

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