Dirac Notation in *Mathematica*

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**Introduction**

This is a tutorial on the use of Quantum *Mathematica* add-on to enter kets, bras and other quantum objects in Dirac notation.

**Load the Package**

First load the Quantum’Notation’ package. Write:

```mathematica
Needs["Quantum`Notation""];
```

then press at the same time the keys `Alt-Enter` to evaluate. *Mathematica* will load the package and print a welcome message:

```
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:

```mathematica
SetQuantumAliases[];
```

then press at the same time the keys `Alt-Enter` to evaluate. Remember that `SetQuantumAliases[]` must be evaluated again in each new notebook:
SetQuantumAliases[]

ALIASES:

- [ESC]ket[ESC] ket template
- [ESC]bra[ESC] bra template
- [ESC]braket[ESC] braket template
- [ESC]op[ESC] operator template
- [ESC].[ESC] quantum concatenation infix symbol
- [ESC]on[ESC] quantum concatenation infix symbol
- [ESC]tp[ESC] tensor product infix symbol
- [ESC]qp[ESC] quantum product template
- [ESC]qs[ESC] sigma notation for sums template
- [ESC]si[ESC] sigma notation for sums template
- [ESC]ev[ESC] eigenvalue-label template
- [ESC]eket[ESC] eigenstate template
- [ESC]eeket[ESC] two-operators-eigenstate template
- [ESC]eeeeket[ESC] three-operators-eigenstate template
- [ESC]ebra[ESC] bra of eigenstate template
- [ESC]eebra[ESC] bra of two-operators-eigenstate template
- [ESC]eeebra[ESC] bra of three-operators-eigenstate template
- [ESC]ebraket[ESC] braket of eigenstates template
- [ESC]eebraket[ESC] bra of two-operators-eigenstate template
- [ESC]eebrakket[ESC] braket of three-operators-eigenstate template
- [ESC]ketbra[ESC] operator (matrix) element template
- [ESC]eketbra[ESC] operator (matrix) element template
- [ESC]eeketbra[ESC] operator (matrix) element template
- [ESC]eeeketbra[ESC] operator (matrix) element template
- [ESC]her[ESC] hermitian conjugate template
- [ESC]con[ESC] complex conjugate template
- [ESC]norm[ESC] quantum norm template
- [ESC]trace[ESC] partial trace template
- [ESC]comm[ESC] commutator template
- [ESC]anti[ESC] anticommutator template
- [ESC]su[ESC] subscript template
- [ESC]po[ESC] power template

The quantum concatenation infix symbol [ESC]on[ESC] is used for operator application, inner product and outer product.

SetQuantumAliases[] must be executed again in each new notebook that is created, only one time per notebook.

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Entering Kets, Bras and Brakets

In order to write a ket in Dirac's notation, place the cursor in a new Mathematica cell and press the keyboard keys:

- [ESC]ket[ESC]

The ket template will appear. In order to select and fill in the "place holder" (square) press the keys:

- [TAB] z

Finally press at the same time the keys[SHIFT] and[ENTER] to evaluate.
In a similar way you can enter a bra:
[ESC]bra[ESC]
then press [TAB] and fill in the "place holder" (square) with label z:

\[ \langle z | \]
\[ \langle z | \]

Here is a braket:
[ESC]braket[ESC]
[TAB]a[TAB]b

\[ \langle a | b \rangle \]
\[ \langle a | b \rangle \]

The internal product of a bra and a ket is entered by pressing the keys:
[ESC]bra[ESC] [ESC]on[ESC] [ESC]ket[ESC]
press [TAB] one or two times to select the first "place holder" (square) and press:
a[TAB]b
finally press at the same time [SHIFT]-[ENTER]

\[ \langle a | \cdot | b \rangle \]
\[ \langle a | b \rangle \]

**Entering Kets of orthonormal states**

In order to write the eigenket of operator \( p \) with eigenvalue 3, place the cursor in a new Mathematica cell and press the keyboard keys:
[ESC]eket[ESC]
The eigenket template will appear. Next press the keys:
[TAB]3[TAB]p
Finally press at the same time the keys [SHIFT] and [ENTER] to evaluate:

\[ | 3_p \rangle \]
\[ | 3_p \rangle \]

In order to write the operator \( h \) acting on its eigenket with eigenvalue 3 press the keys:
[ESC]op[ESC] [ESC]on[ESC] [ESC]eket[ESC]
The operator and eigenket templates will appear. Next press [TAB] several times till the first place holder (square) is selected. Then press the keys:
h[TAB]3[TAB]h
Finally press at the same time the keys [SHIFT] and [ENTER] to evaluate. The result of the calculation is the same ket multiplied by its eigenvalue:
In order to write a ket that is eigenket of two operators press the keys:
[ESC]eket[ESC]
The corresponding eigenket template will appear. Next press the keys:
[TAB][TAB][TAB][TAB][TAB][TAB]
c
Finally press at the same time the keys [SHIFT] and [ENTER] to evaluate.

\[ 3_{p}\hat{\cdot} 3_{h} \]

Another example of an operator acting on its eigenket:
[ESC]op[ESC][ESC]on[ESC][ESC]eket[ESC]
The operator and eigenket templates will appear. Next press [TAB] several times till the first place holder (square) is selected. Then press the keys:
b[TAB][TAB][TAB][TAB][TAB][TAB]
b
Finally press at the same time the keys [SHIFT] and [ENTER] to evaluate. The result of the calculation is the same ket multiplied by its eigenvalue:

\[ 4_{p}\hat{\cdot} 4_{h}, 3_{p} \]

In order to enter the bra that corresponds to an eigenket press:
[ESC]ebra[ESC]
then press [TAB] and fill in the first "place holder" (square) with 6. Press [TAB] again and fill in the second "place holder" with m:

\[ 6_{p} \left\langle \begin{array}{c}
\end{array}\right. \]

Next calculation gives one because eigenstates of the same operator are assumed to be orthonormal:
[ESC]ebra[ESC][ESC]on[ESC][ESC]eket[ESC]
Next press [TAB] several times till the first place holder (square) is selected. Then press:
2[TAB][TAB][TAB][TAB][TAB][TAB]

\[ 2_{p}\left\langle \begin{array}{c}
\end{array}\right. \]

Next calculation gives zero because eigenstates of the same operator are assumed to be orthonormal:
This calculation gives a KroneckerDelta because eigenstates of the same operator are assumed to be orthonormal:

\[ \langle a_n | \cdot | b_n \rangle \]

KroneckerDelta[a - b]

Here is a braket made of eigenstates

\[ \langle 2_q, 3_r | 2_q, 3_r \rangle \]

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In order to write a tensor product of kets press the keys:

\[ \langle \text{eket} | \text{on} | \text{ebra} | \text{eeket} \rangle \]

Then press:

\[ 3[q] | 1[c] \]

Using tensor products you can generate a ket of any length:

\[ \langle 2_q, 8_r, 9_s | 2_q, 3_r \rangle \]

You can apply an operator in a subspace to a ket of the space:

\[ \langle \text{eket} | \text{on} | \text{ebra} | \text{eeket} \rangle \]

Then press:

\[ a[q] | 0[c] \]

and press at the same time[SHIFT]-[ENTER]
Hermitian Conjugate

In order to calculate the Hermitian Conjugate of a ket press the keys:

\[ \text{ESC}\text{her}\text{ESC} \text{[TAB]} \text{ESC}\text{ket}\text{ESC} \text{[TAB]}a \]
and press at the same time [SHIFT]-[ENTER]

\[
( | a \rangle )^\dagger
\]

In order to calculate the Hermitian Conjugate of an expression press the following keys (Notice that the imaginary \(i\) is entered with two \(ii\) between two \(\text{ESC}\)):

\[ \text{ESC}\text{her}\text{ESC}\text{[TAB]}(8+9\text{ESC}ii\text{ESC})^*\text{eket}\text{ESC}+(5+7\text{ESC}ii\text{ESC})^*\text{eket}\text{ESC}\]

Next press [TAB] several times till the first place holder (square) is selected. Then press:

\[0\text{[TAB]}b\text{[TAB]}3\text{[TAB]}a\text{[TAB]}q\text{[TAB]}\text{[TAB]}c\text{[TAB]}-5\text{[TAB]}q\]

and press at the same time [SHIFT]-[ENTER]

\[
( (8 + 9 i) \begin{pmatrix} 0 \ 3 \ 1 \ -5 \end{pmatrix} + (5 + 7 i) \begin{pmatrix} 1 \ -5 \ 0 \ 0 \end{pmatrix} )^\dagger
\]

It also works in symbolic expressions

\[ \text{ESC}\text{her}\text{ESC}\text{[TAB]}a\text{SPACE}\text{ESC}\text{ket}\text{ESC}+\text{ESC}\text{con}\text{ESC}\text{SPACE}\text{ESC}\text{ket}\text{ESC}\]

Next press [TAB] several times till the first place holder (square) is selected. Then press:

\[x\text{[TAB]}b\text{[TAB]}y\]

and press at the same time [SHIFT]-[ENTER]

\[
( a \ | x \rangle + (b)^* \ | y \rangle )^\dagger
\]

Superpositions of Kets and Operators

This is the way to define a ket:

\[\text{ESC}\text{ket}\text{ESC}^=a\text{ESC}\text{eket}\text{ESC}+b\text{ESC}\text{eket}\text{ESC}+c\text{ESC}\text{eket}\text{ESC}+d\text{ESC}\text{eket}\text{ESC}+e\text{ESC}\text{eket}\text{ESC}\]

Next press [TAB] several times till the first place holder (square) is selected. Then press:

\[\text{ESC}\text{psi}\text{ESC}\text{[TAB]}1\text{[TAB]}q\text{[TAB]}2\text{[TAB]}q\text{[TAB]}3\text{[TAB]}q\text{[TAB]}4\text{[TAB]}q\text{[TAB]}5\text{[TAB]}q\]

finally press at the same time [SHIFT]-[ENTER]

\[
\begin{pmatrix} \psi \end{pmatrix} = a \begin{pmatrix} 1 \end{pmatrix} + b \begin{pmatrix} 2 \end{pmatrix} + c \begin{pmatrix} 3 \end{pmatrix} + d \begin{pmatrix} 4 \end{pmatrix} + e \begin{pmatrix} 5 \end{pmatrix}
\]

\[
a \begin{pmatrix} 1 \end{pmatrix} + b \begin{pmatrix} 2 \end{pmatrix} + c \begin{pmatrix} 3 \end{pmatrix} + d \begin{pmatrix} 4 \end{pmatrix} + e \begin{pmatrix} 5 \end{pmatrix}
\]
The internal product of a ket with its dual is a real number (square of its norm)
Here we define another ket
\[ | \text{m} \rangle = u | 1_q \rangle + v | 2_q \rangle + w | 3_q \rangle + x | 4_q \rangle + y | 5_q \rangle \]

Next press [TAB] several times till the first place holder (square) is selected. Then press:
\[ m | 1 \rangle q | 2 \rangle q | 3 \rangle q | 4 \rangle q | 5 \rangle q \]
finally press at the same time [SHIFT]-[ENTER]

Note for advanced Mathematica users: The definition is stored as an upvalue of the variable m:

\[ ? m \]

\[ m^\_ = u | 1_q \rangle + v | 2_q \rangle + w | 3_q \rangle + x | 4_q \rangle + y | 5_q \rangle \]

Here is an operator made of the states that were defined before:

\[
\text{Expand}\left[ | \psi \rangle \cdot X_m \right]
\]

We can obtain the partial trace of the operator. The base-operator template \( \hat{q} \) is entered [ESC]op[ESC]:

\[
\text{QuantumPartialTrace}\left[ | \psi \rangle \cdot \langle m |, \hat{q} \right]
\]

Here we apply the "base" operator q to the ket. Notice that q is inside the operator template [ESC]op[ESC]

\[
\hat{q} \cdot | \psi \rangle
\]

This is one way to define another operator. Notice that p is not inside the operator template:
\[ p = f \cdot \langle 1_q | + g \rangle \cdot \langle 2_q | \cdot + g \rangle \cdot \langle 4_q | \]

\[ f = \langle 1_q | + \langle 2_q | + g \rangle \cdot \langle 4_q | \]

Now the operator and ket that were defined can be used. Notice that \( p \) is **not** inside the operator template:

\[ p \cdot | \psi \rangle 
\]

\[ b f = \langle 1_q | + d g \rangle \cdot \langle 2_q | \]

Notice that \( p \) is **not** inside the operator template, but **base** operator \( q \) is inside the template:

\[ p \cdot \hat{q} \cdot | \psi \rangle 
\]

\[ 2 b f = \langle 1_q | + 4 d g \rangle \cdot \langle 2_q | \]

Hermitian conjugate

\[ (p)' 
\]

\[ f' = \langle 2_q | \cdot \langle 1_q | + g^* \rangle \cdot \langle 4_q | \cdot \langle 2_q | \]

An expression involving a bra, an operator and a ket:

\[ \langle \psi | \cdot p \cdot | \psi \rangle 
\]

\[ b f a^* + d g b^* 
\]

Another expression involving a bra, an operator and a ket:

\[ \langle \psi | \cdot \hat{q} \cdot | \psi \rangle 
\]

\[ a a^* + 2 b b^* + 3 c c^* + 4 d d^* + 5 e e^* 
\]

Here is another operator:

\[ \text{ope} = a \cdot \langle 1_q, 3_s | + b \rangle \cdot \langle 2_q, 4_s | \cdot \langle 3_q, 2_s | + c \rangle \cdot \langle 3_q, 5_s | \cdot \langle 4_q, 5_s | 
\]

\[ a \cdot \langle 1_q, 3_s | + \rangle \cdot \langle 2_q, 4_s | \cdot \langle 3_q, 2_s | + \rangle \cdot \langle 3_q, 5_s | \cdot \langle 4_q, 5_s | 
\]

*Mathematica* can calculate the partial trace with respect to operator \( \hat{q} \):

\[ [\text{ESC}]\text{trace}[/\text{ESC}] 
\]

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Mathematica can calculate the partial trace with respect to operator \( \hat{s} \):

\[
\text{Tr}[s] = \text{Tr}_{\hat{s}}[\text{ope}]
\]

\[
a \ | 3_s \rangle \cdot (3_s | + c \ | 3_q \rangle \cdot (4_q |
\]

**Undefined Symbols are Assumed to be Scalars**

Any undefined name, like \( B \), is assumed to be a complex scalar:

\[
\text{Clear}[B];
\]

\[
(\langle \alpha | \cdot B \cdot | \beta \rangle)^\dagger
\]

\[
B^* \langle \beta | \alpha \rangle
\]

SetQuantumObject[\( B \)] specifies that \( B \) is not a complex scalar:

\[
\text{SetQuantumObject}[B]
\]

\[
\begin{align*}
\text{The object } B & \text{ will Not be considered as a complex scalar} \\
\text{The object } B[\text{args}] & \text{ will Not be considered as a complex scalar} \\
\text{The object } \text{Subscript}[B, \text{__}] & \text{ will Not be considered as a complex scalar} \\
\text{The object } \text{Subscript}[B, \text{__}][\text{args}] & \text{ will Not be considered as a complex scalar} \\
\text{The object } \text{Subscript}[B[\text{__}], \text{__}][\text{args}] & \text{ will Not be considered as a complex scalar}
\end{align*}
\]

After executing SetQuantumObject[\( B \)], \( B \) is considered an operator:

\[
(\langle \alpha | \cdot B \cdot | \beta \rangle)^\dagger
\]

\[
\langle \beta | \cdot B^\dagger \cdot | \alpha \rangle
\]

Finally we clear the definitions made in this document:

\[
\text{Clear}[m, p, \text{ope}, \psi, B]
\]
ReplaceAll versus QuantumReplaceAll

ReplaceAll is a standard Mathematica command that can take advantage of the pattern recognition language of Mathematica. The "delayed rule" symbol \( \rightarrow \) can be entered by pressing the keys [ESC]:\[Esc\]-\[Esc\].

```
ReplaceAll[a | \[Phi]\[Ket] + b | \[Psi]\[Ket], | \[Phi]\[Ket] \rightarrow (| 0\Ket + | 1\Ket)/\[Sqrt]2]
```

\[
a (| 0\Ket + | 1\Ket)/\sqrt{2} + b | \[Psi]\[Ket]
\]

However, ReplaceAll will not make any replacement in the following case, because the expression \(| \[Phi]\[Ket] \otimes | \[Psi]\[Ket]\) evolves to \(| \[Phi], \[Psi]\)[Ket], and the Mathematica command ReplaceAll does not recognize the ket \(| \[Phi]\)[Ket] in this evolved expression:

```
ReplaceAll[| \[Phi]\[Ket] \otimes | \[Psi]\[Ket], | \[Phi]\[Ket] \rightarrow (| 0\Ket + | 1\Ket)/\[Sqrt]2]
```

\[
| \[Phi], \[Psi]\rangle
\]

On the other hand, the Quantum Mathematica command QuantumReplace does recognize the ket and performs the replacement:

```
QuantumReplace[| \[Phi]\[Ket] \otimes | \[Psi]\[Ket], | \[Phi]\[Ket] \rightarrow (| 0\Ket + | 1\Ket)/\[Sqrt]2]
```

\[
| 0, \[Psi]\rangle + | 1, \[Psi]\rangle/\sqrt{2}
\]

QuantumReplaceAll will also work on bras:

```
QuantumReplace[| \[Psi]\[Ket] \cdot \langle \[Phi] |, | \[Phi]\[Ket] \rightarrow (| 0\Ket + | 1\Ket)/\[Sqrt]2]
```

\[
| \[Psi]\rangle \cdot ((| 0 \rangle + | 1 \rangle)/\sqrt{2})
\]

Expand[QuantumReplace[| \[Psi]\[Ket] \cdot \langle \[Phi] |, | \[Phi]\[Ket] \rightarrow (| 0\Ket + | 1\Ket)/\[Sqrt]2]]

\[
| \[Psi]\rangle \cdot (| 0 \rangle + | 1 \rangle)/\sqrt{2}
\]
Questions and Exercises

1. What command is used to load the Quantum Notation package in a fresh Mathematica session?
   Answer:

2. What command is used to load the Dirac Notation's keyboard aliases in a new Mathematica document (notebook)?
   Answer:

3. Select the correct sentence. There is only one:
   a) SetQuantumAliases[] must be executed after evaluating Needs["Quantum`Notation"] in a fresh Mathematica session
   b) SetQuantumAliases[] can be executed before evaluating Needs["Quantum`Notation"] in a fresh Mathematica session
   c) SetQuantumAliases[] must be executed before evaluating Needs["Quantum`Notation"] in a fresh Mathematica session
   The correct sentence is:_____

4. Select the correct sentence. There is only one:
   a) SetQuantumAliases[] must be evaluated before executing each command in Mathematica
   b) SetQuantumAliases[] must be evaluated in each new document (notebook) in Mathematica
   c) SetQuantumAliases[] must be evaluated in each fresh session in Mathematica
   The correct sentence is:_____

5. What combination of keys (keyboard alias) must be pressed in order to obtain the "CenterDot"
   Answer:

6. Select the correct sentences for the Quantum Package. There is more than one correct sentence:
   a) CenterDot · represents the internal product of a bra and a ket
   b) CenterDot · represents the hermitian conjugate operation
   c) CenterDot · represents the external product of a ket and a bra
   d) CenterDot · represents the partial trace operation
   e) CenterDot · represents the application of an operator to a ket
   The correct sentences are:_____

7. What is the difference between $| 3 \rangle \ y \ | 3 \rangle$ in the Quantum Mathematica Package?
   Answer:

8. What differences are there between the Dirac notation as used in Quantum Mechanics textbooks and the notation used in the Quantum Mathematica package?
   Answer:
9. What **similarities** are there between the Dirac notation as used in Quantum Mechanics textbooks and the notation used in the Quantum *Mathematica* package?

**Answer:**

10. Why the following command generates an error message?

   \[ | 3 \rangle = | a \rangle + | b \rangle \]

Why the following command **does not** generate the same error message?

\[ | m \rangle = | a \rangle + | b \rangle \]

**Answer:**

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