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:
Needs["Quantum`Notation`"];
then press at the same time the keys SHIFT-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:
SetQuantumAliases[ ];
then press at the same time the keys SHIFT-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]eeeket[ESC]     three-operators-eigentstate template
[ESC]ebra[ESC]       bra of eigenstate template
[ESC]eebra[ESC]      bra of two-operators-eigenstate template
[ESC]eeebra[ESC]     bra of three-operators-eigentstate template
[ESC]ebraket[ESC]    braket of eigenstates template
[ESC]eebraket[ESC]   braket of two-operators-eigenstates template
[ESC]eeebraket[ESC]  braket of three-operators-eigentstate 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.
```

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.

```
| z〉
```

```
| z〉
```

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:

```
⟨z |
```

```
⟨z |
```

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

```
⟨a | b⟩
```

```
⟨a | b⟩
```

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]

```
⟨a | · | b⟩
```

```
⟨a | b⟩
```

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:

$$\left| 3_{\hat{p}} \right\rangle$$

$$\left| 3_{\hat{p}} \right\rangle$$

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:

$\hat{h} \cdot \left| 3_{\hat{h}} \right\rangle$

$3 \left| 3_{\hat{h}} \right\rangle$

In order to write a ket that is eigenket of two operators press the keys:
[ESC]eeket[ESC]
The corresponding eigenket template will appear. Next press the keys:
[TAB]3[TAB]p[TAB]1[TAB]c
Finally press at the same time the keys [SHIFT] and [ENTER] to evaluate.

$\left| 3_{\hat{p}}, 1_{\hat{c}} \right\rangle$

$\left| 1_{\hat{c}}, 3_{\hat{p}} \right\rangle$

Another example of an operator acting on its eigenket:
[ESC]op[ESC] [ESC]on[ESC] [ESC]eeeket[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]2[TAB]c[TAB]3[TAB]a[TAB]4[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:

$\hat{b} \cdot \left| 2_{\hat{c}}, 3_{\hat{a}}, 4_{\hat{b}} \right\rangle$

$4 \left| 3_{\hat{a}}, 4_{\hat{b}}, 2_{\hat{c}} \right\rangle$

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:

$\left\langle 6_{\hat{m}} \right|$

$\left\langle 6_{\hat{m}} \right|$

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]m[TAB]2[TAB]m

$\left\langle 2_{\hat{m}} \right| \cdot \left| 2_{\hat{m}} \right\rangle$

1

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

$\langle 2_{\hat{m}} | \cdot | 3_{\hat{m}} \rangle$

0

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

$\langle a_{\hat{m}} | \cdot | b_{\hat{m}} \rangle$

KroneckerDelta[a - b]

Here is a braket made of eigenstates
[ESC]eebraket[ESC]
[TAB]2[TAB]q[TAB]3[TAB]c[TAB]2[TAB]q[TAB]3[TAB]c

$\langle 2_{\hat{q}}, 3_{\hat{c}} | 2_{\hat{q}}, 3_{\hat{c}} \rangle$

1

In order to write a tensor product of kets press the keys:
[ESC]eket[ESC] [ESC]on[ESC] [ESC]eket[ESC]
Next press[TAB] several times till the first place holder (square) is selected. Then press:
3[TAB]q[TAB]1[TAB]c

$| 3_{\hat{q}} \rangle \cdot | 1_{\hat{c}} \rangle$

$| 1_{\hat{c}}, 3_{\hat{q}} \rangle$

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

$| 2_{\hat{v}}, 8_{\hat{r}}, 9_{\hat{t}} \rangle \cdot | 5_{\hat{a}}, 6_{\hat{c}} \rangle \cdot | 3_{\hat{w}}, -7_{\hat{z}}, a_{\hat{f}} \rangle$

$| 5_{\hat{a}}, 6_{\hat{c}}, a_{\hat{f}}, 8_{\hat{r}}, 9_{\hat{t}}, 2_{\hat{v}}, 3_{\hat{w}}, (-7)_{\hat{z}} \rangle$

You can apply an operator in a subspace to a ket of the space:
[ESC]eket[ESC] [ESC]on[ESC] [ESC]ebra[ESC] [ESC]on[ESC] [ESC]eeket[ESC]
Next press[TAB] several times till the first place holder (square) is selected.Then press:
a[TAB]q[TAB]j[TAB]q[TAB]0[TAB]c[TAB]j[TAB]q
and press at the same time[SHIFT]-[ENTER]

$| a_{\hat{q}} \rangle \cdot \langle j_{\hat{q}} | \cdot | 0_{\hat{c}}, j_{\hat{q}} \rangle$

$| 0_{\hat{c}}, a_{\hat{q}} \rangle$

Hermitian Conjugate

In order to calculate the Hermitian Conjugate of a ket press the keys:
[ESC]her[ESC] [TAB] [ESC]ket[ESC] [TAB]a
and press at the same time [SHIFT]-[ENTER]

$$\left(\,|\,a\rangle\right)^{\dagger}$$

$$\langle a\,|$$

In order to calculate the Hermitian Conjugate of an expresion press the following keys (Notice that the imaginary i is entered with two ii between two [ESC]):
[ESC]her[ESC][TAB]
(8+9[ESC]ii[ESC])*[ESC]eeket[ESC]+(5+7[ESC]ii[ESC])*[ESC]eeket[ESC]
Next press [TAB] several times till the first place holder (square) is selected. Then press:
0[TAB]c[TAB]3[TAB]q[TAB]1[TAB]c[TAB]-5[TAB]q
and press at the same time [SHIFT]-[ENTER]

$$\left((8+9\,i)\,\left|\,0_{\hat{c}},\,3_{\hat{q}}\right\rangle+(5+7\,i)*\left|\,1_{\hat{c}},\,-5_{\hat{q}}\right\rangle\right)^{\dagger}$$

$$(8-9\,i)\left\langle 0_{\hat{c}},\,3_{\hat{q}}\right|+(5-7\,i)\left\langle 1_{\hat{c}},\,(-5)_{\hat{q}}\right|$$

It also works in symbolic expressions
[ESC]her[ESC][TAB]
a[SPACE][ESC]ket[ESC]+[ESC]con[ESC][SPACE][ESC]ket[ESC]
Next press [TAB] several times till the first place holder (square) is selected. Then press:
x[TAB]b[TAB]y
and press at the same time [SHIFT]-[ENTER]

$$\left(a\,\,|\,x\rangle+(b)^{*}\,\,|\,y\rangle\right)^{\dagger}$$

$$a^{*}\langle x\,|+b\,\langle y\,|$$

Superpositions of Kets and Operators

This is the way to define a ket:
[ESC]ket[ESC]=a[ESC]eket[ESC]+b[ESC]eket[ESC]+c[ESC]eket[ESC]+d[ESC]eket[ESC]+e[ESC]eket[ESC]
Next press [TAB] several times till the first place holder (square) is selected. Then press:
[ESC]psi[ESC][TAB]1[TAB]q[TAB]2[TAB]q[TAB]3[TAB]q[TAB]4[TAB]q[TAB]5[TAB]q
finally press at the same time [SHIFT]-[ENTER]

$$|\,\psi\rangle=a\,\left|\,1_{\hat{q}}\right\rangle+b\,\left|\,2_{\hat{q}}\right\rangle+c\,\left|\,3_{\hat{q}}\right\rangle+d\,\left|\,4_{\hat{q}}\right\rangle+e\,\left|\,5_{\hat{q}}\right\rangle$$

$$a\,\left|\,1_{\hat{q}}\right\rangle+b\,\left|\,2_{\hat{q}}\right\rangle+c\,\left|\,3_{\hat{q}}\right\rangle+d\,\left|\,4_{\hat{q}}\right\rangle+e\,\left|\,5_{\hat{q}}\right\rangle$$

Mathematica calculates the corresponding bra:
[ESC]bra[ESC] [TAB] [ESC]psi[ESC]
finally press at the same time [SHIFT]-[ENTER]

```
⟨ψ |
```

$a^* \langle 1_{\hat{q}} | + b^* \langle 2_{\hat{q}} | + c^* \langle 3_{\hat{q}} | + d^* \langle 4_{\hat{q}} | + e^* \langle 5_{\hat{q}} |$

The internal product of a ket with its dual is a real number (square of its norm)
[ESC]bra[ESC] [ESC]on[ESC] [ESC]ket[ESC]
press [TAB] one or two times to select the first "place holder" (square) and press:
[ESC]psi[ESC] [TAB] [ESC]psi[ESC]
finally press at the same time [SHIFT]-[ENTER]

```
⟨ψ | · | ψ⟩
```

$a\, a^* + b\, b^* + c\, c^* + d\, d^* + e\, e^*$

Mathematica calculates the corresponding norm:
[ESC]norm[ESC] [TAB] [ESC]ket[ESC] [TAB] [ESC]psi[ESC]
finally press at the same time [SHIFT]-[ENTER]

```
‖ | ψ⟩‖
```

$\sqrt{a\, a^* + b\, b^* + c\, c^* + d\, d^* + e\, e^*}$

This external product is not immediately calculated:

```
| ψ⟩ · ⟨ψ |
```

$\left(a\, | 1_{\hat{q}} \rangle + b\, | 2_{\hat{q}} \rangle + c\, | 3_{\hat{q}} \rangle + d\, | 4_{\hat{q}} \rangle + e\, | 5_{\hat{q}} \rangle\right) \cdot \left(a^* \langle 1_{\hat{q}} | + b^* \langle 2_{\hat{q}} | + c^* \langle 3_{\hat{q}} | + d^* \langle 4_{\hat{q}} | + e^* \langle 5_{\hat{q}} |\right)$

The command Expand[] can be used to calculate the external product

```
Expand[ | ψ⟩ · ⟨ψ |]
```

$$
\begin{aligned}
&a\, a^* | 1_{\hat{q}} \rangle \cdot \langle 1_{\hat{q}} | + b\, a^* | 2_{\hat{q}} \rangle \cdot \langle 1_{\hat{q}} | + c\, a^* | 3_{\hat{q}} \rangle \cdot \langle 1_{\hat{q}} | + \\
&d\, a^* | 4_{\hat{q}} \rangle \cdot \langle 1_{\hat{q}} | + e\, a^* | 5_{\hat{q}} \rangle \cdot \langle 1_{\hat{q}} | + a\, b^* | 1_{\hat{q}} \rangle \cdot \langle 2_{\hat{q}} | + \\
&b\, b^* | 2_{\hat{q}} \rangle \cdot \langle 2_{\hat{q}} | + c\, b^* | 3_{\hat{q}} \rangle \cdot \langle 2_{\hat{q}} | + d\, b^* | 4_{\hat{q}} \rangle \cdot \langle 2_{\hat{q}} | + \\
&e\, b^* | 5_{\hat{q}} \rangle \cdot \langle 2_{\hat{q}} | + a\, c^* | 1_{\hat{q}} \rangle \cdot \langle 3_{\hat{q}} | + b\, c^* | 2_{\hat{q}} \rangle \cdot \langle 3_{\hat{q}} | + c\, c^* | 3_{\hat{q}} \rangle \cdot \langle 3_{\hat{q}} | + \\
&d\, c^* | 4_{\hat{q}} \rangle \cdot \langle 3_{\hat{q}} | + e\, c^* | 5_{\hat{q}} \rangle \cdot \langle 3_{\hat{q}} | + a\, d^* | 1_{\hat{q}} \rangle \cdot \langle 4_{\hat{q}} | + b\, d^* | 2_{\hat{q}} \rangle \cdot \langle 4_{\hat{q}} | + \\
&c\, d^* | 3_{\hat{q}} \rangle \cdot \langle 4_{\hat{q}} | + d\, d^* | 4_{\hat{q}} \rangle \cdot \langle 4_{\hat{q}} | + e\, d^* | 5_{\hat{q}} \rangle \cdot \langle 4_{\hat{q}} | + a\, e^* | 1_{\hat{q}} \rangle \cdot \langle 5_{\hat{q}} | + \\
&b\, e^* | 2_{\hat{q}} \rangle \cdot \langle 5_{\hat{q}} | + c\, e^* | 3_{\hat{q}} \rangle \cdot \langle 5_{\hat{q}} | + d\, e^* | 4_{\hat{q}} \rangle \cdot \langle 5_{\hat{q}} | + e\, e^* | 5_{\hat{q}} \rangle \cdot \langle 5_{\hat{q}} |
\end{aligned}
$$

Here we define another ket
[ESC]ket[ESC]=u[ESC]eket[ESC]+v[ESC]eket[ESC]+w[ESC]eket[ESC]+x[ESC]eket[ESC]+y[ESC]eket[ESC]
Next press [TAB] several times till the first place holder (square) is selected. Then press:
m[TAB]1[TAB]q[TAB]2[TAB]q[TAB]3[TAB]q[TAB]4[TAB]q[TAB]5[TAB]q
finally press at the same time [SHIFT]-[ENTER]

$$| m\rangle = u\ |1_{\hat{q}}\rangle + v\ |2_{\hat{q}}\rangle + w\ |3_{\hat{q}}\rangle + x\ |4_{\hat{q}}\rangle + y\ |5_{\hat{q}}\rangle$$

$$u\ |1_{\hat{q}}\rangle + v\ |2_{\hat{q}}\rangle + w\ |3_{\hat{q}}\rangle + x\ |4_{\hat{q}}\rangle + y\ |5_{\hat{q}}\rangle$$

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

```
? m
```

```
Global`m
```

$$| m\rangle \mathrel{\wedge}= u\ |1_{\hat{q}}\rangle + v\ |2_{\hat{q}}\rangle + w\ |3_{\hat{q}}\rangle + x\ |4_{\hat{q}}\rangle + y\ |5_{\hat{q}}\rangle$$

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

$$\text{Expand}[\ |\psi\rangle \cdot \langle m\ |]$$

$$\begin{aligned}
&a\,u^*\ |1_{\hat{q}}\rangle\cdot\langle 1_{\hat{q}}| + b\,u^*\ |2_{\hat{q}}\rangle\cdot\langle 1_{\hat{q}}| + c\,u^*\ |3_{\hat{q}}\rangle\cdot\langle 1_{\hat{q}}| +\\
&d\,u^*\ |4_{\hat{q}}\rangle\cdot\langle 1_{\hat{q}}| + e\,u^*\ |5_{\hat{q}}\rangle\cdot\langle 1_{\hat{q}}| + a\,v^*\ |1_{\hat{q}}\rangle\cdot\langle 2_{\hat{q}}| +\\
&b\,v^*\ |2_{\hat{q}}\rangle\cdot\langle 2_{\hat{q}}| + c\,v^*\ |3_{\hat{q}}\rangle\cdot\langle 2_{\hat{q}}| + d\,v^*\ |4_{\hat{q}}\rangle\cdot\langle 2_{\hat{q}}| +\\
&e\,v^*\ |5_{\hat{q}}\rangle\cdot\langle 2_{\hat{q}}| + a\,w^*\ |1_{\hat{q}}\rangle\cdot\langle 3_{\hat{q}}| + b\,w^*\ |2_{\hat{q}}\rangle\cdot\langle 3_{\hat{q}}| + c\,w^*\ |3_{\hat{q}}\rangle\cdot\langle 3_{\hat{q}}| +\\
&d\,w^*\ |4_{\hat{q}}\rangle\cdot\langle 3_{\hat{q}}| + e\,w^*\ |5_{\hat{q}}\rangle\cdot\langle 3_{\hat{q}}| + a\,x^*\ |1_{\hat{q}}\rangle\cdot\langle 4_{\hat{q}}| + b\,x^*\ |2_{\hat{q}}\rangle\cdot\langle 4_{\hat{q}}| +\\
&c\,x^*\ |3_{\hat{q}}\rangle\cdot\langle 4_{\hat{q}}| + d\,x^*\ |4_{\hat{q}}\rangle\cdot\langle 4_{\hat{q}}| + e\,x^*\ |5_{\hat{q}}\rangle\cdot\langle 4_{\hat{q}}| + a\,y^*\ |1_{\hat{q}}\rangle\cdot\langle 5_{\hat{q}}| +\\
&b\,y^*\ |2_{\hat{q}}\rangle\cdot\langle 5_{\hat{q}}| + c\,y^*\ |3_{\hat{q}}\rangle\cdot\langle 5_{\hat{q}}| + d\,y^*\ |4_{\hat{q}}\rangle\cdot\langle 5_{\hat{q}}| + e\,y^*\ |5_{\hat{q}}\rangle\cdot\langle 5_{\hat{q}}|
\end{aligned}$$

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

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

$$a\,u^* + b\,v^* + c\,w^* + d\,x^* + e\,y^*$$

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

$$\hat{q}\cdot\ |\psi\rangle$$

$$a\ |1_{\hat{q}}\rangle + 2\,b\ |2_{\hat{q}}\rangle + 3\,c\ |3_{\hat{q}}\rangle + 4\,d\ |4_{\hat{q}}\rangle + 5\,e\ |5_{\hat{q}}\rangle$$

This is one way to define another operator. Notice that p is **not** inside the operator template:

$$p = f \left| 1_{\hat{q}} \right\rangle \cdot \left\langle 2_{\hat{q}} \right| + g \left| 2_{\hat{q}} \right\rangle \cdot \left\langle 4_{\hat{q}} \right|$$

$$f \left| 1_{\hat{q}} \right\rangle \cdot \left\langle 2_{\hat{q}} \right| + g \left| 2_{\hat{q}} \right\rangle \cdot \left\langle 4_{\hat{q}} \right|$$

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

$$p \cdot \left| \psi \right\rangle$$

$$b\, f \left| 1_{\hat{q}} \right\rangle + d\, g \left| 2_{\hat{q}} \right\rangle$$

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

$$p \cdot \hat{q} \cdot \left| \psi \right\rangle$$

$$2\, b\, f \left| 1_{\hat{q}} \right\rangle + 4\, d\, g \left| 2_{\hat{q}} \right\rangle$$

Hermitian conjugate
[ESC]her[ESC]

$$(p)^{\dagger}$$

$$f^{*} \left| 2_{\hat{q}} \right\rangle \cdot \left\langle 1_{\hat{q}} \right| + g^{*} \left| 4_{\hat{q}} \right\rangle \cdot \left\langle 2_{\hat{q}} \right|$$

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

$$\left\langle \psi \right| \cdot p \cdot \left| \psi \right\rangle$$

$$b\, f\, a^{*} + d\, g\, b^{*}$$

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

$$\left\langle \psi \right| \cdot \hat{q} \cdot \left| \psi \right\rangle$$

$$a\, a^{*} + 2\, b\, b^{*} + 3\, c\, c^{*} + 4\, d\, d^{*} + 5\, e\, e^{*}$$

Here is another operator :

$$ope = a \left| 1_{\hat{q}}, 3_{\hat{s}} \right\rangle \cdot \left\langle 1_{\hat{q}}, 3_{\hat{s}} \right| + b \left| 2_{\hat{q}}, 4_{\hat{s}} \right\rangle \cdot \left\langle 3_{\hat{q}}, 2_{\hat{s}} \right| + c \left| 3_{\hat{q}}, 5_{\hat{s}} \right\rangle \cdot \left\langle 4_{\hat{q}}, 5_{\hat{s}} \right|$$

$$a \left| 1_{\hat{q}}, 3_{\hat{s}} \right\rangle \cdot \left\langle 1_{\hat{q}}, 3_{\hat{s}} \right| + b \left| 2_{\hat{q}}, 4_{\hat{s}} \right\rangle \cdot \left\langle 3_{\hat{q}}, 2_{\hat{s}} \right| + c \left| 3_{\hat{q}}, 5_{\hat{s}} \right\rangle \cdot \left\langle 4_{\hat{q}}, 5_{\hat{s}} \right|$$

Mathematica can calculate the partial trace with respect to operator $\hat{q}$:
[ESC]trace[ESC]

```
Tr_q̂[ope]
```

```
a |3_ŝ⟩ · ⟨3_ŝ|
```

Mathematica can calculate the partial trace with respect to operator $\hat{s}$:
[ESC]trace[ESC]

```
Tr_ŝ[ope]
```

```
a |1_q̂⟩ · ⟨1_q̂| + c |3_q̂⟩ · ⟨4_q̂|
```

Undefined Symbols are Assumed to be Scalars

Any undefined name, like B, is assumed to be a complex scalar:
[ESC]her[ESC]

```
Clear[B];
(⟨α| · B · |β⟩)†
```

```
B* ⟨β | α⟩
```

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

```
SetQuantumObject[B]
```

```
The object B will Not be considered as a complex scalar
The object B[args] will Not be considered as a complex scalar
The object Subscript[B, __] will Not be considered as a complex scalar
The object Subscript[B, __][args] will Not be considered as a complex scalar
 The object Subscript[B[___], __] will Not be considered as a complex scalar
The object Subscript[B[___], __][args] will Not be considered as a complex scalar
```

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

```
(⟨α| · B · |β⟩)†
```

```
⟨β| · B† · |α⟩
```

Finally we clear the definitions made in this document:

```
Clear[m, p, ope, ψ, B]
```

ReplaceAll versus QuantumReplaceAll

ReplaceAll is a standard *Mathematica* command that can take advantage of the pattern recognitizion language of *Mathematica.* The "delayed rule" symbol :→ can be entered by pressing the keys [ESC]:>[ESC]

```
ReplaceAll[a |ϕ⟩ + b |ψ⟩, |ϕ⟩ :→ (|0⟩ + |1⟩) / √2]
```

$$\frac{a\,(|0\rangle + |1\rangle)}{\sqrt{2}} + b\,|\psi\rangle$$

However, ReplaceAll will not make any replacement in the following case, because the expression $|\phi\rangle \otimes |\psi\rangle$ evolves to $|\phi, \psi\rangle$, and the *Mathematica* command ReplaceAll does not recognize the ket $|\phi\rangle$ in this evolved expression:

```
ReplaceAll[|ϕ⟩ ⊗ |ψ⟩, |ϕ⟩ :→ (|0⟩ + |1⟩) / √2]
```

$$|\phi, \psi\rangle$$

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

```
QuantumReplace[|ϕ⟩ ⊗ |ψ⟩, |ϕ⟩ :→ (|0⟩ + |1⟩) / √2]
```

$$\frac{|0, \psi\rangle + |1, \psi\rangle}{\sqrt{2}}$$

QuantumReplaceAll will also work on bras:

```
QuantumReplace[|ψ⟩ · ⟨ϕ|, |ϕ⟩ :→ (|0⟩ + |1⟩) / √2]
```

$$\frac{|\psi\rangle \cdot (\langle 0| + \langle 1|)}{\sqrt{2}}$$

```
Expand[QuantumReplace[|ψ⟩ · ⟨ϕ|, |ϕ⟩ :→ (|0⟩ + |1⟩) / √2]]
```

$$\frac{|\psi\rangle \cdot \langle 0|}{\sqrt{2}} + \frac{|\psi\rangle \cdot \langle 1|}{\sqrt{2}}$$

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 $|\,3_{\hat{A}}\rangle$ 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⟩ = | a⟩ + | b⟩
```

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

```
| m⟩ = | a⟩ + | b⟩
```

Answer:

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