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# Two Different Ways of Creating Quantum Symbolic Operators

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## Introduction

This document shows different ways to create operators in the Quantum *Mathematica* add-on. The main characteristic of an operator is that its "noncommutative quantum application" is **not** transformed into a normal, commutative multiplication.

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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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## Undefined Symbols are Assumed to be Scalars

First we clear (erase) values and definitions for the symbols that will be used in the examples:

```
Clear[a, b]
```

Symbols are assumed to be scalars by default. This means that their "noncommutative quantum application" is automatically transformed into an ordinary commutative multiplication.

Press the keys:

b [ESC]on[ESC] a

then press at the same time [SHIFT]-[ENTER] to evaluate. Notice that the "noncommutative quantum application" b·a is transformed into the ordinary commutative multiplication ab:

b · a

a b

Scalars are pulled out as multiplicative factors, and the hermitian conjugate of scalars becomes the ordinary complex conjugate.

Press the keys:

[ESC]her[ESC][TAB][ESC]bra[ESC][ESC]on[ESC] b [ESC]on[ESC][ESC]ket[ESC]

press [TAB] one or two times to select the first place-holder (square) and press:

x[TAB]y

finally press at the same time [SHIFT]-[ENTER] to evaluate. Notice that b is pulled out as a multiplicative factor, and that the hermitian conjugate  $b^+$  becomes the complex conjugate  $b^*$ :

(⟨x | · b · | y⟩)<sup>†</sup>

b\* ⟨y | x⟩

The commutator of scalars is zero  $[[a, b]]_ = a \cdot b - b \cdot a = ab - ab = 0$

Press the keys:

[ESC]comm[ESC][TAB]a[TAB]b

finally press at the same time [SHIFT]-[ENTER] to evaluate.

[[a, b]]\_

0

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## First way to define new symbolic operators: Use SetQuantumObject[]

First we clear (erase) values and definitions for the symbols that will be used in the examples:

Clear[c, d]

The command SetQuantumObject[] is used to specify that c and d are operators. The semicolon ; prevents *Mathematica* from printing a confirmation message:

SetQuantumObject[c, d];

This time the "noncommutative quantum application" is **not** transformed into a multiplication:

d [ESC]on[ESC] c

then press at the same time [SHIFT]-[ENTER] to evaluate:

$$\mathbf{d} \cdot \mathbf{c}$$

$$d \cdot c$$

This time the hermitian conjugate is **not** transformed into a complex conjugate:

[ESC]her[ESC][TAB][ESC]bra[ESC][ESC]on[ESC] c [ESC]on[ESC][ESC]ket[ESC]

press [TAB] one or two times to select the first place-holder (square) and press:

x[TAB]y

finally press at the same time [SHIFT]-[ENTER] to evaluate. Hermitian conjugation rules are applied, but  $c^\dagger$  is **not** transformed into  $c^*$

$$(\langle \mathbf{x} | \cdot \mathbf{c} \cdot | \mathbf{y} \rangle)^\dagger$$

$$\langle \mathbf{y} | \cdot \mathbf{c}^\dagger \cdot | \mathbf{x} \rangle$$

This time the commutator  $[[c, d]]_- = c \cdot d - d \cdot c$  is **not** equal to zero:

Press the keys:

[ESC]comm[ESC][TAB]c[TAB]d

finally press at the same time [SHIFT]-[ENTER] to evaluate.

$$[[c, d]]_-$$

$$[[c, d]]_-$$

The commutator can be evaluated using the command EvaluateCommutators

$$\text{EvaluateCommutators}[[c, d]]_-$$

$$-d \cdot c + c \cdot d$$


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## Second way to define new symbolic operators: Use DefineOperatorOnKets[]

First we clear (erase) values and definitions for the symbols that will be used in the examples:

$$\text{Clear}[e, f]$$

Here we define "e" as an operator that will have a specific effect on kets. The standard *Mathematica* symbol  $\Rightarrow$  can be entered by pressing [ESC]:>[ESC]

$$\text{DefineOperatorOnKets}[e, \{ | \mathbf{x}_- \rangle \Rightarrow | \mathbf{x} + 1 \rangle \}]$$

$$| \mathbf{x}_- \rangle \Rightarrow | \mathbf{x} + 1 \rangle$$

This is the operator "e" acting on a ket:

$$\mathbf{e} \cdot |4\rangle$$

$$|5\rangle$$

Here we define "f" as an operator that will have a specific effect on kets. The standard *Mathematica* symbol  $\rightarrow$  can be entered by pressing [ESC]:>[ESC]

$$\text{DefineOperatorOnKets}[\mathbf{f}, \{ |x\rangle \rightarrow |x-1\rangle \}]$$

$$|x\rangle \rightarrow |x-1\rangle$$

This is the operator "f" acting on a ket:

$$\mathbf{f} \cdot |4\rangle$$

$$|3\rangle$$

This time the "noncommutative quantum application" is **not** transformed into a multiplication:

f[ESC]on[ESC] e

then press at the same time [SHIFT]-[ENTER] to evaluate:

$$\mathbf{f} \cdot \mathbf{e}$$

$$\mathbf{f} \cdot \mathbf{e}$$

This time the hermitian conjugate is **not** transformed into a complex conjugate.

Press [ESC]her[ESC][TAB]f

$$(\mathbf{f})^\dagger$$

$$\mathbf{f}^\dagger$$

This time the commutator  $[[e, f]] = e \cdot f - f \cdot e$  is **not** equal to zero:

Press the keys:

[ESC]comm[ESC][TAB]c[TAB]d

finally press at the same time [SHIFT]-[ENTER] to evaluate.

$$[[\mathbf{e}, \mathbf{f}]]$$

$$[[\mathbf{e}, \mathbf{f}]]$$