Step-by-step setup of Kets, Operators, Commutators and Algebra for the Quantum Harmonic Oscillator in *Mathematica*

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Introduction

This is a step-by-step tutorial on the use of Quantum *Mathematica* add-on to define kets, operators and commutators properties of the Harmonic Oscillator. This tutorial uses the notation of the book by C. Cohen-Tannoudji, B. Diu and F. Laloë, "Quantum Mechanics", Volume 1, Chapter V

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[];
```

Step-by-step implementation of the harmonic oscillator

In order to enter a ket similar to those that appear in the book of Cohen-Tannoudji, Chapter V, press the keyboard keys (this will only work in a *Mathematica* document where SetQuantumAliases[] has been executed):
[ESC]ket[ESC]
The ket template will appear. Next press the keys:
[TAB][ESC]su[ESC]
A subscript template will appear inside the ket. Next press the keys:
[TAB][ESC]phi[ESC][TAB]n
Finally press at the same time the keys SHIFT-ENTER to evaluate:

```
| ϕn〉
```

```
| ϕn〉
```

Here we define the effect of the operator "a" on the ket $|\phi_n\rangle$. The standard *Mathematica* symbol :→ can be entered pressing the keys [ESC]:>[ESC], and the square root symbol can be entered by pressing at the same time the keys [CTRL]2. Notice the use of the underscore _ on the left hand side of the assignment, in the subscript $|\phi_{n\_}\rangle$:

```
DefineOperatorOnKets[a, {| ϕn_〉 :→ √n | ϕn-1〉}]
```

```
| ϕn_〉 :→ √n | ϕn-1〉
```

In order to enter the operator in the appropiate syntax press the keys:
a[ESC]on[ESC]
after that enter $|\phi_n\rangle$ as it was done above.
Finally press at the same time the keys [SHIFT] and [ENTER] to evaluate:

```
a · | ϕn〉
```

$$\sqrt{n}\ |\phi_{-1+n}\rangle$$

Powers of the operator on the ket are also calculated (in order to write the power superscript, you can either use the standard *Mathematica* shortcut, pressing at the same time the keys [CTRL]6 or you can use the Quantum shortcut [ESC]po[ESC]):

```
a³ · | ϕn〉
```

$$\sqrt{-2+n}\ \sqrt{-1+n}\ \sqrt{n}\ |\phi_{-3+n}\rangle$$

The definition works for numerical states (copy-paste the previous input from your *Mathematica* document and change "n" to 7):

```
a · | ϕ7〉
```

$$\sqrt{7}\ |\phi_6\rangle$$

The definition of an operator on a ket also defines the operation of a bra on the hermitian conjugate of the operator (press [ESC]bra[ESC] for the bra template, [ESC]on[ESC] for the infix symbol "·" and [ESC]her[ESC] for the hermitian conjugate template):

$\langle \phi_7 \,| \cdot (\mathbf{a})^\dagger$

$\sqrt{7}\ \langle \phi_6 \,|$

In order to enter a power of the hermitian conjugate of operator a, press the keys:
a[CTRL]6[ESC]dg [ESC][SPACE]3

$\langle \phi_7 \,| \cdot \mathbf{a}^{\dagger\, 3}$

$\sqrt{210}\ \langle \phi_4 \,|$

However the effect of the hermitian conjugate of the operator on a ket is undefined (press [ESC]her[ESC] for the hermitian conjugate template, or press a[CTRL]6[ESC]dg[ESC]):

$\mathbf{a}^\dagger \cdot \,| \phi_7 \rangle$

$a^\dagger \cdot \,| \phi_7 \rangle$

The effect of the hermitian conjugate of the operator on a ket can be defined using DefineOperatorOnKets. Notice the use of the underscore _ on the left hand side of the assignment, in the subscript

$\mathbf{DefineOperatorOnKets}\left[\mathbf{a}^\dagger, \left\{ \,\middle| \phi_{n\_} \right\rangle :\!\to \sqrt{n+1}\ \,| \phi_{n+1} \rangle \right\}\Big]$

$\left| \phi_{n\_} \right\rangle :\!\to \sqrt{n+1}\ \,| \phi_{n+1} \rangle$

This time $a^\dagger$ acts on the ket:

$\mathbf{a}^\dagger \cdot \,| \phi_7 \rangle$

$2\sqrt{2}\ \,| \phi_8 \rangle$

In order to enter a power of the hermitian conjugate of operator a, press the keys:
a[CTRL]6[ESC]dg [ESC][SPACE]3

$\mathbf{a}^{\dagger\, 3} \cdot \,| \phi_7 \rangle$

$12\sqrt{5}\ \,| \phi_{10} \rangle$

We can try calculating matrix elements, however *Mathematica* does not know (yet) that these vectors are orthonormal:

```
⟨ϕ8 | · a† · | ϕ7⟩
```

$2\sqrt{2}\ \langle \phi_8 \mid \phi_8 \rangle$

Next we indicate that the kets are orthonormal. The standard *Mathematica* command KroneckerDelta is used. Notice that no output will be generated after pressing SHIFT-ENTER in this command, because it is a delayed assignment (using := instead of =), and also notice the use of the underscores _ in the left-hand side of the assignment:

```
⟨ϕj_ | · | ϕk_⟩ := KroneckerDelta[j - k]
```

Now the vectors are orthonormal:

```
⟨ϕ8 | · | ϕ8⟩
```

1

```
⟨ϕ8 | · | ϕ9⟩
```

0

```
⟨ϕm | · | ϕn⟩
```

KroneckerDelta[m - n]

Now we can get our matrix element:

```
⟨ϕ8 | · a† · | ϕ7⟩
```

$2\sqrt{2}$

We can use the standard *Mathematica* command Table to generate a matrix representing the operator "a" for a finite number of states. This matrix corresponds to the matrix (C-24-a) in the page 499 in the book of Cohen-Tannoudji.

```
mymatrix = Table[⟨ϕj | · a · | ϕk⟩, {j, 1, 8}, {k, 1, 8}];
MatrixForm[mymatrix]
```

$$\begin{pmatrix} 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\sqrt{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Mathematica can calculate the effect of "algebraic" expressions including the operators and kets that were defined above (in order to write the power superscript, you can either use the standard *Mathematica* shortcut, pressing at the same time the keys CTRL6 or you can use the Quantum shortcut [ESC]po[ESC]):

```
(a + a†)² · |ϕ₇⟩
```

```
√42 |ϕ₅⟩ + 15 |ϕ₇⟩ + 6 √2 |ϕ₉⟩
```

Here is a TEX version of the result:

```
TeXForm[√42 |ϕ₅⟩ + 15 |ϕ₇⟩ + 6 √2 |ϕ₉⟩]
```

```
\sqrt{42} \left|\phi _5\right\rangle +15 \left|\phi
   _7\right\rangle +6 \sqrt{2} \left|\phi
   _9\right\rangle
```

On the other hand, the expression itself does not evolve to any result:

```
(a + a†)²
```

```
(a + a†)²
```

We can expand the expression using the command Expand:

```
Expand[(a + a†)²]
```

```
a² + a† · a + a · a† + (a†)²
```

The expansion has exactly the same effect on a ket as the original expresion:

```
(a² + a† · a + a · a† + (a†)²) · |ϕ₇⟩
```

```
√42 |ϕ₅⟩ + 15 |ϕ₇⟩ + 6 √2 |ϕ₉⟩
```

Another type of expansion (using commutators) is obtained with the Quantum *Mathematica* command CommutatorExpand. However, *Mathematica* does not know (yet) that the commutator of these operators is equal to one.

```
CommutatorExpand[(a + a†)²]
```

```
a² - ⟦a, a†⟧₋ + 2 a · a† + (a†)²
```

A different expansion is obtained with the option ReverseOrdering → True (the standard *Mathematica* symbol -> can be entered pressing the keys [ESC]->[ESC]):

```
CommutatorExpand[(a + a†)^2, ReverseOrdering → True]
```

$a^2 - [\![a^\dagger, a]\!]_- + 2\, a^\dagger \cdot a + (a^\dagger)^2$

The expansion has exactly the same effect on a ket as the original expresion:

```
(a^2 - ⟦a†, a⟧_ + 2 a† · a + (a†)^2) · |ϕ7⟩
```

$\sqrt{42}\ |\phi_5\rangle + 15\ |\phi_7\rangle + 6\sqrt{2}\ |\phi_9\rangle$

The Quantum *Mathematica* command EvaluateCommutators forces the evaluation of commutators. Notice that the result is the same as before:

```
EvaluateCommutators[(a^2 - ⟦a†, a⟧_ + 2 a† · a + (a†)^2)]
```

$a^2 + a^\dagger \cdot a + a \cdot a^\dagger + (a^\dagger)^2$

The TraditionalForm of an expression is usually easier to read:

```
TraditionalForm[a^2 + a† · a + a · a† + (a†)^2]
```

$a^\dagger a + a a^\dagger + (a^\dagger)^2 + a^2$

Here the value "one" is assigned to the commutator. Press the keys [ESC]comm[ESC] in order to enter the commutator template:

```
⟦a, a†⟧_ = 1
```

1

This time QuantumExpand uses the value of the commutator:

```
CommutatorExpand[(a + a†)^2]
```

$-1 + a^2 + 2\, a \cdot a^\dagger + (a^\dagger)^2$

The TraditionalForm representation can be easier to read:

```
TraditionalForm[CommutatorExpand[(a + a†)^2]]
```

$2\, a a^\dagger + (a^\dagger)^2 + a^2 - 1$

Here is a $\TeX$ version of the TraditionalForm:

```
TeXForm[TraditionalForm[CommutatorExpand[(a + a†)^2]]]
```

```
2 aa^{\dagger }+\left(a^{\dagger }\right)^2+a^2-1
```

Symbolic calculations can be performed:

$(a + a^\dagger)^2 \cdot |\phi_k\rangle$

$\sqrt{-1+k}\ \sqrt{k}\ |\phi_{-2+k}\rangle + k\ |\phi_k\rangle + (1+k)\ |\phi_k\rangle + \sqrt{1+k}\ \sqrt{2+k}\ |\phi_{2+k}\rangle$

Standard *Mathematica* commands (for example Collect) can be used on the expression:

$\text{Collect}\left[(a + a^\dagger)^2 \cdot |\phi_k\rangle,\ |\phi_k\rangle\right]$

$\sqrt{-1+k}\ \sqrt{k}\ |\phi_{-2+k}\rangle + (1+2k)\ |\phi_k\rangle + \sqrt{1+k}\ \sqrt{2+k}\ |\phi_{2+k}\rangle$

Here is another simple example

$(a^\dagger \cdot a)^3 \cdot |\phi_k\rangle$

$k^3\ |\phi_k\rangle$

This is the corresponding commutator expansion. It is using the known value for the commutator of these two operators:

$\text{CommutatorExpand}\left[(a^\dagger \cdot a)^3\right]$

$-1 + a \cdot a^\dagger - 3\left(-2a + a^2 \cdot a^\dagger\right) \cdot a^\dagger + \left(-3a^2 + a^3 \cdot a^\dagger\right) \cdot (a^\dagger)^2$

Expand and CommutatorExpand can be combined:

$\text{Expand}\left[\text{CommutatorExpand}\left[(a^\dagger \cdot a)^3\right]\right]$

$-1 + 7a \cdot a^\dagger - 6a^2 \cdot (a^\dagger)^2 + a^3 \cdot (a^\dagger)^3$

Quantum *Mathematica* commands as CollectFromRight can be used on this expression:

$\text{CollectFromRight}\left[-1 + 7a \cdot a^\dagger - 6a^2 \cdot (a^\dagger)^2 + a^3 \cdot (a^\dagger)^3\right]$

$-1 + \left(7a + \left(-6a^2 + a^3 \cdot a^\dagger\right) \cdot a^\dagger\right) \cdot a^\dagger$

The result of the quantum expansion on a ket is the same as with the original expression:

```
Simplify[(-1 + (7 a + (-6 a^2 + a^3 · a†) · a†) · a†) ·  | ϕk〉]
```

```
k^3  | ϕk〉
```

We define the position representation using the standard *Mathematica* command HermiteH and the standard *Mathematica* pattern _?NumberQ, which means that this definition will be used only when x is a number:

```
〈x_?NumberQ | ·  | ϕk_〉 := Exp[-x^2 / 2] * HermiteH[k, x] / Sqrt[2^k * k! * Sqrt[Pi]]
```

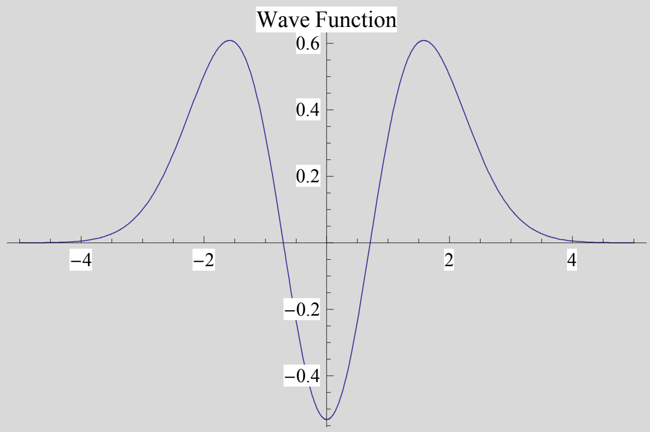
This is the value of the wave function when x=0.5

```
〈0.5 | ·  | ϕ2〉
```

```
-0.234359
```

We can plot the wave function:

```
Plot[〈x | ·  | ϕ2〉, {x, -5, 5}, PlotLabel → "Wave Function"]
```



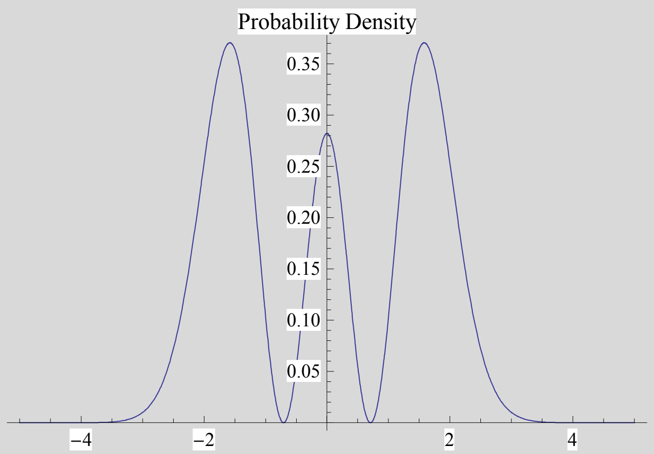
This is the value of the probability density function when x=0.5
(press the keys [ESC]norm[ESC] in order to write the quantum Norm template)

```
‖〈0.5 | ·  | ϕ2〉‖^2
```

```
0.0549239
```

We can plot the probability density
(press the keys [ESC]norm[ESC] in order to write the quantum Norm template)

```
Plot[‖⟨x | · | ϕ₂⟩‖², {x, -5, 5}, PlotLabel → "Probability Density"]
```



Next we verify that the function is normalized:

```
NIntegrate[‖⟨x | · | ϕ₂⟩‖², {x, -5, 5}]
```

```
1.
```

Summary

These are all the definitions that were explained above. They correspond to the Quantum Harmonic Oscillator:

```
Needs["Quantum`Notation`"];
⟨ϕj_ | · | ϕk_⟩ := KroneckerDelta[j - k];
DefineOperatorOnKets[a, { | ϕn_⟩ :→ √n | ϕn-1⟩}];
DefineOperatorOnKets[(a)†, { | ϕn_⟩ :→ √(n + 1) | ϕn+1⟩}];
⟦a, a†⟧_ = 1;
⟨x_?NumberQ | · | ϕk_⟩ := Exp[-x^2 / 2] * HermiteH[k, x] / √(2^k * k! * √Pi);
```

Simple and complex operations can be performed after evaluating those definitions:

```
a^4 · | ϕ7⟩
```

```
2 √210 | ϕ3⟩
```

Simple and complex operations can be performed after evaluating those definitions:

```
CommutatorExpand[(a + a†)^3]
```

```
-3 a + a^3 + 3 a^2 · a† + 3 a · (a†)^2 - 3 a† + (a†)^3
```

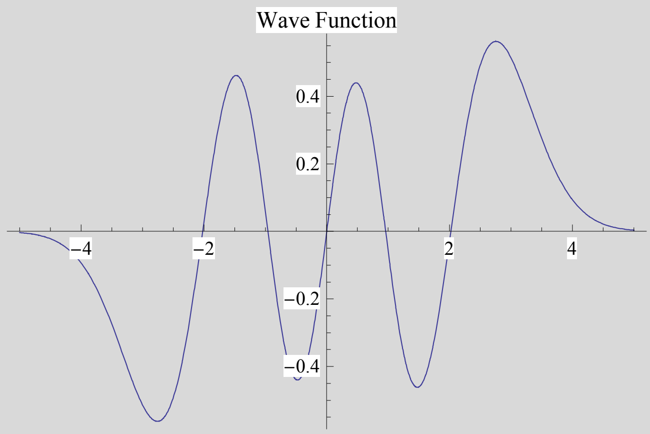
Simple and complex operations can be performed after evaluating those definitions:

```
mymatrix = Table[⟨ϕj | · (a + a†)^3 · | ϕk⟩, {j, 1, 8}, {k, 1, 8}];
MatrixForm[mymatrix]
```

$$\begin{pmatrix} 0 & 6\sqrt{2} & 0 & 2\sqrt{6} & 0 & 0 & 0 & 0 \\ 6\sqrt{2} & 0 & 9\sqrt{3} & 0 & 2\sqrt{15} & 0 & 0 & 0 \\ 0 & 9\sqrt{3} & 0 & 24 & 0 & 2\sqrt{30} & 0 & 0 \\ 2\sqrt{6} & 0 & 24 & 0 & 15\sqrt{5} & 0 & \sqrt{210} & 0 \\ 0 & 2\sqrt{15} & 0 & 15\sqrt{5} & 0 & 18\sqrt{6} & 0 & 4\sqrt{21} \\ 0 & 0 & 2\sqrt{30} & 0 & 18\sqrt{6} & 0 & 21\sqrt{7} & 0 \\ 0 & 0 & 0 & \sqrt{210} & 0 & 21\sqrt{7} & 0 & 48\sqrt{2} \\ 0 & 0 & 0 & 0 & 4\sqrt{21} & 0 & 48\sqrt{2} & 0 \end{pmatrix}$$

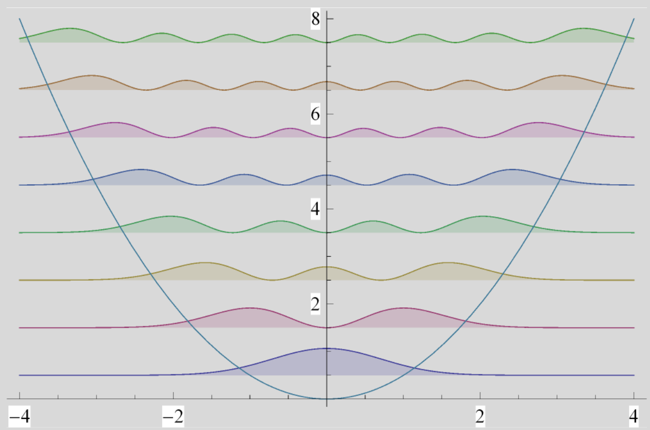
Simple and complex operations can be performed after evaluating those definitions:

```
Plot[⟨x | · | ϕ5⟩, {x, -5, 5}, PlotLabel → "Wave Function"]
```



Simple and complex operations can be performed after evaluating those definitions:

```
Plot[
 Evaluate[Append[Table[‖⟨x | · | ϕn⟩‖^2 + n + 1/2, {n, 0, 7}], x^2/2]],
 {x, -4, 4}, Filling -> Table[n → n - 1/2, {n, 1, 8}]]
```



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