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 I, Chapter V

**Load the Package**

First load the Quantum`Notation` package. Write:

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

then press at the same time the keys `Shift-Enter` to evaluate. *Mathematica* will load the package:

```
Needs["Quantum`Notation`"]
```

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 `Shift-Enter` to evaluate. The semicolon prevents *Mathematica* from printing the help message. Remember that `SetQuantumAliases[]` must be evaluated again in each new notebook:
**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:

```
| φ_n >
| φ_n >
```

Here we define the effect of the operator "a" on the ket `| φ_n >`. 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 `| φ_n_`

```
DefineOperatorOnKets[a, { | φ_n_ -> Sqrt[n] | φ_{n-1} > }]
```

In order to enter the operator in the appropriate syntax press the keys:

```
a[ESC]on[ESC]
```

after that enter `| φ_n >` as it was done above.

Finally press at the same time the keys `SHIFT` and `ENTER` to evaluate:

```
a · | φ_n >
| Sqrt[n] | φ_{n-1} >
```

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]`):

```
a^3 · | φ_n >
| Sqrt[-2 + n] · Sqrt[-1 + n] · Sqrt[n] | φ_{3+n} >
```

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

```
a · | φ_7 >
| Sqrt[7] | φ_6 >
```
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 \[\cdot\] and [ESC]her[ESC] for the hermitian conjugate template):

\[ \langle \phi_7 | \cdot (a)^\dagger \]
\[ \sqrt{7} \langle \phi_6 | \]

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

\[ \langle \phi_7 | \cdot a^{13} \]
\[ \sqrt{210} \langle \phi_4 | \]

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]):

\[ a^\dagger \cdot | \phi_7 \rangle \]
\[ a^\dagger \cdot | \phi_7 \rangle \]

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

\[
\text{DefineOperatorOnKets}[a^\dagger, \{ | \phi_{n..} \rangle \mapsto \sqrt{n+1} \ | \phi_{n+1} \rangle \}]
\]

\[ | \phi_{n..} \rangle \mapsto \sqrt{n+1} \ | \phi_{n+1} \rangle \]

This time \(a^\dagger\) acts on the ket:

\[ a^\dagger : | \phi_7 \rangle \]
\[ 2 \sqrt{2} | \phi_8 \rangle \]

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

\[ a^{13} \cdot | \phi_7 \rangle \]
\[ 12 \sqrt{5} | \phi_{10} \rangle \]

We can try calculating matrix elements, however Mathematica does not know (yet) that these vectors are orthonormal:
Next we indicate that the kets are orthonormal. The standard Mathematica command KroneckerDelta is used. Notice that no output will be generated after pressing \[\text{\textasciitilde}-\text{\textasciitilde}\] in this command, because it is a delayed assignment (using \texttt{:=} instead of \texttt{=}), and also notice the use of the underscores \_ in the left-hand side of the assignment:

\[
\langle \phi_j \mid \cdot \mid \phi_k \rangle := \text{KroneckerDelta}[j - k]
\]

Now the vectors are orthonormal:

\[
\langle \phi_8 \mid \cdot \mid \phi_8 \rangle = 1
\]

\[
\langle \phi_8 \mid \cdot \mid \phi_9 \rangle = 0
\]

\[
\langle \phi_m \mid \cdot \mid \phi_n \rangle = \text{KroneckerDelta}[m - n]
\]

Now we can get our matrix element:

\[
\langle \phi_8 \mid \cdot \mid a^\dagger \cdot \mid \phi_7 \rangle = 2 \sqrt{2}
\]

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.

\[
\text{mymatrix} = \text{Table}[\langle \phi_j \mid \cdot \mid a \cdot \mid \phi_k \rangle, \{j, 1, 8\}, \{k, 1, 8\}];
\]

\[
\text{MatrixForm}[\text{mymatrix}]
\]
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 \[CTRL\]6 or you can use the Quantum shortcut [ESC]po[ESC]):

\[(a + a^\dagger)^2 \cdot |\phi\rangle\]

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

Here is a \TeX version of the result:

\[\text{TeXForm}\left[\sqrt{42} |\phi_5\rangle + 15 |\phi_7\rangle + 6 \sqrt{2} |\phi_9\rangle\right]\]

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

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

\[(a + a^\dagger)^2\]

\[(a + a^\dagger)^2\]

We can expand the expression using the command Expand:

\[\text{Expand}\left[(a + a^\dagger)^2\right]\]

\[a^2 + a^\dagger \cdot a + a \cdot a^\dagger + (a^\dagger)^2\]

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

\[(a^2 + a^\dagger \cdot a + a \cdot a^\dagger + (a^\dagger)^2) \cdot |\phi\rangle\]

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

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.

\[\text{CommutatorExpand}\left[(a + a^\dagger)^2\right]\]

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

A different expansion is obtained with the option ReverseOrdering \rightarrow True (the standard Mathematica symbol \rightarrow can be entered pressing the keys [ESC]\rightarrow[ESC]):
The expansion has exactly the same effect on a ket as the original expression:

\[
\left( a^2 - [a', a]_+ + 2 a' \cdot a + (a')^2 \right) \cdot | \phi_7 \rangle \\
\sqrt{42} | \phi_5 \rangle + 15 | \phi_7 \rangle + 6 \sqrt{2} | \phi_9 \rangle
\]

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

\[
\text{EvaluateCommutators} \left[ \left( a^2 - [a', a]_+ + 2 a' \cdot a + (a')^2 \right) \right]
\]

\[
a^2 + a' \cdot a + a \cdot a' + (a')^2
\]

The TraditionalForm of an expression is usually easier to read:

\[
\text{TraditionalForm} \left[ a^2 + a' \cdot a + a \cdot a' + (a')^2 \right]
\]

\[
a' a + a a' + (a')^2 + a^2
\]

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:

\[
\text{CommutatorExpand} \left[ (a + a')^2 \right]
\]

\[
-1 + a^2 + 2 a \cdot a' + (a')^2
\]

The TraditionalForm representation can be easier to read:

\[
\text{TraditionalForm} \left[ \text{CommutatorExpand} \left[ (a + a')^2 \right] \right]
\]

\[
2 a a' + (a')^2 + a^2 - 1
\]

Here is a \TeX version of the TraditionalForm:
Symbolic calculations can be performed:

\[(a + a\dagger)^2 \cdot |\psi_k\rangle\]

\[\sqrt{1+k} \sqrt{k} |\phi_{2,k}\rangle + k |\phi_{k}\rangle + (1+k) |\phi_{k}\rangle + \sqrt{1+k} \sqrt{2+k} |\phi_{2,k}\rangle\]

Here is another simple example

\[(a\dagger \cdot a)^3 \cdot |\psi_k\rangle\]

\[k^3 |\psi_k\rangle\]

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

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

\[-1 + a \cdot a\dagger - 3 (-2 a + a^2 \cdot a\dagger) \cdot a\dagger + (-3 a^2 + a^3 \cdot a\dagger) \cdot (a\dagger)^2\]

Expand and CommutatorExpand can be combined:

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

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

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

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

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

The result of the quantum expansion on a ket is the same as with the original expression:
\[ \text{Simplify}\left\{ -1 + \left( 7a + \left( -6a^2 + a^3 \cdot a' \cdot a' \right) \cdot a' \right) \cdot \phi_k \right\} \]

\[ k^3 \cdot \phi_k \]

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:

\[ \langle x \_?NumberQ | \cdot | \phi_k \rangle := \text{Exp}[-x^2/2] \cdot \text{HermiteH}[k, x] / \sqrt{2^k \cdot k! \cdot \sqrt{\pi}} \]

This is the value of the wave function when \( x = 0.5 \)

\[ \langle 0.5 | \cdot | \phi_2 \rangle \]

\[-0.234359 \]

We can plot the wave function:

\[ \text{Plot}[(x | \cdot | \phi_2), \{x, -5, 5\}, \text{PlotLabel} \rightarrow \text{"Wave Function"}] \]

This is the value of the probability density function when \( x = 0.5 \)

(press the keys \([\text{ESC}]\text{norm}[\text{ESC}]\) in order to write the quantum Norm template)

\[ \|\langle 0.5 | \cdot | \phi_2 \rangle\|^2 \]

\[ 0.0549239 \]

We can plot the probability density

(press the keys \([\text{ESC}]\text{norm}[\text{ESC}]\) in order to write the quantum Norm template)
Next we verify that the function is normalized:

\[
\text{NIntegrate}\left[\|\langle x \mid \cdot \mid \phi_2\rangle\|^2, \{x, -5, 5\}\right]
\]

1.

**Summary**

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

\[
\begin{align*}
\text{Needs} & \left[\text{"Quantum`Notation`"}\right]; \\
\langle \phi_j \mid \cdot \mid \phi_k \rangle & := \text{KroneckerDelta}[j - k]; \\
\text{DefineOperatorOnKets} & \left[a, \{\mid \phi_n \rangle \mapsto \sqrt{n} \mid \phi_{n-1} \rangle\}\right]; \\
\text{DefineOperatorOnKets} & \left[(a)^\dagger, \{\mid \phi_n \rangle \mapsto \sqrt{n+1} \mid \phi_{n+1} \rangle\}\right]; \\
[a, a^\dagger] & = 1; \\
\langle x \_\text{?NumberQ} \mid \cdot \mid \phi_k \rangle & := \text{Exp}\left[-x^2/2\right] * \text{HermiteH}[k, x] / \sqrt{2^k * k! * \sqrt{\pi}} ;
\end{align*}
\]

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

\[
a^4 \cdot \mid \phi_1\rangle
\]

\[
2 \sqrt{210} \mid \phi_1\rangle
\]

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

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

\[
-3a + a^3 + 3a^2 \cdot a^\dagger + 3a \cdot (a^\dagger)^2 - 3a^\dagger + (a^\dagger)^3
\]
Simple and complex operations can be performed after evaluating those definitions:

```math
\text{mymatrix} = \text{Table}\left(\left(\phi_j \cdot (a + a')^3 \cdot \phi_k\right), \{j, 1, 8\}, \{k, 1, 8\}\right);
\text{MatrixForm}[\text{mymatrix}]
```

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

```math
\text{Plot}\left[\left(x \cdot \phi_5\right), \{x, -5, 5\}\right], \text{PlotLabel} \rightarrow \text{"Wave Function"}
```

Simple and complex operations can be performed after evaluating those definitions:
Plot[
  Evaluate[Append[Table[\[\langle x | \phi_n \rangle \|^2 + n + \frac{1}{2}, (n, 0, 7)], \frac{x^2}{2}],
  {x, -4, 4}, Filling -> Table[n \rightarrow n - \frac{1}{2}, (n, 1, 8)]]
]

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