Pauli Gates vs Pauli Operators and the PauliExpand Command

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Introduction

This is a tutorial explains the difference between Pauli gates $\mathcal{I}_{\hat{\square}}$, $\mathcal{X}_{\hat{\square}}$, $\mathcal{Y}_{\hat{\square}}$, $\mathcal{Z}_{\hat{\square}}$ and Pauli operators $\sigma_{0,\hat{\square}}$, $\sigma_{\mathcal{X},\hat{\square}}$, $\sigma_{\mathcal{Y},\hat{\square}}$, and the use of the PauliExpand command to represent any combination of quantum gates in terms of Pauli operators.

Load the Package

First load the Quantum`Computing` package. Write:
Needs["Quantum`Computing`"];
then press at the same time the keys SHIFT-ENTER to evaluate. *Mathematica* will load the package:

```
Needs["Quantum`Computing`"]
```

```
Quantum`Computing` Version 2.2.0. (June 2010)
A Mathematica package for Quantum Computing
  in Dirac bra-ket notation and plotting of quantum circuits
by José Luis Gómez-Muñoz

Execute SetComputingAliases[] in order to use
  the keyboard to enter quantum objects in Dirac's notation
SetComputingAliases[] must be executed again in each new notebook that is created
```

In order to use the keyboard to enter quantum objects write:
SetComputingAliases[ ];
then press at the same time the keys SHIFT-ENTER to evaluate. The semicolon prevents *Mathematica* from printing the help message. Remember that SetComputingAliases[ ] must be evaluated again in each new notebook:

```
SetComputingAliases[];
```

Pauli Gates and Pauli Operators: The Similarities

Press the keys [ESC]xg[ESC] in order to obtain the template for the 1st Pauli **gate**: $\mathcal{X}_{\hat{\square}}$. Then press [TAB] to select the place holder □ and write a qubit number or label (for example, 7)

$\mathcal{X}_{\hat{7}}$

$\mathcal{X}_{\hat{7}}$

This is the Dirac representation of the 1st Pauli **gate**:

```
QuantumEvaluate[𝒳₇̂]
```

$| 1_{\hat{7}} \rangle \cdot \langle 0_{\hat{7}} | + | 0_{\hat{7}} \rangle \cdot \langle 1_{\hat{7}} |$

This is the matrix representation of the 1st Pauli **gate**:

```
QuantumMatrixForm[𝒳₇̂]
```

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

This *Mathematica* package includes also Pauli **operators**, which are similar in many aspects to Pauli **gates**. Press the keys [ESC]sx[ESC] in order to obtain the template for the 1st Pauli **operator**: $\sigma_{\mathcal{X},\hat{\square}}$. Then press [TAB] to select the place holder □ and write a qubit number or label (for example, 7)

$\sigma_{\mathcal{X},\hat{7}}$

$\sigma_{\mathcal{X},\hat{7}}$

This is the Dirac representation of the 1st Pauli **operator**, which is the same as for the corresponding Pauli **gate**:

```
QuantumEvaluate[σ𝒳,₇̂]
```

$| 1_{\hat{7}} \rangle \cdot \langle 0_{\hat{7}} | + | 0_{\hat{7}} \rangle \cdot \langle 1_{\hat{7}} |$

This is the matrix representation of the 1st Pauli **operator**, which is the same as for the corresponding Pauli **gate**:

```
QuantumMatrixForm[σ𝒳,₇̂]
```

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Pauli Gates vs Pauli Operators: The Differences

A noncommutative product of Pauli **gates** is "stable", *Mathematica* returns as output exactly the input in this example. Press the keys:
[ESC]xg[ESC][ESC]on[ESC][ESC]yg[ESC][TAB]5[TAB]5
finally press at the same time [SHIFT]-[ENTER] to evaluate:

$\mathcal{X}_{\hat{5}} \cdot \mathcal{Y}_{\hat{5}}$

$\mathcal{X}_{\hat{5}} \cdot \mathcal{Y}_{\hat{5}}$

On the other hand, a noncommutative product of Pauli **operators** is automatically simplified, Quantum *Mathematica* "knows" their algebraic properties. Press the keys:
[ESC]sx[ESC][ESC]on[ESC][ESC]sy[ESC][TAB]5[TAB]5
finally press at the same time [SHIFT]-[ENTER] to evaluate:

$$\sigma_{x,\hat{5}} \cdot \sigma_{y,\hat{5}}$$

$$i\,\sigma_{z,\hat{5}}$$

A stable noncommutative product of Pauli **gates**:

$$y_{\hat{5}} \cdot (z_{\hat{5}})^7 \cdot y_{\hat{5}}$$

$$y_{\hat{5}} \cdot z_{\hat{5}}^7 \cdot y_{\hat{5}}$$

The equivalent noncommutative product of Pauli **operators** is automatically simplified:

$$\sigma_{y,\hat{5}} \cdot (\sigma_{z,\hat{5}})^7 \cdot \sigma_{y,\hat{5}}$$

$$-\sigma_{z,\hat{5}}$$

The PauliExpand Command

The PauliExpand[] command transforms any noncommutative product of **gates** into the corresponding Pauli **operators**. Here the simplest example:

PauliExpand$[y_{\hat{5}}]$

$$\sigma_{y,\hat{5}}$$

These Pauli **gates** are transformed to Pauli **operators**, and those Pauli operators are simplified using their algebraic properties:

PauliExpand$[y_{\hat{5}} \cdot (z_{\hat{5}})^7 \cdot y_{\hat{5}}]$

$$-\sigma_{z,\hat{5}}$$

Any combination of quantum **gates** can be transformed to Pauli **operators**:

```
PauliExpand[C^{1̂}[NOT_2̂] · H_1̂]
```

$$\frac{\sigma_{0,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{0,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}$$

Copy-paste the previous output inside the QuantumTableForm[] command in order to get the truth table of the Pauli operators expression:

QuantumTableForm$\left[\frac{\sigma_{0,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{0,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}\right]$

	Input	Output
0	$\lvert 0_{\hat{1}}, 0_{\hat{2}}\rangle$	$\frac{\lvert 0_{\hat{1}},0_{\hat{2}}\rangle}{\sqrt{2}}+\frac{\lvert 1_{\hat{1}},1_{\hat{2}}\rangle}{\sqrt{2}}$
1	$\lvert 0_{\hat{1}}, 1_{\hat{2}}\rangle$	$\frac{\lvert 0_{\hat{1}},1_{\hat{2}}\rangle}{\sqrt{2}}+\frac{\lvert 1_{\hat{1}},0_{\hat{2}}\rangle}{\sqrt{2}}$
2	$\lvert 1_{\hat{1}}, 0_{\hat{2}}\rangle$	$\frac{\lvert 0_{\hat{1}},0_{\hat{2}}\rangle}{\sqrt{2}}-\frac{\lvert 1_{\hat{1}},1_{\hat{2}}\rangle}{\sqrt{2}}$
3	$\lvert 1_{\hat{1}}, 1_{\hat{2}}\rangle$	$\frac{\lvert 0_{\hat{1}},1_{\hat{2}}\rangle}{\sqrt{2}}-\frac{\lvert 1_{\hat{1}},0_{\hat{2}}\rangle}{\sqrt{2}}$

Compare with the truth-table of the original expression:

```
QuantumTableForm[C^{1̂}[NOT_2̂] · H_1̂]
```

	Input	Output
0	$\lvert 0_{\hat{1}}, 0_{\hat{2}}\rangle$	$\frac{\lvert 0_{\hat{1}},0_{\hat{2}}\rangle}{\sqrt{2}}+\frac{\lvert 1_{\hat{1}},1_{\hat{2}}\rangle}{\sqrt{2}}$
1	$\lvert 0_{\hat{1}}, 1_{\hat{2}}\rangle$	$\frac{\lvert 0_{\hat{1}},1_{\hat{2}}\rangle}{\sqrt{2}}+\frac{\lvert 1_{\hat{1}},0_{\hat{2}}\rangle}{\sqrt{2}}$
2	$\lvert 1_{\hat{1}}, 0_{\hat{2}}\rangle$	$\frac{\lvert 0_{\hat{1}},0_{\hat{2}}\rangle}{\sqrt{2}}-\frac{\lvert 1_{\hat{1}},1_{\hat{2}}\rangle}{\sqrt{2}}$
3	$\lvert 1_{\hat{1}}, 1_{\hat{2}}\rangle$	$\frac{\lvert 0_{\hat{1}},1_{\hat{2}}\rangle}{\sqrt{2}}-\frac{\lvert 1_{\hat{1}},0_{\hat{2}}\rangle}{\sqrt{2}}$

TraditionalForm[] gives a format closer to the format of papers and textbooks:

$$\text{TraditionalForm}\left[\frac{\sigma_{o,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{o,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}\right]$$

$$-\frac{i\,\sigma_1^{\mathcal{Y}}\sigma_2^{\mathcal{X}}}{2\sqrt{2}}+\frac{\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}}{2\sqrt{2}}+\frac{\sigma_1^{\mathcal{X}}\sigma_2^{\mathit{0}}}{2\sqrt{2}}-\frac{\sigma_1^{\mathit{0}}\sigma_2^{\mathcal{X}}}{2\sqrt{2}}+\frac{\sigma_1^{\mathcal{X}}\sigma_2^{\mathcal{X}}}{2\sqrt{2}}+\frac{i\,\sigma_1^{\mathcal{Y}}\sigma_2^{\mathit{0}}}{2\sqrt{2}}+\frac{\sigma_1^{\mathcal{Z}}\sigma_2^{\mathit{0}}}{2\sqrt{2}}+\frac{\sigma_1^{\mathit{0}}\sigma_2^{\mathit{0}}}{2\sqrt{2}}$$

This is the TeXForm[] of the TraditionalForm of the expression:

$$\text{TeXForm}\left[\text{TraditionalForm}\left[\frac{\sigma_{o,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{o,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}\right]\right]$$

```
-\frac{i \sigma _1^{\mathcal{Y}}\sigma
   _2^{\mathcal{X}}}{2 \sqrt{2}}+\frac{\sigma
   _1^{\mathcal{Z}}\sigma _2^{\mathcal{X}}}{2
   \sqrt{2}}+\frac{\sigma _1^{\mathcal{X}}\sigma
   _2^{\mathit{0}}}{2 \sqrt{2}}-\frac{\sigma
   _1^{\mathit{0}}\sigma _2^{\mathcal{X}}}{2
   \sqrt{2}}+\frac{\sigma _1^{\mathcal{X}}\sigma
   _2^{\mathcal{X}}}{2 \sqrt{2}}+\frac{i \sigma
   _1^{\mathcal{Y}}\sigma _2^{\mathit{0}}}{2
   \sqrt{2}}+\frac{\sigma _1^{\mathcal{Z}}\sigma
   _2^{\mathit{0}}}{2 \sqrt{2}}+\frac{\sigma
   _1^{\mathit{0}}\sigma _2^{\mathit{0}}}{2 \sqrt{2}}
```

Noncommutative Algebraic commands from Quantum`Notation` can be used. Here is CollectFromLeft[], which can be typed or pasted from the "Quantum Algebra" palette, in the "Palettes" menu of *Mathematica:*

$$\text{CollectFromLeft}\left[\frac{\sigma_{o,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{o,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{o,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}\right]$$

$$\sigma_{o,\hat{1}}\cdot\left(\frac{\sigma_{o,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)+\sigma_{y,\hat{1}}\cdot\left(\frac{i\,\sigma_{o,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)+\sigma_{x,\hat{1}}\cdot\left(\frac{\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)+\sigma_{z,\hat{1}}\cdot\left(\frac{\sigma_{o,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)$$

Noncommutative Algebraic commands from Quantum`Notation` can be used. Here is CollectFromRight[], which can be typed or pasted from the "Quantum Algebra" palette, in the "Palettes" menu of *Mathematica:*

```
CollectFromRight[σ_{0,1̂}·σ_{0,2̂}/(2√2) + σ_{x,1̂}·σ_{0,2̂}/(2√2) + ⅈ σ_{y,1̂}·σ_{0,2̂}/(2√2) +
  σ_{z,1̂}·σ_{0,2̂}/(2√2) - σ_{0,1̂}·σ_{x,2̂}/(2√2) + σ_{x,1̂}·σ_{x,2̂}/(2√2) - ⅈ σ_{y,1̂}·σ_{x,2̂}/(2√2) + σ_{z,1̂}·σ_{x,2̂}/(2√2)]
```

$$\left(\frac{\sigma_{0,\hat{1}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}}{2\sqrt{2}}\right)\cdot\sigma_{0,\hat{2}}+\left(-\frac{\sigma_{0,\hat{1}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}}{2\sqrt{2}}\right)\cdot\sigma_{x,\hat{2}}$$

Collecting from left and the from right:

```
CollectFromRight[CollectFromLeft[σ_{0,1̂}·σ_{0,2̂}/(2√2) + σ_{x,1̂}·σ_{0,2̂}/(2√2) +
  ⅈ σ_{y,1̂}·σ_{0,2̂}/(2√2) + σ_{z,1̂}·σ_{0,2̂}/(2√2) - σ_{0,1̂}·σ_{x,2̂}/(2√2) + σ_{x,1̂}·σ_{x,2̂}/(2√2) - ⅈ σ_{y,1̂}·σ_{x,2̂}/(2√2) + σ_{z,1̂}·σ_{x,2̂}/(2√2)]]
```

$$\sigma_{0,\hat{1}}\cdot\left(\frac{\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)+\sigma_{y,\hat{1}}\cdot\left(\frac{i\,\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)+\left(\sigma_{x,\hat{1}}+\sigma_{z,\hat{1}}\right)\cdot\left(\frac{\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)$$

Expand recovers the original expression (copy-paste the previous output):

```
Expand[σ_{0,1̂}·(σ_{0,2̂}/(2√2) - σ_{x,2̂}/(2√2)) + σ_{y,1̂}·(ⅈ σ_{0,2̂}/(2√2) - ⅈ σ_{x,2̂}/(2√2)) + (σ_{x,1̂} + σ_{z,1̂})·(σ_{0,2̂}/(2√2) + σ_{x,2̂}/(2√2))]
```

$$\frac{\sigma_{0,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{0,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}$$

This is the tensor representation. Remember that for further calculations you must use **QuantumTensor** instead of **QuantumTensorForm**:

```
QuantumTensorForm[
 σ_{0,1̂}·(σ_{0,2̂}/(2√2) - σ_{x,2̂}/(2√2)) + σ_{y,1̂}·(ⅈ σ_{0,2̂}/(2√2) - ⅈ σ_{x,2̂}/(2√2)) + (σ_{x,1̂} + σ_{z,1̂})·(σ_{0,2̂}/(2√2) + σ_{x,2̂}/(2√2))]
```

$$\begin{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}} & 0\\ 0 & \frac{1}{\sqrt{2}}\end{pmatrix} & \begin{pmatrix}\frac{1}{\sqrt{2}} & 0\\ 0 & \frac{1}{\sqrt{2}}\end{pmatrix}\\ \begin{pmatrix}0 & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & 0\end{pmatrix} & \begin{pmatrix}0 & -\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}} & 0\end{pmatrix}\end{pmatrix}$$

This is the matrix representation. Remember that for further calculations you must use **QuantumMatrix** instead of **QuantumMatrixForm**:

$$\text{QuantumMatrix}\Big[\sigma_{0,\hat{1}}\cdot\left(\frac{\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)+\sigma_{y,\hat{1}}\cdot\left(\frac{i\,\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)+\left(\sigma_{x,\hat{1}}+\sigma_{z,\hat{1}}\right)\cdot\left(\frac{\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{2}}}{2\sqrt{2}}\right)\Big]$$

$$\left\{\left\{\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}},0\right\},\left\{0,\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}}\right\},\left\{0,\frac{1}{\sqrt{2}},0,-\frac{1}{\sqrt{2}}\right\},\left\{\frac{1}{\sqrt{2}},0,-\frac{1}{\sqrt{2}},0\right\}\right\}$$

PauliExpand and MatrixQuantum can be used to transform from a matrix to Pauli operators (copy-paste the previous output):

$$\text{PauliExpand}\Big[\text{MatrixQuantum}\Big[\left\{\left\{\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}},0\right\},\left\{0,\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}}\right\},\left\{0,\frac{1}{\sqrt{2}},0,-\frac{1}{\sqrt{2}}\right\},\left\{\frac{1}{\sqrt{2}},0,-\frac{1}{\sqrt{2}},0\right\}\right\}\Big]\Big]$$

$$\frac{\sigma_{0,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{0,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}$$

This is the Dirac notation representation:

$$\text{QuantumEvaluate}\Big[\frac{\sigma_{0,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{0,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}\Big]$$

$$\frac{|0_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},0_{\hat{2}}|}{\sqrt{2}}+\frac{|1_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},0_{\hat{2}}|}{\sqrt{2}}+\frac{|0_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},1_{\hat{2}}|}{\sqrt{2}}+\frac{|1_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},1_{\hat{2}}|}{\sqrt{2}}+\frac{|0_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},0_{\hat{2}}|}{\sqrt{2}}-\frac{|1_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},0_{\hat{2}}|}{\sqrt{2}}+\frac{|0_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},1_{\hat{2}}|}{\sqrt{2}}-\frac{|1_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},1_{\hat{2}}|}{\sqrt{2}}$$

We can use PauliExpand to go from Dirac Notation to Pauli Operators. The Dirac expression must represent a unitary operator (copy-paste the previous output):

$$\mathbf{PauliExpand}\Big[\frac{|0_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},0_{\hat{2}}|}{\sqrt{2}}+\frac{|1_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},0_{\hat{2}}|}{\sqrt{2}}+\frac{|0_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},1_{\hat{2}}|}{\sqrt{2}}+\frac{|1_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 0_{\hat{1}},1_{\hat{2}}|}{\sqrt{2}}+\frac{|0_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},0_{\hat{2}}|}{\sqrt{2}}-\frac{|1_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},0_{\hat{2}}|}{\sqrt{2}}+\frac{|0_{\hat{1}},1_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},1_{\hat{2}}|}{\sqrt{2}}-\frac{|1_{\hat{1}},0_{\hat{2}}\rangle\cdot\langle 1_{\hat{1}},1_{\hat{2}}|}{\sqrt{2}}\Big]$$

$$\frac{\sigma_{0,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{0,\hat{2}}}{2\sqrt{2}}-\frac{\sigma_{0,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{x,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}-\frac{i\,\sigma_{y,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}+\frac{\sigma_{z,\hat{1}}\cdot\sigma_{x,\hat{2}}}{2\sqrt{2}}$$

This is the TraditionalForm[] of a larger expansion in terms of Pauli operators. Remember that TraditionalForm[] is only for displaying purposes, not for further calculations. This operation takes several seconds to evaluate:

$$\mathbf{TraditionalForm}\Big[\mathbf{PauliExpand}\Big[\bigotimes_{k=1}^{3}\mathcal{C}^{\{\hat{k}\}}\big[\mathcal{NOT}_{\widehat{k+1}}\big]\Big]\Big]$$

$$\frac{1}{8}\sigma_1^0\sigma_2^0\sigma_3^0\sigma_4^0+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^0\sigma_3^0\sigma_4^0+\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{X}}\sigma_3^0\sigma_4^0-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^0\sigma_4^0-\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{Y}}\sigma_3^0\sigma_4^0+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^0\sigma_4^0+\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{Z}}\sigma_3^0\sigma_4^0+$$
$$\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^0\sigma_4^0+\frac{1}{8}\sigma_1^0\sigma_2^0\sigma_3^{\mathcal{X}}\sigma_4^0+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^0\sigma_3^{\mathcal{X}}\sigma_4^0+\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{X}}\sigma_4^0-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{X}}\sigma_4^0+\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{X}}\sigma_4^0-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{X}}\sigma_4^0-$$
$$\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{X}}\sigma_4^0-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{X}}\sigma_4^0-\frac{1}{8}i\,\sigma_1^0\sigma_2^0\sigma_3^{\mathcal{Y}}\sigma_4^0-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^0\sigma_3^{\mathcal{Y}}\sigma_4^0-\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Y}}\sigma_4^0+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Y}}\sigma_4^0+$$
$$\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Y}}\sigma_4^0-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Y}}\sigma_4^0+\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}\sigma_4^0+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}\sigma_4^0+\frac{1}{8}\sigma_1^0\sigma_2^0\sigma_3^{\mathcal{Z}}\sigma_4^0+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^0\sigma_3^{\mathcal{Z}}\sigma_4^0+\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Z}}\sigma_4^0-$$
$$\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Z}}\sigma_4^0-\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Z}}\sigma_4^0+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Z}}\sigma_4^0+\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}\sigma_4^0+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}\sigma_4^0+\frac{1}{8}\sigma_1^0\sigma_2^0\sigma_3^0\sigma_4^{\mathcal{X}}+$$
$$\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^0\sigma_3^0\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{X}}\sigma_3^0\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^0\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{Y}}\sigma_3^0\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^0\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{Z}}\sigma_3^0\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^0\sigma_4^{\mathcal{X}}+$$
$$\frac{1}{8}\sigma_1^0\sigma_2^0\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^0\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-$$
$$\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^0\sigma_2^0\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^0\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}-$$
$$\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^0\sigma_2^0\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^0\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-$$
$$\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^0\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^0\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}$$

Use the option **PauliIdentities->False** inside the PauliExpand command in order to transform each identity operators σ_0 into the number 1. This can be useful for displaying purposes, **it is not a good idea in actual calculations:**

```
TraditionalForm[PauliExpand[⊗_{k=1}^{3} C^{k̂}[NOT_{k+1̂}], PauliIdentities → False]]
```

$$
\begin{aligned}
&-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}+\frac{1}{8}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{X}}+\frac{1}{8}i\,\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{X}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_3^{\mathcal{X}}-\frac{1}{8}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{X}}+\frac{1}{8}\sigma_2^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_2^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\\
&\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_2^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}-\frac{1}{8}i\,\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Y}}+\frac{1}{8}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Y}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}+\frac{1}{8}i\,\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}+\\
&\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}+\frac{1}{8}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Z}}-\frac{1}{8}i\,\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Z}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}+\frac{1}{8}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{X}}-\\
&\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}-\\
&\frac{1}{8}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\\
&\frac{1}{8}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Y}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Y}}+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Z}}+\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Z}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}-\\
&\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{X}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Y}}\sigma_4^{\mathcal{X}}+\\
&\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{X}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}i\,\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Y}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}-\frac{1}{8}\sigma_1^{\mathcal{Z}}\sigma_2^{\mathcal{Z}}\sigma_3^{\mathcal{Z}}\sigma_4^{\mathcal{X}}+\frac{\sigma_2^{\mathcal{X}}}{8}+\frac{\sigma_3^{\mathcal{X}}}{8}+\frac{\sigma_4^{\mathcal{X}}}{8}-\frac{i\,\sigma_2^{\mathcal{Y}}}{8}-\frac{i\,\sigma_3^{\mathcal{Y}}}{8}+\frac{\sigma_1^{\mathcal{Z}}}{8}+\frac{\sigma_2^{\mathcal{Z}}}{8}+\frac{\sigma_3^{\mathcal{Z}}}{8}+\frac{1}{8}
\end{aligned}
$$

Sample Application: Bloch Equations for Resonance Fluorescence

This is Moritz Schubotz's solution of exercises 3.10 from the textbook **QUANTUM MEASUREMENT AND CONTROL by H., Wiseman and G. Milburn 2010** www.cambridge.org/9780521804424

Every density matrix for a two level system can be written as a linear combination of Pauli-matrices, see next definition of ρ. Creation and annihilation operators σ_+ σ_- are also defined.

```
ρ = (σ_{0,1̂} + x[t] σ_{X,1̂} + y[t] σ_{Y,1̂} + z[t] σ_{Z,1̂}) / 2
σ₊ = (σ_{X,1̂} + I σ_{Y,1̂}) / 2
σ₋ = (σ₊)†
```

$$\frac{1}{2}\left(\sigma_{0,\hat{1}}+x[t]\,\sigma_{\mathcal{X},\hat{1}}+y[t]\,\sigma_{\mathcal{Y},\hat{1}}+z[t]\,\sigma_{\mathcal{Z},\hat{1}}\right)$$

$$\frac{1}{2}\left(\sigma_{\mathcal{X},\hat{1}}+i\,\sigma_{\mathcal{Y},\hat{1}}\right)$$

$$\frac{1}{2}\left(\sigma_{\mathcal{X},\hat{1}}-i\,\sigma_{\mathcal{Y},\hat{1}}\right)$$

The effective Hamilton operator of an externally driven system is given by equation (3.31) of Wiseman and Milburn, where Ω stands for the Rabi - frequency and Δ is the effective deturning of the atom:

```
H = Ω/2 σ_{x,î} + Δ/2 σ_{z,î}
```

$$\frac{1}{2}\Omega\,\sigma_{x,\hat{\imath}} + \frac{1}{2}\Delta\,\sigma_{z,\hat{\imath}}$$

Furthermore the Lindblad super operator is given by equation (3.29) of Wiseman and Milburn. The evaluation of next definition does not produce any output, however it stores the definition of DD[]:

```
DD[A_] := Function[{ope}, A · ope · (A)† - ((A)† · A · ope + ope · (A)† · A)/2 ]
```

The Born - Markov Master Equation are given by equation (3.28) of Wiseman and Milburn. Here it is evaluated in the Hamiltonian that was previously defined:

```
dtρ = Simplify[Expand[ - ⅈ * 〚H, ρ〛_ + γ * DD[σ_][ρ] ]];
TraditionalForm[dtρ]
```

$$\frac{1}{4}\left(x(t)\left(2\,\Delta\,\sigma_1^y - \gamma\,\sigma_1^x\right) - y(t)\left(2\,\Delta\,\sigma_1^x + \gamma\,\sigma_1^y - 2\,\Omega\,\sigma_1^z\right) - 2\left(\Omega\,z(t)\,\sigma_1^y + \gamma\,z(t)\,\sigma_1^z + \gamma\,\sigma_1^z\right)\right)$$

Density matrices in Pauli basis, have the feature that the components x,y,z can be calculated by $x = \mathrm{Tr}(\sigma_1\,\rho)$ etc. The same holds true for $d_t\,x$ etc. The Pauli − Matrices are all traceless with the exception of σ_0 where the trace is 2. So the equations of movement for x,z,t read:

```
Blochxyz =
  Simplify[Table[Expand[σ_{k,î} · dtρ] /. {σ_{x,î} → 0, σ_{y,î} → 0, σ_{z,î} → 0, σ_{o,î} → 2}, {k, 3}]];
TraditionalForm[MatrixForm[Blochxyz]]
```

$$\begin{pmatrix} \frac{1}{2}(-\gamma\,x(t) - 2\,\Delta\,y(t)) \\ \Delta\,x(t) - \frac{1}{2}\gamma\,y(t) - \Omega\,z(t) \\ \Omega\,y(t) - \gamma\,(z(t) + 1) \end{pmatrix}$$

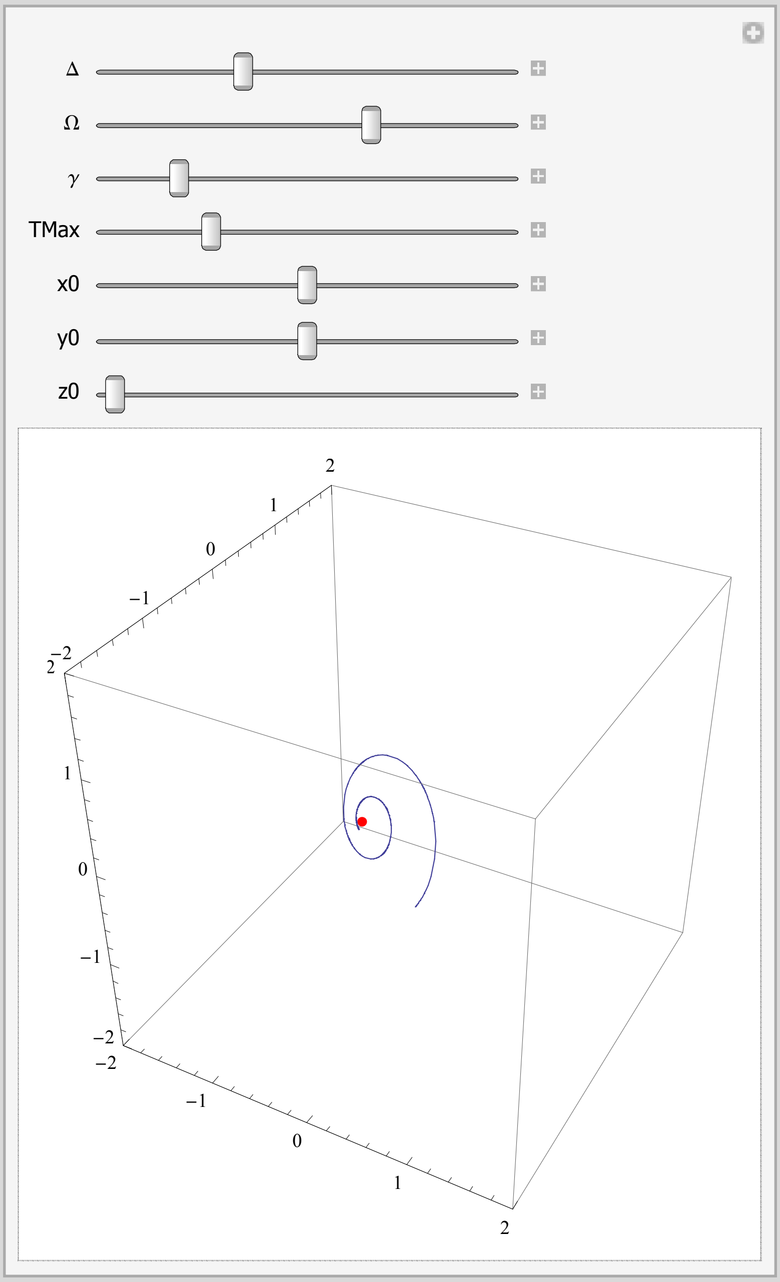
Furthermore the goal is to calculate a steady state for this equations.

```
X = {x[t], y[t], z[t]};
BlochStat[Δ_, Ω_, γ_] = Solve[Blochxyz == {0, 0, 0}, X];
X /. BlochStat[Δ, Ω, γ]
```

$$\left\{\left\{-\frac{4\,\Delta\,\Omega}{\gamma^2 + 4\,\Delta^2 + 2\,\Omega^2},\ \frac{2\,\gamma\,\Omega}{\gamma^2 + 4\,\Delta^2 + 2\,\Omega^2},\ -\frac{\gamma^2 + 4\,\Delta^2}{\gamma^2 + 4\,\Delta^2 + 2\,\Omega^2}\right\}\right\}$$

This can be visualized. The red dot is the steady state and the blue curve shows the movement of the density matrix in Bloch space for given initial conditions.

```
GLN[Δ_, Ω_, γ_] = Table[D[X[[k]], t] == Blochxyz[[k]], {k, 3}];
Manipulate[
 LSG = NDSolve[{GLN[Δ, Ω, γ], x[0] == x0, y[0] == y0, z[0] == z0}, X, {t, 0, TMax}]; P1 =
  ParametricPlot3D[X /. LSG, {t, 0, TMax}, PlotRange → {{-2, 2}, {-2, 2}, {-2, 2}}];
 P2 = Graphics3D[{Red, PointSize[Medium], Point[X /. BlochStat[Δ, Ω, γ]]}];
 Show[P1, P2],
 {{Δ, 1}, 0, 3}, {{Ω, 2}, 0, 3}, {{γ, 1 / 2}, 0, 3},
 {{TMax, 5}, 0, 20}, {{x0, 0}, -1, 1}, {{y0, 0}, -1, 1}, {{z0, -1}, -1, 1},
 SaveDefinitions → True
]
```



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