Working in Different Bases

Why not just in the computational basis?

- One important motivation did we already see in **E. 06**, "**Measurements.**" Recall that one must expand a given quantum state $|\psi\rangle$ in the eigenbasis $\{|a\rangle | \hat{A} | a\rangle = |a\rangle a\}$ of the observable $\hat{A} = \sum_{a} |a\rangle a \langle a|$. That is, $|\psi\rangle = \sum_{a} |a\rangle c_a$.
- Here is another motivation.

Consider a quantum register of qubits, referred to by symbol s.

Here is a dynamic way of constructing the spin XX Hamiltonian.

```
In[\circ] := xx = Total@ChainBy[Through[ss[1]], Multiply] Out[\circ] = S_1^x S_2^x + S_2^x S_3^x + S_3^x S_4^x
```

In the same manner, construct the spin YY Hamiltonian.

```
\label{eq:chainBy} $$\inf_{s \in \mathbb{R}^y := \mathbb{R}^y := \mathbb{R}^y := \mathbb{R}^y := \mathbb{R}^y := \mathbb{R}^y : \mathbb{R}^y := \mathbb{R}^y : \mathbb{R
```

Finally, construct the spin ZZ Hamiltonian.

```
\label{eq:chainBy} $$\inf_{s \in \mathbb{R}^z} zz = Total@ChainBy[Through[ss[3]], Multiply]$$ $$Out[s] = $S_1^z S_2^z + S_2^z S_3^z + S_3^z S_4^z$$$
```

Here is the total Hamiltonian.

$$\label{eq:continuous} \begin{split} & \textit{In[\circ} \ \) := \ \ \textbf{H = xx + yy + zz} \\ & \textit{Out[\circ} \ \) = \\ & S_1^x \ S_2^x + S_1^y \ S_2^y + S_1^z \ S_2^z + S_2^x \ S_3^x + S_2^y \ S_3^y + S_2^z \ S_3^z + S_3^x \ S_4^x + S_3^y \ S_4^y + S_3^z \ S_4^z \end{split}$$

The Hamiltonian has so many zeros. That is why matrix representations are treated in **SparseArray** form in Q3.

```
In[*]:= mat = Matrix[H];
     mat // MatrixForm
Out[•]//MatrixForm=
     3 0
                    0 0 0 0
                                  0
          0
      0 1 2
                   0 0 0 0
                             0 0 0 0
                                      0 0
      0 0 0 1
              0
                 2
                   0 0 0 0
                                      0 0
      0 0
          2
            0 -1 0
                   0 0 2 0
                             0 0 0 0
                                      0 0
            2
              0
                -3 2 0 0
                                      0 0
          0 0 0
                 2 -1 0 0 0
                             2 0 0 0 0 0
                0 0 1 0 0
      0 0 0 0 2 0 0 0 1 0
                             0 0 0 0 0 0
           0 0 2 0 0 0 -1 2
                               0 0
       0
          0 0 0
                0 2 0 0 2
                            -3 0
         0 0 0 0 0 2 0 0
      0 0
                            0 -1 0
      0 0 0 0 0 0 0 0 0 0
                             0 2 0 -1 2 0
                                    2
                                      1 0
      0 0 0 0
                0 0 0 0
                          0
                             0
                               0 0
```

Anyway, how can we diagonalize Hamiltonian?

What about working in a different basis?

Construct a different basis where elements are characterized by the total angular momentum.

In[0]:= bs = QubitAdd[ss]

$$\begin{split} & \langle \left| \left\{ 0,0 \right\} \rightarrow \left\{ \frac{1}{2} \mid \left| 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle - \frac{1}{2} \mid \left| 0_{S_1} 1_{S_2} 1_{S_3} 0_{S_4} \right\rangle - \frac{1}{2} \mid \left| 1_{S_1} 0_{S_2} 0_{S_3} 1_{S_4} \right\rangle + \frac{1}{2} \mid \left| 1_{S_1} 0_{S_2} 1_{S_3} 0_{S_4} \right\rangle, \\ & \frac{\left| 0_{S_1} 0_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{3}} - \frac{\left| 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle}{2 \sqrt{3}} - \frac{\left| 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle}{2 \sqrt{3}} + \frac{\left| 1_{S_1} 0_{S_2} 1_{S_3} 0_{S_4} \right\rangle}{\sqrt{3}} \right\}, \left\{ 1, -1 \right\} \rightarrow \\ & \left\{ \frac{\left| 0_{S_1} 1_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{2}} - \frac{\left| 1_{S_1} 0_{S_1} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{2}} + \frac{\left| 1_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle}{\sqrt{6}} + \frac{\left| 1_{S_1} 0_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{6}} - \sqrt{\frac{2}{3}} \mid \left| 1_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle, \\ & \frac{\left| 0_{S_1} 1_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{2}} - \frac{\left| 1_{S_1} 0_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{2}} + \frac{\left| 1_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle}{\sqrt{6}} + \frac{\left| 1_{S_1} 0_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{6}} - \sqrt{\frac{2}{3}} \mid \left| 1_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle, \\ & \frac{\left| 0_{S_1} 1_{S_2} 1_{S_3} 1_{S_3} \right\rangle}{2 \sqrt{3}} + \frac{\left| 1_{S_1} 0_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{2 \sqrt{3}} - \frac{1}{2} \cdot \sqrt{3} \mid \left| 1_{S_1} 1_{S_2} 1_{S_2} 0_{S_4} \right\rangle, \\ & \left\{ 1, 0 \right\} \rightarrow \left\{ \frac{1}{2} \mid \left| 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle + \frac{1}{2} \mid \left| 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle - \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 1_{S_4} \right\rangle - \frac{1}{2} \mid \left| 1_{S_1} 0_{S_2} 1_{S_3} 0_{S_4} \right\rangle, \\ & \left\{ 1, 0 \right\} \rightarrow \left\{ \frac{1}{2} \mid \left| 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle + \frac{1}{2} \mid \left| 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle - \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 1_{S_4} \right\rangle - \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 1_{S_3} 0_{S_4} \right\rangle, \\ & \left\{ 1, 0 \right\} \rightarrow \left\{ \frac{1}{2} \mid \left| 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle - \frac{1}{2} \mid \left| 0_{S_1} 1_{S_2} 0_{S_3} 0_{S_4} \right\rangle - \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 1_{S_4} \right\rangle + \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 0_{S_4} \right\rangle + \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 0_{S_4} \right\rangle - \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 0_{S_4} \right\rangle + \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 0_{S_4} \right\rangle - \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 0_{S_4} \right\rangle + \frac{1}{2} \cdot \left| 1_{S_1} 0_{S_2} 0_{S_3} 0_{S_4} \right\rangle - \frac{1}{2} \cdot \left| 1_{S_1} 0_$$

The keys label the corresponding angular momentum.

```
In[0]:= Keys[bs]
Out[0]=
       \{\{0,0\},\{1,-1\},\{1,0\},\{1,1\},\{2,-2\},\{2,-1\},\{2,0\},\{2,1\},\{2,2\}\}
```

Group the labels according to the magnitude of the total angular momentum.

In[*]:= GroupBy[Keys[bs], First] // Normal // TableForm

```
Out[*]//TableForm=  0 \to \{\{0,0\}\}   1 \to \{\{1,-1\},\{1,0\},\{1,1\}\}   2 \to \{\{2,-2\},\{2,-1\},\{2,0\},\{2,1\},\{2,2\}\}
```

To compare this basis, arrange all elements in the given order.

$$\label{eq:out_solution} \begin{split} &\text{bb} = \text{Catenate[bs];} \\ &\text{bb} \text{ [; ; 3]]} \\ &\text{Out[\circ] =} \\ & \left\{ \frac{1}{2} \; \left| \; 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle - \frac{1}{2} \; \left| \; 0_{S_1} 1_{S_2} 1_{S_3} 0_{S_4} \right\rangle - \frac{1}{2} \; \left| \; 1_{S_1} 0_{S_2} 0_{S_3} 1_{S_4} \right\rangle + \frac{1}{2} \; \left| \; 1_{S_1} 0_{S_2} 1_{S_3} 0_{S_4} \right\rangle, \\ & \frac{\left| \; 0_{S_1} 0_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{3}} - \frac{\left| \; 0_{S_1} 1_{S_2} 0_{S_3} 1_{S_4} \right\rangle}{2 \; \sqrt{3}} - \frac{\left| \; 0_{S_1} 1_{S_2} 1_{S_3} 0_{S_4} \right\rangle}{2 \; \sqrt{3}} - \frac{\left| \; 1_{S_1} 0_{S_2} 0_{S_3} 1_{S_4} \right\rangle}{2 \; \sqrt{3}} - \\ & \frac{\left| \; 1_{S_1} 0_{S_2} 1_{S_3} 0_{S_4} \right\rangle}{2 \; \sqrt{3}} + \frac{\left| \; 1_{S_1} 1_{S_2} 0_{S_3} 0_{S_4} \right\rangle}{\sqrt{3}} \; , \; \frac{\left| \; 0_{S_1} 1_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{2}} - \frac{\left| \; 1_{S_1} 0_{S_2} 1_{S_3} 1_{S_4} \right\rangle}{\sqrt{2}} \right\} \end{split}$$

Now, calculate the matrix representation of the Hamiltonian in this new basis.

```
In[*]:= EchoTiming[
    new = Outer[Multiply, Dagger[bb], H ** bb];
]
new // MatrixForm
```

0.505931

Out[•]//MatrixForm=

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                                              \sqrt{3}
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```

The Outer function

Observe how the Outer function works.

```
In[*]:= Outer[f, {1, 2, 3}, {a, b}] // MatrixForm
Out[•]//MatrixForm=
        f[1, a] f[1, b]
        f[2, a] f[2, b]
       f[3, a] f[3, b]
```

Let us go back to the previous example, and consider different options for calculating the matrix representation in the new basis.

```
■ Choice 1
EchoTiming[
 mm = Outer[Dagger[#1] ** H ** #2 &, bb, bb];
]
mm // MatrixForm
```

0 8.60772

Out[•]//MatrixForm=

```
\sqrt{3}
- 6
                                                                    0 0 0 0 0
\sqrt{3}
      0
            0
                         0
                                                                    0 0 0 0 0
                  0
                               0
                                     0
                                            0
                                                   0
                                                         0
                                                               0
                 \sqrt{3}
           - 2
                         0
0
      0
                               0
                                     0
                                            0
                                                         0
                                                               0
                                                                    0 0 0 0 0
                                                  0
                       4 √2
          \sqrt{3}
      0
                                     0
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0
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                                            0
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                         3
                <u>4 √</u>2
                         1
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                                    \sqrt{3}
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      0
            0
                  0
                         0
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                                          4\sqrt{2}
                              \sqrt{3}
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0
      0
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                                                       4\sqrt{2}
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0
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                                                                    0 0 0 3 0
      0
            0
                  0
                         0
                               0
0
                  0
                                     0
                                            0
                                                                    0 0 0 0 3
```

■ Choice 2

In[@]:= EchoTiming[mm = Outer[#1 ** H ** #2 &, Dagger[bb], bb];] mm // MatrixForm

8.75689

Out[•]//MatrixForm=

| - 6 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
|------------|------------|------------|-----------------------|------------------------|------------|-----------------------|------------------------|------------|------------------------|-----------------------|---|---|---|---|---|--|
| $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4 \sqrt{2}}{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | $\frac{4\sqrt{2}}{3}$ | $\frac{1}{3}$ | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4 \sqrt{2}}{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | $\frac{4\sqrt{2}}{3}$ | $\frac{1}{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4\sqrt{2}}{3}$ | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $\frac{4 \sqrt{2}}{3}$ | <u>1</u> 3 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | Θ | 0 | 0 | Θ | 0 | 0 | 0 | 3 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | |

■ Choice 3

In[*]:= EchoTiming[mm = Outer[#1 ** #2 &, Dagger[bb], H ** bb];] mm // MatrixForm

0.547041

Out[•]//MatrixForm=

| 1 | _ 6 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
|---|------------|------------|------------|------------------------|------------------------|------------|-----------------------|------------------------|------------|------------------------|-----------------------|---|---|---|---|---|--|
| | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4 \sqrt{2}}{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | $\frac{4 \sqrt{2}}{3}$ | $\frac{1}{3}$ | 0 | 0 | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4 \sqrt{2}}{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | $\frac{4\sqrt{2}}{3}$ | $\frac{1}{3}$ | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | Θ | 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4\sqrt{2}}{3}$ | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | Θ | 0 | 0 | Θ | $\frac{4 \sqrt{2}}{3}$ | <u>1</u> 3 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 3 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | |
| | . 0 | 0 | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | |

In[o]:= EchoTiming[mm = Outer[Multiply, Dagger[bb], H**bb];] mm // MatrixForm

0.555479

Out[•]//MatrixForm=

| - 6 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | ١ |
|------------|------------|------------|-----------------------|------------------------|------------|-----------------------|------------------------|------------|------------------------|-----------------------|---|---|---|---|-----|---|
| $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4 \sqrt{2}}{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | $\frac{4\sqrt{2}}{3}$ | $\frac{1}{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4 \sqrt{2}}{3}$ | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | $\frac{4\sqrt{2}}{3}$ | $\frac{1}{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - 2 | $\sqrt{3}$ | 0 | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $\sqrt{3}$ | $-\frac{4}{3}$ | $\frac{4\sqrt{2}}{3}$ | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $\frac{4 \sqrt{2}}{3}$ | $\frac{1}{3}$ | 0 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 0 | 0 | |
| 0 | 0 | 0 | 0 | Θ | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 0 | |
| 0 | 0 | 0 | 0 | Θ | 0 | 0 | Θ | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | |
| ○ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 / | į |

Summary

Functions

- Outer
- Matrix, ExpressionFor
- QubitAdd
- **■** Chain
- Dagger
- EchoTiming

Related Links

■ Appendix A of the Quantum Workbook (2022, 2023) -- Available for free via the QuantumPlaybook package.