Basis, Matrix, ExpressionFor

In[0]:= << Q3`

Basis

```
In[*]:= Let[Qubit, S]
  In[0]:= bs = Basis[{S[1, $], S[2, $]}]
            \{ | 0_{S_1}0_{S_2} \rangle, | 0_{S_1}1_{S_2} \rangle, | 1_{S_1}0_{S_2} \rangle, | 1_{S_1}1_{S_2} \rangle \}
            Shorthand expressions
  In[*]:= Basis@{S[1, $], S[2, $]}
Out[•]=
            \{ | 0_{S_1}0_{S_2} \rangle, | 0_{S_1}1_{S_2} \rangle, | 1_{S_1}0_{S_2} \rangle, | 1_{S_1}1_{S_2} \rangle \}
  In[*]:= Basis@S[{1, 2}, $]
Out[0]=
            \{ | 0_{S_1}0_{S_2} \rangle, | 0_{S_1}1_{S_2} \rangle, | 1_{S_1}0_{S_2} \rangle, | 1_{S_1}1_{S_2} \rangle \}
  In[0]:= Basis@S@{1, 2}
Out[0]=
            \{ | 0_{S_1} 0_{S_2} \rangle, | 0_{S_1} 1_{S_2} \rangle, | 1_{S_1} 0_{S_2} \rangle, | 1_{S_1} 1_{S_2} \rangle \}
  In[.]:= new = Basis@S@{2, 1}
Out[0]=
            \{ | 0_{S_1}0_{S_2} \rangle, | 1_{S_1}0_{S_2} \rangle, | 0_{S_1}1_{S_2} \rangle, | 1_{S_1}1_{S_2} \rangle \}
  in[o]:= tbl = Transpose@{bb = Row /@ Tuples[{0, 1}, 2], bs, bb, new} // KetRegulate;
            TableForm[tbl,
              TableHeadings \rightarrow {Range[4], {Row@S[{1, 2}, $], "", Row@S[{2, 1}, $], ""}}]
Out[o]//TableForm=
                     S_1 \, S_2
                                                        S_2 \ S_1
            1
                     00
                                      0_{S_1}0_{S_2}
                                                                        0_{S_1}0_{S_2}
            2
                                      0_{S_1}1_{S_2}
                                                                        1<sub>S1</sub>0<sub>S2</sub>
                     01
                                                        01
            3
                                      1_{S_1}0_{S_2}
                                                                        0_{S_1}1_{S_2}
                     10
                                                        10
                     11
                                                                        1_{S_1}1_{S_2}
                                      1_{\mathsf{S}_1}1_{\mathsf{S}_2}
                                                        11
```

In[0]:= Let[Boson, c]

$$\begin{split} & \text{In} \{ \bullet \} \! := \; \mathbf{bs} = \mathbf{Basis} [\mathbf{c}, \mathbf{S} @ \{ \mathbf{1}, \mathbf{2} \}] \\ & \text{Out} \{ \bullet \} \! := \\ & \quad \left\{ \left. \left| \left. 0_{c} 0_{S_{1}} 0_{S_{2}} \right\rangle, \, \left| \left. 0_{c} 0_{S_{1}} 1_{S_{2}} \right\rangle, \, \left| \left. 0_{c} 1_{S_{1}} 0_{S_{2}} \right\rangle, \, \left| \left. 0_{c} 1_{S_{1}} 1_{S_{2}} \right\rangle, \, \left| 1_{c} 0_{S_{1}} 0_{S_{2}} \right\rangle, \, \left| 1_{c} 0_{S_{1}} 1_{S_{2}} \right\rangle, \, \left$$

Matrix vs ExpressionFor

In[0]:= Let[Qubit, S]

Matrix Representation of Vectors

Consider a typical initialization state.

$$In[\circ]:= in = Ket[S@{1,2} \rightarrow 0]$$

$$Out[\circ]:= \left| O_{S_1}O_{S_2} \right\rangle$$

Construct a superposition state by applying the Hadamard operator on each qubit.

In[•]:=
$$\mathbf{v} = \mathbf{S[1, 6]} ** \mathbf{S[2, 6]} ** in$$

Out[•]:=
$$\frac{1}{2} \left| \mathbf{0}_{S_1} \mathbf{0}_{S_2} \right\rangle + \frac{1}{2} \left| \mathbf{0}_{S_1} \mathbf{1}_{S_2} \right\rangle + \frac{1}{2} \left| \mathbf{1}_{S_1} \mathbf{0}_{S_2} \right\rangle + \frac{1}{2} \left| \mathbf{1}_{S_1} \mathbf{1}_{S_2} \right\rangle$$

Represent the state vector in a matrix form.

In[0]:= col // MatrixForm

Out[
$$\circ$$
]//MatrixForm=
$$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

Shorthand expressions

$$ln[*]:= Matrix[v, S[{1, 2}]] // Normal Out[*]:$$
 $\left\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right\}$

In[
$$\circ$$
]:= Matrix[v, S@{1, 2}] // Normal Out[\circ]= $\left\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right\}$

Convert it back to the state expression form.

$$\begin{array}{l} & \textit{In[*]:=} & \textit{new = ExpressionFor[col, S[\{1,2\},\$]]} \\ & \textit{Out[*]:=} \\ & & \frac{1}{2} \quad \left| \, \theta_{S_1} \theta_{S_2} \, \right\rangle + \frac{1}{2} \quad \left| \, \theta_{S_1} \mathbf{1}_{S_2} \, \right\rangle + \frac{1}{2} \quad \left| \, \mathbf{1}_{S_1} \theta_{S_2} \, \right\rangle + \frac{1}{2} \quad \left| \, \mathbf{1}_{S_1} \mathbf{1}_{S_2} \, \right\rangle \\ & \textit{In[*]:=} \quad \textit{new - v} \\ & \textit{Out[*]:=} \\ & & \theta \end{array}$$

Shorthand expressions

$$\begin{array}{ll} & & & \\ & \text{Out}[\circ] := & & \\ & & \frac{1}{2} & \left| \left. 0_{S_1} 0_{S_2} \right\rangle + \frac{1}{2} & \left| \left. 0_{S_1} 1_{S_2} \right\rangle + \frac{1}{2} & \left| \left. 1_{S_1} 0_{S_2} \right\rangle + \frac{1}{2} & \left| 1_{S_1} 1_{S_2} \right\rangle \\ & & & \\ & & \text{In}[\circ] := & \\ & & \frac{1}{2} & \left| \left. 0_{S_1} 0_{S_2} \right\rangle + \frac{1}{2} & \left| \left. 0_{S_1} 1_{S_2} \right\rangle + \frac{1}{2} & \left| \left. 1_{S_1} 0_{S_2} \right\rangle + \frac{1}{2} & \left| \left. 1_{S_1} 1_{S_2} \right\rangle \\ & & & \\ & & \frac{1}{2} & \left| \left. 0_{S_1} 0_{S_2} \right\rangle + \frac{1}{2} & \left| \left. 0_{S_1} 1_{S_2} \right\rangle + \frac{1}{2} & \left| \left. 1_{S_1} 0_{S_2} \right\rangle + \frac{1}{2} & \left| \left. 1_{S_1} 1_{S_2} \right\rangle \\ \end{array}$$

Matrix Representation of Operators

Consider a typical two-qubit Hamiltonian. For your information, this is the famous Heisenberg model of interacting spins.

$$\label{eq:continuous} \begin{split} &\inf \{\cdot \} := & \ \ \, \text{H = Total[S[1, All] **S[2, All]]} \\ & \textit{Out[*]} = \\ & S_1^x \ S_2^x + S_1^y \ S_2^y + S_1^z \ S_2^z \\ & \text{Represent it in a matrix form.} \end{split}$$

$$\label{eq:out_objective} \begin{tabular}{ll} \textit{Out[0]//MatrixForm} & & & & & & & \\ & 1 & 0 & 0 & 0 & \\ & 0 & -1 & 2 & 0 & \\ & 0 & 2 & -1 & 0 & \\ & 0 & 0 & 0 & 1 & \\ \end{tabular}$$

Convert it back to an operator expression.

```
In[o]:= op = ExpressionFor[mat, S@{1, 2}]
Out[0]=
           S_1^z S_2^z + 2 S_1^+ S_2^- + 2 S_1^- S_2^+
  In[•]:= PauliForm[op]
Out[0]=
           Z \otimes Z + 2 \quad X^- \otimes X^+ + 2 \quad X^+ \otimes X^-
  In[0]:= new = Elaborate[op]
Out[0]=
           S_1^X S_2^X + S_1^Y S_2^Y + S_1^Z S_2^Z
  In[0]:= PauliForm[new]
Out[0]=
           X\otimes X\,+\,Y\otimes Y\,+\,Z\otimes Z
```

Application: Eigenvalue Problem

Suppose you want to calculate the eigenvalues and corresponding eigenvectors of the following operator.

```
In[*]:= H = Total[S[1, All] ** S[2, All]]
Out[0]=
         S_1^X S_2^X + S_1^Y S_2^Y + S_1^Z S_2^Z
```

First, calculate the matrix representation of the operator.

```
In[*]:= mat = Matrix[H, S@{1, 2}];
       mat // MatrixForm
Out[•]//MatrixForm=
        1 0 0 0
        0 - 1 2 0
        0 \ 2 \ -1 \ 0
```

Calculate the eigenvalues.

```
In[.]:= Eigenvalues[mat]
Out[0]=
        \{-3, 1, 1, 1\}
```

Calculate the corresponding eigenvectors.

```
In[*]:= vv = Eigenvectors[mat]
Out[0]=
        \{\{0, -1, 1, 0\}, \{0, 0, 0, 1\}, \{0, 1, 1, 0\}, \{1, 0, 0, 0\}\}
```

In the result above, there are four eigenvectors that are represented in the column-vector form.

Convert the eigenvectors into the state expression form.

$$\label{eq:continuous} \begin{split} &\inf\{\circ\}:=\text{ vec = Map[ExpressionFor[\#, S@\{1,2\}] \&, vv]}\\ &\inf\{\circ\}:=\\ &\left\{-\left|0_{S_{1}}1_{S_{2}}\right\rangle+\left|1_{S_{1}}0_{S_{2}}\right\rangle,\,\left|1_{S_{1}}1_{S_{2}}\right\rangle,\,\left|0_{S_{1}}1_{S_{2}}\right\rangle+\left|1_{S_{1}}0_{S_{2}}\right\rangle,\,\left|0_{S_{1}}0_{S_{2}}\right\rangle\right\}\\ &\inf\{\circ\}:=\text{ ExpressionFor[\#, S@\{1,2\}] \&/@vv}\\ &\inf\{\circ\}:=\\ &\left\{-\left|0_{S_{1}}1_{S_{2}}\right\rangle+\left|1_{S_{1}}0_{S_{2}}\right\rangle,\,\left|1_{S_{1}}1_{S_{2}}\right\rangle,\,\left|0_{S_{1}}1_{S_{2}}\right\rangle+\left|1_{S_{1}}0_{S_{2}}\right\rangle,\,\left|0_{S_{1}}0_{S_{2}}\right\rangle\right\} \end{split}$$

You can get the eigenvalues and corresponding eigenvectors at once.

```
In[*]:= Eigensystem[mat]
Out[•]=
        \{\{-3, 1, 1, 1\}, \{\{0, -1, 1, 0\}, \{0, 0, 0, 1\}, \{0, 1, 1, 0\}, \{1, 0, 0, 0\}\}\}
 In[0]:= {val, vec} = Eigensystem[mat]
Out[0]=
        \{\{-3, 1, 1, 1\}, \{\{0, -1, 1, 0\}, \{0, 0, 0, 1\}, \{0, 1, 1, 0\}, \{1, 0, 0, 0\}\}\}
        Check the eigenvalues.
 In[•]:= val
Out[0]=
        \{-3, 1, 1, 1\}
        Check the eigenvectors.
 In[0]:= vec
Out[0]=
```

Converting an operator to matrix and then back to state expression is boring.

 $\{\{0, -1, 1, 0\}, \{0, 0, 0, 1\}, \{0, 1, 1, 0\}, \{1, 0, 0, 0\}\}$

```
In[*]:= H = Total[S[1, All] ** S[2, All]]
Out[0]=
            S_1^X S_2^X + S_1^Y S_2^Y + S_1^Z S_2^Z
  In[*]:= ProperValues[H]
Out[0]=
             \{-3, 1, 1, 1\}
  In[*]:= ProperStates[H]
Out[0]=
             \{- | O_{S_1} I_{S_2} \rangle + | I_{S_1} O_{S_2} \rangle, | I_{S_1} I_{S_2} \rangle, | O_{S_1} I_{S_2} \rangle + | I_{S_1} O_{S_2} \rangle, | O_{S_1} O_{S_2} \rangle \}
  In[o]:= {val, vec} = ProperSystem[H]
Out[0]=
             \{\{-3, 1, 1, 1\}, \{-|0_{S_1}1_{S_2}\rangle + |1_{S_1}0_{S_2}\rangle, |1_{S_1}1_{S_2}\rangle, |0_{S_1}1_{S_2}\rangle + |1_{S_1}0_{S_2}\rangle, |0_{S_1}0_{S_2}\rangle\}\}
```

```
In[•]:= val
Out[0]=
                           \{-3, 1, 1, 1\}
     In[0]:= vec
Out[0]=
                           \left\{-\left.\left|0_{S_{1}}1_{S_{2}}\right.\right\rangle + \left.\left|1_{S_{1}}0_{S_{2}}\right.\right\rangle , \right. \left|1_{S_{1}}1_{S_{2}}\right.\right\rangle , \left.\left|0_{S_{1}}1_{S_{2}}\right.\right\rangle + \left.\left|1_{S_{1}}0_{S_{2}}\right.\right\rangle , \left.\left|0_{S_{1}}0_{S_{2}}\right.\right\rangle \right\}
```

Summary

Functions

- Basis
- Matrix
- ExpressionFor
- Eigenvalues, Eigenvectors, Eigensystem
- ProperValues, ProperStates, ProperSystem

Related Links

- S. Wolfram (2017), "An Elementary Introduction to Wolfram Language," 2nd edition (2017).
- The Wolfram Language: Fast Introduction for Math Students
- The Wolfram Language: Fast Introduction for Programmers