

In[1]:= Needs ["SpinDynamica`"]

SpinDynamica version 3.0.1 loaded

... **ModifyBuiltin**: The following built-in routines have been modified in SpinDynamica:  
{Chop, Dot, Duration, Exp, Expand, ExpandAll, NumericQ, Plus, Power, Simplify, Times, WignerD}.  
Evaluate ??symbol to generate the additional definitions for symbol.

## opl (angular momentum operators)

In[2]:= ? opI

opl[spin,  $\mu$ ] defines an angular momentum operator for the indicated spin. If the symbol spin is a List, a sum over the spins in the list is implied, and if the symbol spin is absent, a sum over all spins in the current spin system is taken. The label  $\mu$  may be a phase  $\phi$  (indicating the phase angle of the spin angular momentum in the xy-plane), or may specify the polar angles  $\{\theta, \phi\}$  (indicating spin angular momentum in an arbitrary direction in 3D space). The label  $\mu$  may also take the values "x", "y", "z", indicating spin angular momentum operators along one of the Cartesian axes. Shift operators are indicated by using labels "+", "-", while polarization operators for spins-1/2 are indicated by using labels " $\alpha$ ", " $\beta$ ". If the label  $\mu$  is absent, a vector of the three Cartesian angular momentum components is generated. Hence opl[i].opl[j] defines the dot product of the angular momenta of spins i and j.

## 2 spins-1/2

In[3]:= SetSpinSystem[2]

... **SetSpinSystem**: the spin system has been set to  $\left\{\left\{1, \frac{1}{2}\right\}, \left\{2, \frac{1}{2}\right\}\right\}$

... **SetBasis**: the state basis has been set to ZeemanBasis $\left[\left\{\left\{1, \frac{1}{2}\right\}, \left\{2, \frac{1}{2}\right\}\right\}, \text{BasisLabels} \rightarrow \text{Automatic}\right]$ .

In[4]:= opI["x"]

Out[4]=  $I_{1x} + I_{2x}$

In[5]:= opI[3, "x"]

... **SpinSystem**: spin index 3 is not in current spin system. Use SetSpinSystem or SetBasis to set up spin system.

Out[5]= \$Failed

In[6]:= opI[{1, 2}, "x"]

Out[6]=  $I_{1x} + I_{2x}$

In[7]:= opI[{1, 2, 3}, "x"]

... **SpinSystem**: spin index {1, 2, 3} is not in current spin system. Use SetSpinSystem or SetBasis to set up spin system.

Out[7]= \$Failed

In[8]:= MatrixRepresentation[opI["x"]] // MatrixForm

Out[8]//MatrixForm=

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

In[9]:= **MatrixRepresentation**[opI[1, "x"]] // **MatrixForm**

Out[9]//MatrixForm=

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

In[10]:= **MatrixRepresentation**[opI[2, "x"]] // **MatrixForm**

Out[10]//MatrixForm=

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

In[11]:= **MatrixRepresentation**[2 opI[1, "z"].opI[2, "x"]] // **MatrixForm**

Out[11]//MatrixForm=

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

In[12]:= **MatrixRepresentation**[2 opI[1, "z"].opI[2, "+"]] // **MatrixForm**

Out[12]//MatrixForm=

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

In[13]:= **MatrixRepresentation**[opI[1, "α"].opI[2, "β"]] // **MatrixForm**

Out[13]//MatrixForm=

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

In[14]:= **opI**[1,  $\pi/4$ ]

$$\text{Out[14]} = \frac{\mathbf{I}_{1x}}{\sqrt{2}} + \frac{\mathbf{I}_{1y}}{\sqrt{2}}$$

In[15]:= **opI**[1, { $\pi/3$ ,  $\pi/4$ }]

$$\text{Out[15]} = \frac{1}{2} \sqrt{3} \left( \frac{\mathbf{I}_{1x}}{\sqrt{2}} + \frac{\mathbf{I}_{1y}}{\sqrt{2}} \right) + \frac{\mathbf{I}_{1z}}{2}$$

In[16]:= **opI**[{ $\pi/3$ ,  $\pi/4$ }]

$$\text{Out[16]} = \frac{1}{2} \sqrt{3} \left( \frac{\mathbf{I}_{1x}}{\sqrt{2}} + \frac{\mathbf{I}_{1y}}{\sqrt{2}} \right) + \frac{\mathbf{I}_{1z}}{2} + \frac{1}{2} \sqrt{3} \left( \frac{\mathbf{I}_{2x}}{\sqrt{2}} + \frac{\mathbf{I}_{2y}}{\sqrt{2}} \right) + \frac{\mathbf{I}_{2z}}{2}$$

In[17]:= **opI**[1].**opI**[2]

$$\text{Out[17]} = \mathbf{I}_{1x} \cdot \mathbf{I}_{2x} + \mathbf{I}_{1y} \cdot \mathbf{I}_{2y} + \mathbf{I}_{1z} \cdot \mathbf{I}_{2z}$$

In[18]:= **opI[1].{a, b, c}**

Out[18]=  $a I_{1x} + b I_{1y} + c I_{1z}$

## spin "I" (quantum number 1) and spin "S" (quantum number 3/2)

In[19]:= **SetSpinSystem[{"I", 1}, {"S", 3/2}]**

... **SetSpinSystem**: the spin system has been set to  $\{\{I, 1\}, \{S, \frac{3}{2}\}\}$

... **SetBasis**: the state basis has been set to  $\text{ZeemanBasis}[\{\{I, 1\}, \{S, \frac{3}{2}\}\}, \text{BasisLabels} \rightarrow \text{Automatic}]$ .

In[20]:= **opI["x"]**

Out[20]=  $I_x + S_x$

In[21]:= **MatrixRepresentation[opI["x"]] // MatrixForm**

Out[21]//MatrixForm=

$$\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

In[22]:= **opI[1, "x"]**

... **SpinSystem**: spin index 1 is not in current spin system. Use SetSpinSystem or SetBasis to set up spin system.

Out[22]= **\$Failed**

In[23]:= **MatrixRepresentation**[opI["I", "x"]] // **MatrixForm**

Out[23]//MatrixForm=

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

In[24]:= **MatrixRepresentation**[opI["S", "x"]] // **MatrixForm**

Out[24]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 \end{pmatrix}$$

