

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.

In[2]:= SetSpinSystem[2]

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

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

default operator basis (ZeemanKetBraOperatorBasis)

natural sorting order

In[3]:= SetOperatorBasis[]

... **SetOperatorBasis**: the operator basis has been set to ShiftAndZOperatorBasis $\{\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}\}, \text{Sorted} \rightarrow \text{CoherenceOrder}\}$.

In[4]:= BasisOperators[]

Out[4]= $\{I_1^- \cdot I_2^-, \sqrt{2} (I_1^- \cdot I_{2z}), \sqrt{2} (I_{1z} \cdot I_2^-), \frac{I_1^-}{\sqrt{2}}, \frac{I_2^-}{\sqrt{2}}, I_1^- \cdot I_2^+, I_1^+ \cdot I_2^-,$
 $2 (I_{1z} \cdot I_{2z}), I_{1z}, I_{2z}, \frac{1}{2}, \sqrt{2} (I_1^+ \cdot I_{2z}), \sqrt{2} (I_{1z} \cdot I_2^+), \frac{I_1^+}{\sqrt{2}}, \frac{I_2^+}{\sqrt{2}}, I_1^+ \cdot I_2^+\}$

In[5]:= CoherenceOrder /@ BasisOperators[]

Out[5]= $\{-2, -1, -1, -1, -1, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 2\}$

sort the basis operators according to the coherence order

In[6]:= SetOperatorBasis[ZeemanKetBraOperatorBasis[Sorted → CoherenceOrder]]

... **SetOperatorBasis**: the operator basis has been set to
ZeemanKetBraOperatorBasis $\{\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}\}, \text{Sorted} \rightarrow \text{CoherenceOrder}\}$.

In[7]:= BasisOperators[]

Out[7]= $\{|\beta\beta\rangle \cdot \langle\alpha\alpha|, |\beta\beta\rangle \cdot \langle\beta\alpha|, |\beta\beta\rangle \cdot \langle\alpha\beta|, |\beta\alpha\rangle \cdot \langle\alpha\alpha|, |\alpha\beta\rangle \cdot \langle\alpha\alpha|,$
 $|\beta\beta\rangle \cdot \langle\beta\beta|, |\beta\alpha\rangle \cdot \langle\beta\alpha|, |\beta\alpha\rangle \cdot \langle\alpha\beta|, |\alpha\beta\rangle \cdot \langle\beta\alpha|, |\alpha\beta\rangle \cdot \langle\alpha\beta|, |\alpha\alpha\rangle \cdot \langle\alpha\alpha|,$
 $|\beta\alpha\rangle \cdot \langle\beta\beta|, |\alpha\beta\rangle \cdot \langle\beta\beta|, |\alpha\alpha\rangle \cdot \langle\beta\alpha|, |\alpha\alpha\rangle \cdot \langle\alpha\beta|, |\alpha\alpha\rangle \cdot \langle\beta\beta|\}$

In[8]:= CoherenceOrder /@ BasisOperators[]

Out[8]= $\{-2, -1, -1, -1, -1, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 2\}$

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In[9]:= OperatorBasisTransformationMatrix[
  ZeemanKetBraOperatorBasis[Sorted → CoherenceOrder],
  ZeemanKetBraOperatorBasis[Sorted → False]
] // MatrixForm
```

Out[9]//MatrixForm=

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

CartesianProductOperatorBasis

default sorting

```
In[10]:= SetOperatorBasis[CartesianProductOperatorBasis[]]
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SetOperatorBasis: the operator basis has been set to

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CartesianProductOperatorBasis[{{1, 1/2}, {2, 1/2}}, Sorted → SpinProductRank].
```

```
In[11]:= BasisOperators[]
```

```
Out[11]= { 1/2, I1x, I1y, I1z, I2x, I2y, I2z, 2 (I1x•I2x), 2 (I1x•I2y), 2 (I1x•I2z),
  2 (I1y•I2x), 2 (I1y•I2y), 2 (I1y•I2z), 2 (I1z•I2x), 2 (I1z•I2y), 2 (I1z•I2z) }
```

```
In[12]:= CoherenceOrder /@ BasisOperators[]
```

```
Out[12]= {0, {-1, 1}, {-1, 1}, 0, {-1, 1}, {-1, 1}, 0, {-2, 0, 2},
  {-2, 0, 2}, {-1, 1}, {-2, 0, 2}, {-2, 0, 2}, {-1, 1}, {-1, 1}, {-1, 1}, 0}
```

```
In[13]:= SpinProductRank /@ BasisOperators[]
```

```
Out[13]= {0, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2}
```

basis transformation matrix

```
In[14]:= OperatorBasisTransformationMatrix[
  ZeemanKetBraOperatorBasis[Sorted → CoherenceOrder],
  CartesianProductOperatorBasis[]
] // MatrixForm
```

Out[14]//MatrixForm=

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

ShiftAndZOperatorBasis

default sorting

```
In[15]:= SetOperatorBasis[ShiftAndZOperatorBasis[]]
```

SetOperatorBasis: the operator basis has been set to ShiftAndZOperatorBasis[{{1, $\frac{1}{2}$ }, {2, $\frac{1}{2}$ }}, Sorted → CoherenceOrder].

```
In[16]:= BasisOperators[]
```

$$\text{Out[16]= } \left\{ \mathbf{I}_1^- \cdot \mathbf{I}_2^-, \sqrt{2} (\mathbf{I}_1^- \cdot \mathbf{I}_{2z}), \sqrt{2} (\mathbf{I}_{1z} \cdot \mathbf{I}_2^-), \frac{\mathbf{I}_1^-}{\sqrt{2}}, \frac{\mathbf{I}_2^-}{\sqrt{2}}, \mathbf{I}_1^- \cdot \mathbf{I}_2^+, \mathbf{I}_1^+ \cdot \mathbf{I}_2^-, \right. \\ \left. 2 (\mathbf{I}_{1z} \cdot \mathbf{I}_{2z}), \mathbf{I}_{1z}, \mathbf{I}_{2z}, \frac{1}{2}, \sqrt{2} (\mathbf{I}_1^+ \cdot \mathbf{I}_{2z}), \sqrt{2} (\mathbf{I}_{1z} \cdot \mathbf{I}_2^+), \frac{\mathbf{I}_1^+}{\sqrt{2}}, \frac{\mathbf{I}_2^+}{\sqrt{2}}, \mathbf{I}_1^+ \cdot \mathbf{I}_2^+ \right\}$$

```
In[17]:= CoherenceOrder /@ BasisOperators[]
```

Out[17]= {-2, -1, -1, -1, -1, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 2}

```
In[18]:= SpinProductRank /@ BasisOperators[]
```

Out[18]= {2, 2, 2, 1, 1, 2, 2, 2, 1, 1, 0, 2, 2, 1, 1, 2}

basis transformation matrix

```
In[19]:= OperatorBasisTransformationMatrix[
  ShiftAndZOperatorBasis[],
  CartesianProductOperatorBasis[]
] // MatrixForm
```

Out[19]//MatrixForm=

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