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*.

spherical tensor operators

In[2]:=
```
? opT
```

opT[j,{1,μ}] defines a first–rank spherical tensor operator for spin j.

opT[{1,μ}] defaults to opT[1,{1,μ}].

opT[{j,k},{2,μ}] defines a second–rank spherical tensor operator for spins j and k.

opT[2,μ] defaults to opT[{1,2},{2,μ}]

opT[{{j,λ_j},{k,λ_k}..},{Λ,M}] generates a Λth rank ISTO by coupling together the interactions {{j,λ_j},{k,λ_k}..} where j is a symbol identifying the interaction and λ_j is its rank.

opT[{j,k..},{Λ,M}] defaults to opT[{{j,1},{k,1}..},{Λ,M}].

The option Normalize–>True may be set to generate STOs normalized in the current state basis.

In cases where there are many possible coupling paths to the requested operator, a message is issued and a list of all possible operators is returned. A single operator may be returned using the form opT[{{j,λ_j},{k,λ_k}..},{Λ,M},n], where n is an integer identifying the requested operator.

An explicit coupling pathway may also be specified. For example, a rank–2 operator generated by coupling together the rank–1 operator for spin ♯1 with the rank–1 operator for spin ♯2, and then coupling the resulting rank–1 operator with a rank–2 operator for spin ♯3, may be specified as follows: opT[{{{{1,1},{2,1}},1},{3,2}},{2,M}].

single spin-1/2

In[3]:=
```
SetSpinSystem[1]
```

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

... SetBasis: the state basis has been set to ZeemanBasis$[\{\{1, \frac{1}{2}\}\}$, BasisLabels → Automatic$]$.

In[4]:=
```
opT[1, {1, 0}]
```

Out[4]= I_{1z}

In[5]:=
```
opT[1, {2, 0}]
```

Out[5]= 𝟘

In[6]:=
```
opT[1, {1, 1}]
```

Out[6]= $-\frac{I_1^+}{\sqrt{2}}$

In[7]:=
```
opT[1, {1, -1}]
```

Out[7]= $\frac{I_1^-}{\sqrt{2}}$

single spin-3/2

In[8]:= `SetSpinSystem[{{1, 3/2}}]`

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

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

In[9]:= `opT[1, {1, 0}]`

Out[9]= I_{1z}

In[10]:= `opT[1, {2, 0}]`

Out[10]= $$\frac{-(I_{1x}\cdot I_{1x}) - I_{1y}\cdot I_{1y} + 2\,(I_{1z}\cdot I_{1z})}{\sqrt{6}}$$

In[11]:= `opT[1, {2, 2}]`

Out[11]= $$\frac{1}{2}\,(I_1^+\cdot I_1^+)$$

In[12]:= `opT[1, {3, 0}]`

opT: Spherical tensor operators of high rank are calculated using the Wigner–Eckart theorem and provided in the form of Operator. Explicit expressions may be constructed by applying ExpressOperator. This message appears only once.

Out[12]= Operator[<< .. >>, OperatorType → Hermitian]

In[13]:= `opT[1, {3, 3}]`

Out[13]= Operator[<< .. >>, OperatorType → None]

spin-1/2 pairs

In[14]:= `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$[\{\{1, \frac{1}{2}\}, \{2, \frac{1}{2}\}\}$, BasisLabels → Automatic].

In[15]:= `opT[1, {1, 0}]`

Out[15]= I_{1z}

In[16]:= `opT[{1, 2}, {2, 0}]`

Out[16]= $$-\frac{I_1^-\cdot I_2^+ + I_1^+\cdot I_2^- - 4\,(I_{1z}\cdot I_{2z})}{2\sqrt{6}}$$

In[17]:= `opT[{1, 2}, {1, 1}]`

Out[17]= $$\frac{1}{2}\,(-(I_1^+\cdot I_{2z}) + I_{1z}\cdot I_2^+)$$

In[18]:= `opT[{1, 2}, {2, 2}]`

Out[18]= $\frac{1}{2}\,(I_1^+ \bullet I_2^+)$

3 spins-1/2

In[19]:= `SetSpinSystem[3]`

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

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

In[20]:= `opT[1, {1, 0}]`

Out[20]= $I_{1\,z}$

In[21]:= `opT[{1, 2}, {2, 0}]`

Out[21]= $-\frac{I_1^- \bullet I_2^+ + I_1^+ \bullet I_2^- - 4\,(I_{1\,z} \bullet I_{2\,z})}{2\sqrt{6}}$

In[22]:= `opT[{1, 2}, {1, 1}]`

Out[22]= $\frac{1}{2}\,(-(I_1^+ \bullet I_{2\,z}) + I_{1\,z} \bullet I_2^+)$

In[23]:= `opT[{1, 2}, {2, 2}]`

Out[23]= $\frac{1}{2}\,(I_1^+ \bullet I_2^+)$

In[24]:= `opT[{1, 2, 3}, {3, 3}]`

Out[24]= $-\frac{I_1^+ \bullet I_2^+ \bullet I_3^+}{2\sqrt{2}}$

In[25]:= `opT[{1, 2, 3}, {3, 2}]`

Out[25]= $\frac{I_1^+ \bullet I_2^+ \bullet I_{3\,z} + I_1^+ \bullet I_{2\,z} \bullet I_3^+ + I_{1\,z} \bullet I_2^+ \bullet I_3^+}{2\sqrt{3}}$

In[26]:= `opT[{1, 2, 3}, {2, 2}]`

opT: There are 2 operators with this specification. A list of all possibilities has been returned. Specify a single operator using the form opT[interactions,{Lam,M},index] where index is an integer.

Out[26]= $\left\{\frac{I_1^+ \bullet I_{2\,z} \bullet I_3^+ - I_{1\,z} \bullet I_2^+ \bullet I_3^+}{2\sqrt{2}}, \frac{2\,(I_1^+ \bullet I_2^+ \bullet I_{3\,z}) - I_1^+ \bullet I_{2\,z} \bullet I_3^+ - I_{1\,z} \bullet I_2^+ \bullet I_3^+}{2\sqrt{6}}\right\}$

In[27]:= `opT[{1, 2, 3}, {2, 2}, 1]`

opT: There are 2 operators with this specification. A list of all possibilities has been returned. Specify a single operator using the form opT[interactions,{Lam,M},index] where index is an integer.

Out[27]= $\left\{\frac{I_1^+ \bullet I_{2\,z} \bullet I_3^+ - I_{1\,z} \bullet I_2^+ \bullet I_3^+}{2\sqrt{2}}, \frac{2\,(I_1^+ \bullet I_2^+ \bullet I_{3\,z}) - I_1^+ \bullet I_{2\,z} \bullet I_3^+ - I_{1\,z} \bullet I_2^+ \bullet I_3^+}{2\sqrt{6}}\right\}$

In[28]:=
```
opT[{1, 2, 3}, {2, 2}, 2]
```

opT: failure in opT routine

Out[28]= 𝕆