

Needs["SpinDynamica`"]

spherical tensor operators

? 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.

In cases where there are many possible couplings the form opT[{{j,λ_j},{k,λ_k...},{Λ,M},n]

must be used where n is an integer identifying the coupling scheme.

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.

single spin-1/2

SetSpinSystem[1]

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

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

opT[1, {1, 0}]

I_{1z}

opT[1, {2, 0}]

opT::singlespinranktoohigh : spin system does not support a single-spin irreducible spherical tensor operator of rank 2
0

opT[1, {1, 1}]

$-\frac{I_1^+}{\sqrt{2}}$

opT[1, {1, -1}]

$\frac{I_1^-}{\sqrt{2}}$

single spin-3/2

SetSpinSystem[{1, 3/2}]

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

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

opT[1, {1, 0}]

I_{1z}

opT[1, {2, 0}]

$$-\frac{I_1^- \cdot I_1^+}{2\sqrt{6}} - \frac{I_1^+ \cdot I_1^-}{2\sqrt{6}} + \sqrt{\frac{2}{3}} I_{1z} \cdot I_{1z}$$

opT[1, {2, 2}]

$$\frac{1}{2} I_1^+ \cdot I_1^+$$

opT[1, {3, 0}]

$$-\frac{I_1^- \cdot I_1^+ \cdot I_{1z}}{2\sqrt{10}} - \frac{I_1^- \cdot I_{1z} \cdot I_1^+}{2\sqrt{10}} - \frac{I_1^+ \cdot I_1^- \cdot I_{1z}}{2\sqrt{10}} - \frac{I_1^+ \cdot I_{1z} \cdot I_1^-}{2\sqrt{10}} - \frac{I_{1z} \cdot I_1^- \cdot I_1^+}{2\sqrt{10}} - \frac{I_{1z} \cdot I_1^+ \cdot I_1^-}{2\sqrt{10}} + \sqrt{\frac{2}{5}} I_{1z} \cdot I_{1z} \cdot I_{1z}$$

opT[1, {3, 3}]

$$-\frac{I_1^+ \cdot I_1^+ \cdot I_1^+}{2\sqrt{2}}$$

spin-1/2 pairs

SetSpinSystem[2]

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

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

opT[1, {1, 0}]

I_{1z}

opT[{1, 2}, {2, 0}]

$$-\frac{I_1^- \cdot I_2^+}{2\sqrt{6}} - \frac{I_1^+ \cdot I_2^-}{2\sqrt{6}} + \sqrt{\frac{2}{3}} I_{1z} \cdot I_{2z}$$

opT[{1, 2}, {1, 1}]

$$-\frac{1}{2} I_1^+ \cdot I_{2z} + \frac{1}{2} I_{1z} \cdot I_2^+$$

opT[{1, 2}, {2, 2}]

$$\frac{1}{2} I_1^+ \cdot I_2^+$$

3 spins-1/2

SetSpinSystem[3]

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

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

opT[1, {1, 0}]

$$I_{1z}$$

opT[{1, 2}, {2, 0}]

$$-\frac{I_1^- \cdot I_2^+}{2\sqrt{6}} - \frac{I_1^+ \cdot I_2^-}{2\sqrt{6}} + \sqrt{\frac{2}{3}} I_{1z} \cdot I_{2z}$$

opT[{1, 2}, {1, 1}]

$$-\frac{1}{2} I_1^+ \cdot I_{2z} + \frac{1}{2} I_{1z} \cdot I_2^+$$

opT[{1, 2}, {2, 2}]

$$\frac{1}{2} I_1^+ \cdot I_2^+$$

opT[{1, 2, 3}, {3, 3}]

$$-\frac{I_1^+ \cdot I_2^+ \cdot I_3^+}{2\sqrt{2}}$$

opT[{1, 2, 3}, {3, 2}]

$$\frac{I_1^+ \cdot I_2^+ \cdot I_{3z}}{2\sqrt{3}} + \frac{I_1^+ \cdot I_{2z} \cdot I_3^+}{2\sqrt{3}} + \frac{I_{1z} \cdot I_2^+ \cdot I_3^+}{2\sqrt{3}}$$

opT[{1, 2, 3}, {2, 2}]

opT::multiple :

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.

$$\left\{ \frac{I_1^+ \cdot I_{2z} \cdot I_3^+}{2\sqrt{2}} - \frac{I_{1z} \cdot I_2^+ \cdot I_3^+}{2\sqrt{2}}, \frac{I_1^+ \cdot I_2^+ \cdot I_{3z}}{\sqrt{6}} - \frac{I_1^+ \cdot I_{2z} \cdot I_3^+}{2\sqrt{6}} - \frac{I_{1z} \cdot I_2^+ \cdot I_3^+}{2\sqrt{6}} \right\}$$

opT[{1, 2, 3}, {2, 2}, 1]

$$\frac{I_1^+ \cdot I_{2z} \cdot I_3^+}{2\sqrt{2}} - \frac{I_{1z} \cdot I_2^+ \cdot I_3^+}{2\sqrt{2}}$$

opT[{1, 2, 3}, {2, 2}, 2]

$$\frac{I_1^+ \cdot I_2^+ \cdot I_{3z}}{\sqrt{6}} - \frac{I_1^+ \cdot I_{2z} \cdot I_3^+}{2\sqrt{6}} - \frac{I_{1z} \cdot I_2^+ \cdot I_3^+}{2\sqrt{6}}$$