Understanding of spin orbit interaction with an example of *l* = 1 and *s* = 1/2

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Using the Mathematica (KroneckerProduct and Eigensystem), the eigenvalue problem of the spin-orbit interaction for the orbital angular momentum (*l* =1) and spin angular momentum (*s* = 1/2) is dicussed. This discussion is useful for students in understanding the concept of the Clebsch-Gordan coefficient.

1. Matrix representation for the state vectors

(i) Orbital angular momentum of *l* = 1

$$|l=1, m=1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |1,-1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

(ii) Spin angular momentum

$$|+z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |-z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

(iii) $|l=1, m\rangle \otimes |\pm z\rangle$

$$|\phi_1\rangle = |l=1, m=1\rangle \otimes |+z\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|\phi_2\rangle = |l=1, m=1\rangle \otimes |-z\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\left|\phi_3\right\rangle = \left|l=1, m=0\right\rangle \otimes \left|+z\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\left|\phi_4\right\rangle = \left|l=1, m=0\right\rangle \otimes \left|-z\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\left|\phi_5\right\rangle = \left|l=1, m=-1\right\rangle \otimes \left|+z\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\left|\phi_6\right\rangle = \left|l=1, m=-1\right\rangle \otimes \left|-z\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

2. The matrix representation of the spin-orbit interaction

$$\frac{\hat{L}_x}{\hbar} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \qquad \frac{\hat{L}_y}{\hbar} = \begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}$$

$$\frac{\hat{L}_z}{\hbar} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\frac{\hat{S}_x}{\hbar} = \frac{1}{2}\hat{\sigma}_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \frac{\hat{S}_y}{\hbar} = \frac{1}{2}\hat{\sigma}_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\frac{\hat{S}_z}{\hbar} = \frac{1}{2}\hat{\sigma}_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The spin orbit interaction

$$\hat{H}_{so} = \xi(\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}) = \xi\hbar^2(\frac{\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}}{\hbar^2})$$

$$\xi\frac{\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}}{\hbar^2} = \xi(\frac{\hat{L}_x}{\hbar} \otimes \frac{\hat{S}_x}{\hbar} + \frac{\hat{L}_y}{\hbar} \otimes \frac{\hat{S}_y}{\hbar} + \frac{\hat{L}_z}{\hbar} \otimes \frac{\hat{S}_z}{\hbar})$$

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

under the basis $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle, |\phi_5\rangle, |\phi_6\rangle\}$. We solve the eigenvalue problem.

3. Eigenvalue problem

Eigenvalue

(a) Energy eigenvalue: $\frac{\xi}{2}$

$$|\psi_3\rangle = \left|j=\frac{3}{2}, m=-\frac{3}{2}\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \qquad |\psi_4\rangle = \left|j=\frac{1}{2}, m=-\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \sqrt{2/3} \\ 1/\sqrt{3} \\ 0 \end{pmatrix}$$

$$|\psi_5\rangle = \left|j=\frac{3}{2}, m=\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 1/\sqrt{3} \\ \sqrt{2/3} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_6\rangle = \left|j=\frac{3}{2}, m=\frac{3}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

(b) Energy eigenvalue: $-\xi$

$$|\psi_1\rangle = \left|j=\frac{1}{2}, m=\frac{1}{2}\right\rangle \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1/\sqrt{3} \\ -\sqrt{2/3} \\ 0 \end{pmatrix}, \qquad |\psi_2\rangle = \left|j=\frac{1}{2}, m=-\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ \sqrt{2/3} \\ -1/\sqrt{3} \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

4. Discussion

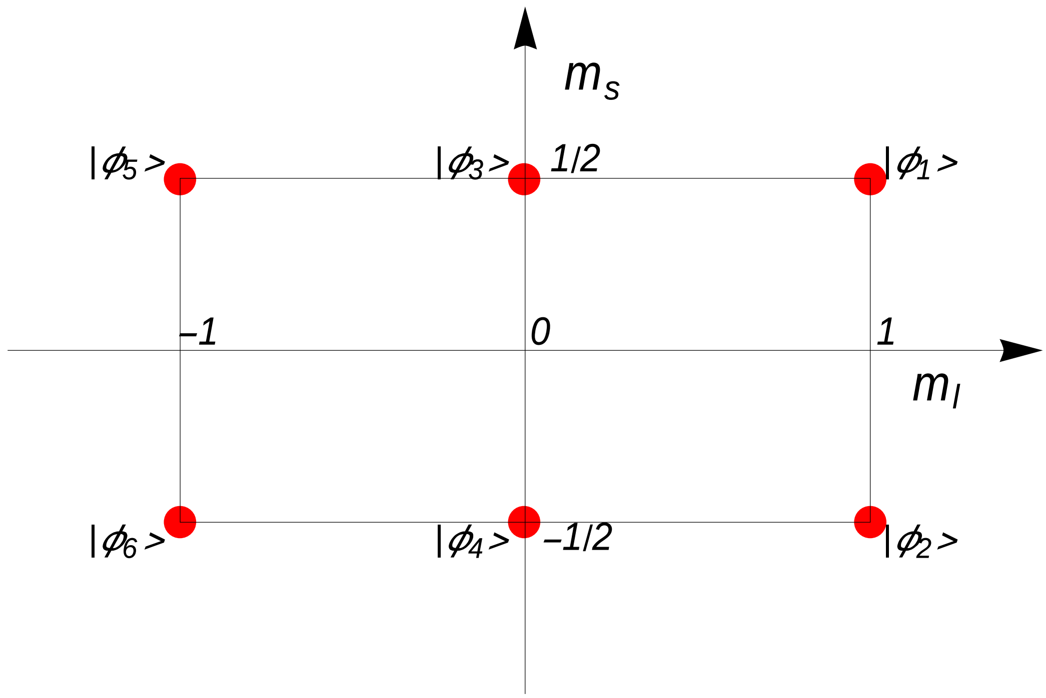

Fig. $\left|\phi_1\right\rangle = \left|m_l = 1, m_s = \frac{1}{2}\right\rangle$. $\left|\phi_2\right\rangle = \left|m_l = 1, m_s = -\frac{1}{2}\right\rangle$, $\left|\phi_3\right\rangle = \left|m_l = 0, m_s = \frac{1}{2}\right\rangle$.
$\left|\phi_4\right\rangle = \left|m_l = 0, m_s = -\frac{1}{2}\right\rangle$, $\left|\phi_5\right\rangle = \left|m_l = -1, m_s = \frac{1}{2}\right\rangle$. $\left|\phi_6\right\rangle = \left|m_l = -1, m_s = -\frac{1}{2}\right\rangle$,

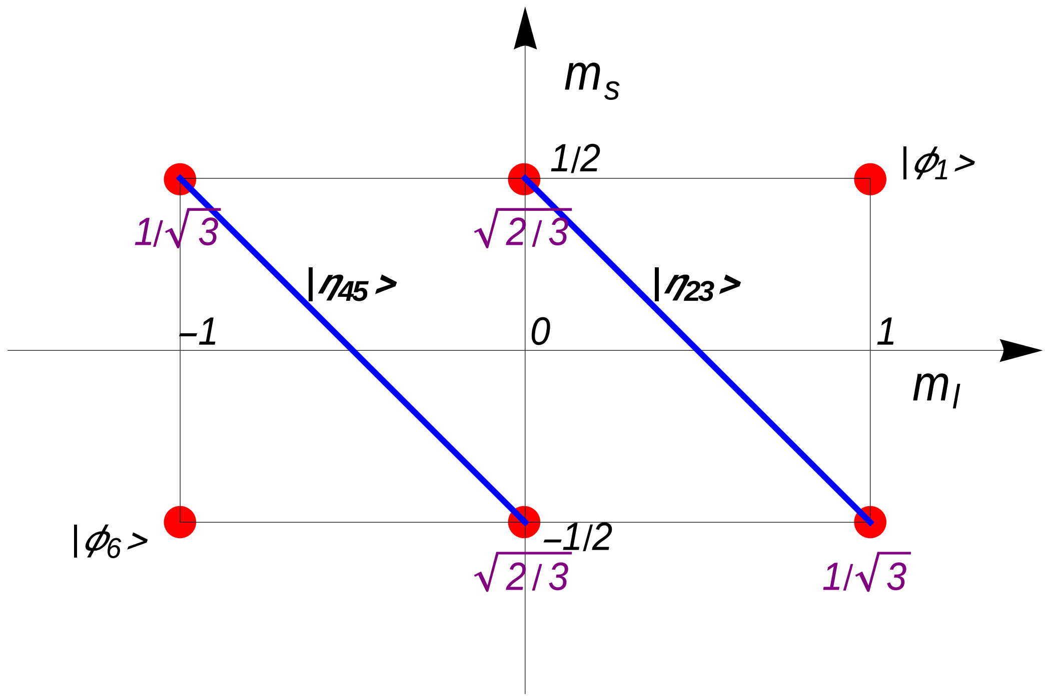

Fig. $\lambda=\frac{1}{2}$. $j=\frac{3}{2}$. $|\eta_{23}\rangle=|\,j=\frac{3}{2},m=\frac{1}{2}>$. $|\eta_{45}\rangle=|\,j=\frac{1}{2},m=-\frac{1}{2}>$. The CG coefficients are denoted next to the red points.

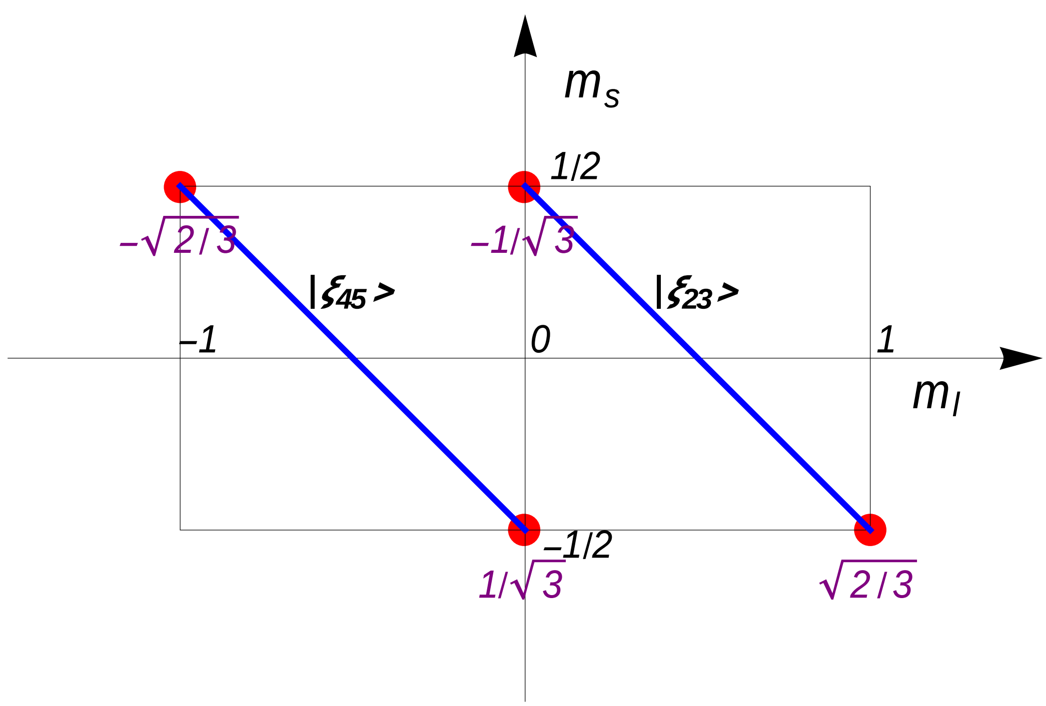

Fig. $\lambda = -1$. $j = \frac{1}{2}$. $|\xi_{23}\rangle = | j = \frac{1}{2}, m = \frac{1}{2} >$. $|\xi_{45}\rangle = | j = \frac{1}{2}, m = -\frac{1}{2} >$

$$\hat{H}_{so} = \xi \frac{\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}}{\hbar^2} = \xi \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

$$\frac{\hat{H}_{so}}{\xi}|\phi_1\rangle = \frac{1}{2}|\phi_1\rangle$$

$$\frac{\hat{H}_{so}}{\xi}|\phi_2\rangle = -\frac{1}{2}|\phi_2\rangle + \frac{1}{\sqrt{2}}|\phi_3\rangle, \qquad \frac{\hat{H}_{so}}{\xi}|\phi_3\rangle = \frac{1}{\sqrt{2}}|\phi_2\rangle$$

$$\frac{\hat{H}_{so}}{\xi}|\phi_4\rangle = \frac{1}{\sqrt{2}}|\phi_5\rangle, \qquad \frac{\hat{H}_{so}}{\xi}|\phi_5\rangle = \frac{1}{\sqrt{2}}|\phi_4\rangle - \frac{1}{2}|\phi_5\rangle$$

$$\frac{\hat{H}_{so}}{\xi}|\phi_6\rangle = \frac{1}{2}|\phi_6\rangle$$

So $|\phi_1\rangle$ and $|\phi_6\rangle$ are the eigenkets of $\frac{\hat{H}_{so}}{\xi}$ with the eigenvalue $\frac{1}{2}$.

(i)

$|\phi_2\rangle$ and $|\phi_3\rangle$ form a subsystem of $\frac{\hat{H}_{so}}{\xi}$. The matrix of $\frac{\hat{H}_{so}}{\xi}$ under the basis $\{|\phi_2\rangle, |\phi_3\rangle\}$ is obtained as

$$\hat{A} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

We solve the eigenvalue problem.

Eigenvalue -1: $\left|\xi_{23}\right\rangle = \sqrt{\frac{2}{3}}\left|\phi_2\right\rangle - \frac{1}{\sqrt{3}}\left|\phi_3\right\rangle$

Eigenvalue $\frac{1}{2}$ $\left|\eta_{23}\right\rangle = \frac{1}{\sqrt{3}}\left|\phi_2\right\rangle + \sqrt{\frac{2}{3}}\left|\phi_3\right\rangle$

(ii)

$\left|\phi_2\right\rangle$ and $\left|\phi_3\right\rangle$ form a subsystem of $\frac{\hat{H}_{so}}{\xi}$. The matrix of $\frac{\hat{H}_{so}}{\xi}$ under the basis $\{\left|\phi_2\right\rangle, \left|\phi_3\right\rangle\}$ is obtained as

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

We solve the eigenvalue problem.

Eigenvalue -1: $\left|\xi_{45}\right\rangle = \frac{1}{\sqrt{3}}\left|\phi_4\right\rangle - \sqrt{\frac{2}{3}}\left|\phi_5\right\rangle$

Eigenvalue $\frac{1}{2}$ $\left|\eta_{45}\right\rangle = \sqrt{\frac{2}{3}}\left|\phi_4\right\rangle + \frac{1}{\sqrt{3}}\left|\phi_5\right\rangle$

We note that

$$2\lambda = j(j+1) - l(l+1) - s(s+1) = j(j+1) - 2 - \frac{3}{4} = j(j+1) - \frac{11}{4}$$

When $\lambda = -1$, $j = \frac{1}{2}$

since

$$j(j+1)-\frac{11}{4}=-2, \qquad \text{or} \qquad j^2+j-\frac{3}{4}=0 \qquad (j+\frac{3}{2})(j-\frac{1}{2})=0.$$

When $\lambda=\frac{1}{2}$, $\qquad j=\frac{3}{2}$

since

$$j(j+1)-\frac{11}{4}=1, \qquad \text{or} \qquad j^2+j-\frac{15}{4}=0 \qquad (j-\frac{3}{2})(j+\frac{5}{2})=0.$$

5. Clebsch-Gordan coefficient

The above discussion is confirmed from the derivation of the Clebsch-Gordan co-efficient for $l = 1$ and $s = 1/2$.

(a) $j=\frac{3}{2}$

$$\left|j=\frac{3}{2},m=\frac{3}{2}\right\rangle=\left|l=1,m_l=1\right\rangle\otimes\left|s=1/2,m_l=1/2\right\rangle$$

$$\left|j=\frac{3}{2},m=\frac{1}{2}\right\rangle=\frac{1}{\sqrt{3}}\left|l=1,m_l=1\right\rangle\otimes\left|s=1/2,m_l=-1/2\right\rangle + \sqrt{\frac{2}{3}}\left|l=1,m_l=0\right\rangle\otimes\left|s=1/2,m_l=1/2\right\rangle$$

$$\left|j=\frac{3}{2},m=-\frac{1}{2}\right\rangle=\sqrt{\frac{2}{3}}\left|l=1,m_l=0\right\rangle\otimes\left|s=1/2,m_l=-1/2\right\rangle + \frac{1}{\sqrt{3}}\left|l=1,m_l=-1\right\rangle\otimes\left|s=1/2,m_l=1/2\right\rangle$$

$$\left|j=\frac{3}{2},m=-\frac{3}{2}\right\rangle=\left|l=1,m_l=-1\right\rangle\otimes\left|s=1/2,m_l=-1/2\right\rangle$$

(b) $j=\frac{1}{2}$

$$\left| j=\frac{1}{2}, m=\frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} \left| l=1, m_l=1 \right\rangle \otimes \left| s=1/2, m_l=-1/2 \right\rangle$$
$$-\frac{1}{\sqrt{3}} \left| l=1, m_l=0 \right\rangle \otimes \left| s=1/2, m_l=1/2 \right\rangle$$

$$\left| j=\frac{1}{2}, m=-\frac{1}{2} \right\rangle = \frac{1}{\sqrt{3}} \left| l=1, m_l=0 \right\rangle \otimes \left| s=1/2, m_l=-1/2 \right\rangle$$
$$-\sqrt{\frac{2}{3}} \left| l=1, m_l=-1 \right\rangle \otimes \left| s=1/2, m_l=1/2 \right\rangle$$

((**Mathematica**))

```
Clear["Global`*"];
```

```
CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], 0]]
```

```
CG[{j_, m_}, j1_, j2_] :=
 Sum[CCGG[{j1, m1}, {j2, m - m1}, {j, m}] a[j1, m1]
   b[j2, m - m1], {m1, -j1, j1}]
```

j1 = 1 and j2 = 1/2

j = 3/2

```
j1 = 1; j2 = 1 / 2;
```

```
CG[{3 / 2, 3 / 2}, j1, j2]
```

$$a[1, 1]\, b\left[\frac{1}{2}, \frac{1}{2}\right]$$

```
CG[{3 / 2, 1 / 2}, j1, j2]
```

$$\frac{a[1, 1]\, b\left[\frac{1}{2}, -\frac{1}{2}\right]}{\sqrt{3}} + \sqrt{\frac{2}{3}}\, a[1, 0]\, b\left[\frac{1}{2}, \frac{1}{2}\right]$$

CG[{3 / 2, -1 / 2}, j1, j2]

$$\sqrt{\frac{2}{3}}\, a[1, 0]\, b\left[\frac{1}{2}, -\frac{1}{2}\right] + \frac{a[1, -1]\, b\left[\frac{1}{2}, \frac{1}{2}\right]}{\sqrt{3}}$$

CG[{3 / 2, -3 / 2}, j1, j2]

$$a[1, -1]\, b\left[\frac{1}{2}, -\frac{1}{2}\right]$$

j =1/2

CG[{1 / 2, 1 / 2}, j1, j2]

$$\sqrt{\frac{2}{3}}\, a[1, 1]\, b\left[\frac{1}{2}, -\frac{1}{2}\right] - \frac{a[1, 0]\, b\left[\frac{1}{2}, \frac{1}{2}\right]}{\sqrt{3}}$$

CG[{1 / 2, -1 / 2}, j1, j2]

$$\frac{a[1, 0]\, b\left[\frac{1}{2}, -\frac{1}{2}\right]}{\sqrt{3}} - \sqrt{\frac{2}{3}}\, a[1, -1]\, b\left[\frac{1}{2}, \frac{1}{2}\right]$$