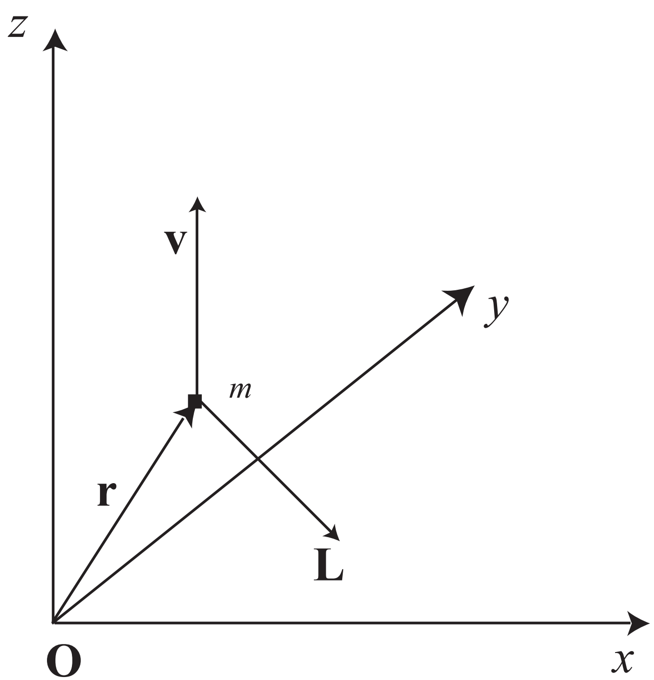
Angular momentum and spin

Orbital angular momentum

1. General properties

$$\mathbf{L} = \boldsymbol{r} \times \boldsymbol{p}$$

⇒ axial vector



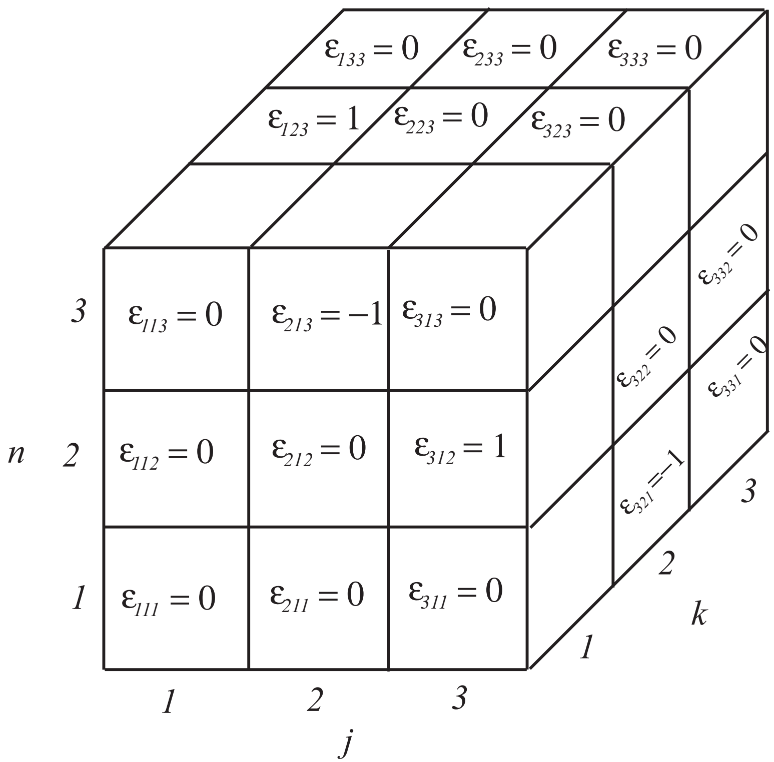
The operator in coordinate representation:

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = -\imath\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = -\imath\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -\imath\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$\hat{L}_j = \epsilon_{jkn}\hat{r}_k\hat{p}_n$$



Commutation relations:

$$
\begin{aligned}
\left[\hat{L}_x, \hat{L}_y\right] &= \left[\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z\right] \\
&= \left[\hat{y}\hat{p}_z, \hat{z}\hat{p}_x\right] + \left[\hat{z}\hat{p}_y, \hat{x}\hat{p}_z\right] \\
&= \hat{y}\left[\hat{p}_z, \hat{z}\right]\hat{p}_x + \hat{p}_y\left[\hat{z}, \hat{p}_z\right]\hat{x} \\
&= \imath\hbar\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right) \\
&= \imath\hbar\hat{L}_z,
\end{aligned}
$$

$$\left[\hat{L}_x, \hat{L}_y\right] = \imath\hbar\hat{L}_z, \quad \left[\hat{L}_y, \hat{L}_z\right] = \imath\hbar\hat{L}_x, \quad \left[\hat{L}_z, \hat{L}_x\right] = \imath\hbar\hat{L}_y$$

$$\left[\hat{L}_j, \hat{L}_k\right] = \imath\hbar\epsilon_{jkn}\hat{L}_n$$

⇒the three components of the angular momentum are not simultaneously measurable.

$$\left[\hat{L}_j, \hat{\mathbf{L}}^2\right] = 0.$$

⇒ it is possible to measure simultaneously $\mathbf{L}^2$ and one (and only one) of the components L_j.

2. Rotations and angular momentum

⇒ consider how a generic state |ψ> is modified by the action of the unitary rotation operator:

$$\hat{U}_\theta = e^{\frac{\imath}{\hbar}\theta\mathbf{n}\cdot\hat{\mathbf{L}}} = e^{\imath\theta\mathbf{n}\cdot\hat{\mathbf{l}}}$$

→ rotation by an angle ϑ around the axis defined by the vector **n**.

$$\hat{\mathbf{l}} = \frac{\hat{\mathbf{L}}}{\hbar} = \hat{\mathbf{r}} \times \hat{\mathbf{k}} \qquad\qquad \hat{\mathbf{k}} = \hat{\mathbf{p}}/\hbar = -\imath\nabla$$

⇒ infinitesimal rotations: δϑ → 0. Taylor expansion of the unitary operator to first order:

$$\hat{U}_{\delta\theta} \simeq 1 + \imath\delta\theta\mathbf{n}\cdot\hat{\mathbf{l}} = 1 + \imath\delta\theta\hat{R}$$

→ generator of the rotation: $\boxed{\hat{R} = \mathbf{n}\cdot\hat{\mathbf{l}}}$

For a generic operator Ô, the rotation induces the following transformation:

$$\hat{O} \mapsto \hat{O}' = \hat{U}_{\delta\theta}\hat{O}\hat{U}^\dagger_{\delta\theta} = \left(1 + \imath\delta\theta\hat{R}\right)\hat{O}\left(1 - \imath\delta\theta\hat{R}\right)$$
$$= \hat{O} + \delta\hat{O},$$

⇒ to first order in δϑ: $$\delta \hat{O} \simeq \imath \delta\theta \left[\hat{R}, \hat{O}\right]$$ If Ô is a scalar for rotations → δÔ = 0.

In the general 3D case: for the Euler angles β, ϕ, ϑ around the axes x, y, z, respectively:

$$\hat{\mathbf{R}}(\beta,\phi,\theta) = \begin{bmatrix} \cos\beta\cos\phi\cos\theta - \sin\beta\sin\theta & \sin\beta\cos\phi\cos\theta + \cos\beta\sin\theta & -\sin\phi\cos\theta \\ -\cos\beta\cos\phi\sin\theta - \sin\beta\cos\theta & -\sin\beta\cos\phi\sin\theta + \cos\beta\cos\theta & \sin\phi\sin\theta \\ \cos\beta\sin\phi & \sin\beta\sin\phi & \cos\phi \end{bmatrix}$$

Rotation by ϑ around the z-axis:

$$\hat{\mathbf{R}}(\theta) = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

For an arbitrary vector: $\mathbf{v} \equiv (v_x, v_y, v_z) \longrightarrow \mathbf{v}' \equiv (v'_x, v'_y, v'_z) \quad (\mathbf{v}' = \mathbf{v} - \delta\mathbf{v})$

$$\begin{aligned} v'_x &= \cos\delta\theta\, v_x + \sin\delta\theta\, v_y, \\ v'_y &= -\sin\delta\theta\, v_x + \cos\delta\theta\, v_y \\ v'_z &= v_z. \end{aligned}$$

δϑ << ⇒ $v'_x \simeq v_x + \delta\theta\, v_y \qquad v'_y \simeq -\delta\theta\, v_x + v_y$

$$\delta v_x = -\delta\theta v_y, \quad \delta v_y = \delta\theta v_x, \quad \delta v_z = 0$$

...compared to $\delta\hat{O} \simeq \imath\delta\theta\left[\hat{R}, \hat{O}\right]$ $\Rightarrow$ $\left[\hat{l}_z, v_x\right] = \imath v_y, \quad \left[\hat{l}_z, v_y\right] = -\imath v_x, \quad \left[\hat{l}_z, v_z\right] = 0$

Since this is valid for any vector **v** → $\left[\hat{L}_z, \hat{x}\right] = \imath\hbar\hat{y}$ and $\left[\hat{L}_z, \hat{p}_x\right] = \imath\hbar\hat{p}_y$

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3. Angular momentum eigenvalues

In contrast to the case of position and momentum, different components of the angular momentum do not commute with each other. We have to choose a pair of commuting observables that can be diagonalized simultaneously:

$$\boxed{\hat{\mathbf{l}}^2 \text{ and } \hat{l}_z} \qquad \hat{\mathbf{l}}^2 - \hat{l}_z^2 = \hat{l}_x^2 + \hat{l}_y^2 \geq 0$$

The basis of the Hilbert space: $\left|l, m_l\right\rangle$ (eigenvalues of $\mathbf{l}^2$ and l_z)

$$\langle l, m_l | \hat{\mathbf{l}}^2 - \hat{l}_z^2 | l, m_l \rangle = \langle l, m_l | \hat{l}_x^2 + \hat{l}_y^2 | l, m_l \rangle \geq 0$$

⇒ the eigenvalues of l_z^2 cannot exceed the eigenvalues of $\mathbf{l}^2$.

$$-l \leq m_l \leq l$$

l → azimuthal quantum number
m_l → magnetic quantum number

$$\hat{l}_z | l, m_l \rangle = m_l | l, m_l \rangle$$

Angular momentum algebra

→ introduce the raising and lowering operators: $\hat{l}_\pm = \hat{l}_x \pm \imath \hat{l}_y \quad \hat{l}_- = \hat{l}_+^\dagger$

Commutation relations: $\left[\hat{l}_z, \hat{l}_\pm\right] = \pm\hat{l}_\pm, \left[\hat{l}_+, \hat{l}_-\right] = 2\hat{l}_z, \left[\hat{\mathbf{l}}^2, \hat{l}_\pm\right] = 0$

$$\begin{aligned} \hat{l}_z\hat{l}_+ | l, m_l \rangle &= \left(\hat{l}_+\hat{l}_z + \left[\hat{l}_z, \hat{l}_+\right]\right) | l, m_l \rangle \\ &= m\hat{l}_+ | l, m_l \rangle + \hat{l}_+ | l, m_l \rangle \\ &= (m_l + 1)\hat{l}_+ | l, m_l \rangle . \end{aligned}$$

$$\hat{l}_+ | l, m_l \rangle \propto | l, m_l + 1 \rangle$$

… in the same way: $\boxed{\hat{l}_- \left| l, m_l \right\rangle \propto \left| l, m_l - 1 \right\rangle}$ eigenvector of the operator l_z.

Since *l* is the maximal eigenvalue of l_z, and –*l* is the minimal eigenvalue, we must also have:

$$\hat{l}_+ \left| l, l \right\rangle = 0 \text{ and } \hat{l}_- \left| l, -l \right\rangle = 0.$$

Table 6.1 Ordering of the "ascending" and "descending" angular momentum eigenstates and corresponding eigenvalues of $\hat{l}_z$

"Ascending" eigenstates	"Descending" eigenstates	Eigenvalue of $\hat{l}_z$
$\hat{l}_+^{2l} \left| l, -l \right\rangle \propto \left| l, l \right\rangle$	$\left| l, l \right\rangle$	l
$\hat{l}_+^{2l-1} \left| l, -l \right\rangle \propto \left| l, l-1 \right\rangle$	$\hat{l}_- \left| l, l \right\rangle \propto \left| l, l-1 \right\rangle$	$l-1$
$\cdots$	$\hat{l}_-^2 \left| l, l \right\rangle \propto \hat{l}_- \left| l, l-1 \right\rangle$	
	$\propto \left| l, l-2 \right\rangle$	$l-2$
$\cdots$	$\cdots$	$\cdots$
$\hat{l}_+^2 \left| l, -l \right\rangle \propto \hat{l}_+ \left| l, -l+1 \right\rangle$		
$\propto \left| l, -l+2 \right\rangle$	$\cdots$	$-l+2$
$\hat{l}_+ \left| l, -l \right\rangle \propto \left| l, -l+1 \right\rangle$	$\hat{l}_-^{2l-1} \left| l, l \right\rangle \propto \left| l, -l+1 \right\rangle$	$-l+1$
$\left| l, -l \right\rangle$	$\hat{l}_-^{2l} \left| l, l \right\rangle \propto \left| l, -l \right\rangle$	$-l$

Eigenvalues of $\mathbf{l}^2$:

$$\hat{l}_-\hat{l}_+ = \left(\hat{l}_x - i\hat{l}_y\right)\left(\hat{l}_x + i\hat{l}_y\right) = \hat{l}_x^2 + \hat{l}_y^2 + i\left[\hat{l}_x, \hat{l}_y\right]$$
$$= \hat{\mathbf{l}}^2 - \hat{l}_z^2 - \hat{l}_z,$$

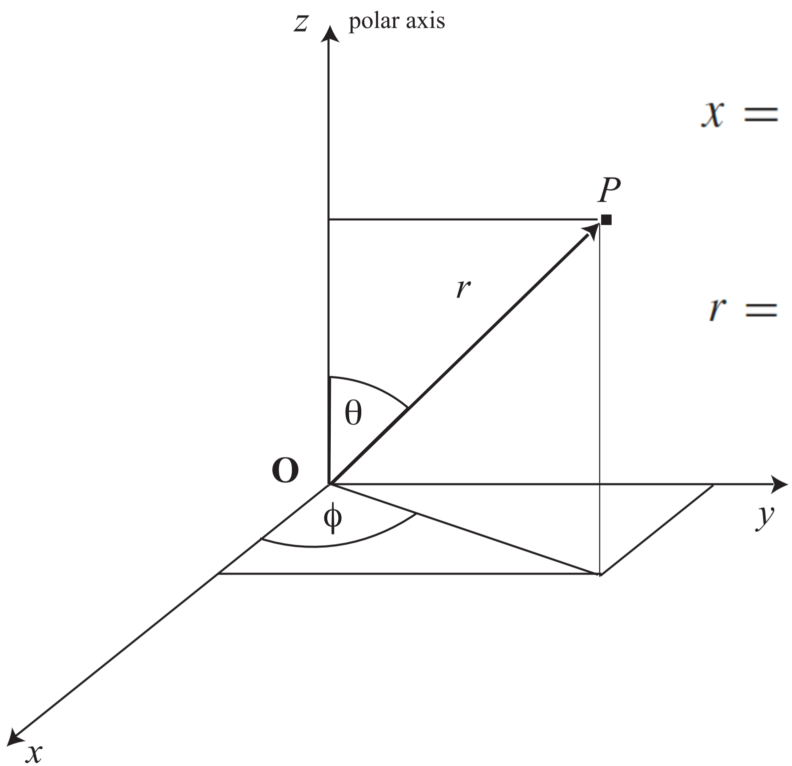
For the state with maximum projection: $$0 = \hat{l}_-\hat{l}_+ \left| l, l \right\rangle = \left(\hat{\mathbf{l}}^2 - \hat{l}_z^2 - \hat{l}_z\right) \left| l, l \right\rangle$$

$\Rightarrow$ $$\left[\hat{\mathbf{l}}^2 - l(l+1)\right] \left| l, l \right\rangle = 0$$ $\Rightarrow$ $$\boxed{\hat{\mathbf{l}}^2 \left| l, l \right\rangle = l(l+1) \left| l, l \right\rangle}$$

This is true for any state in the representation *l*, because of: $$\left[\hat{\mathbf{l}}^2, \hat{l}_\pm\right] = 0$$

$$\hat{\mathbf{l}}^2 \left| l, m_l \right\rangle = l(l+1) \left| l, m_l \right\rangle$$

4. Angular momentum eigenfunctions



$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta$$

$$r = \sqrt{x^2+y^2+z^2}, \quad \phi = \arctan\frac{y}{x}, \quad \theta = \arctan\frac{\sqrt{x^2+y^2}}{z}$$

$$-\imath\hbar\frac{\partial}{\partial\phi} = -\imath\hbar\left(\frac{\partial x}{\partial\phi}\frac{\partial}{\partial x}+\frac{\partial y}{\partial\phi}\frac{\partial}{\partial y}\right) = -\imath\hbar\left(-\hat{y}\frac{\partial}{\partial x}+\hat{x}\frac{\partial}{\partial y}\right) = \hat{L}_z$$

generates a rotation around the z-axis.

Eigenfunctions of the angular momentum: $\psi(r,\theta,\phi)$

$$\hat{l}_z\psi(r,\theta,\phi) = -\imath\frac{\partial}{\partial\phi}\psi(r,\theta,\phi) = m_l\psi(r,\theta,\phi) \quad \Rightarrow \quad \psi(r,\theta,\phi) = f(r,\theta)\frac{e^{\imath m_l\phi}}{\sqrt{2\pi}}$$

→ invariance of the wave function for a rotation of 2π around the z-axis: $\phi \to \phi + 2\pi \Rightarrow m_l \in \mathbf{Z}$.

Orthonormal functions: $\mathrm{F}_m(\phi) = \frac{e^{\imath m_l \phi}}{\sqrt{2\pi}}$

$$\int_0^{2\pi} d\phi \mathrm{F}_m^*(\phi)\mathrm{F}_{m'}(\phi) = \frac{1}{2\pi}\int_0^{2\pi} d\phi e^{\imath(m_l' - m_l)\phi} = \delta_{m_l m_l'}$$

The matrix element:

$$\left\langle l, m_l \left| \hat{l}_- \hat{l}_+ \right| l, m_l \right\rangle = \sum_{j=-l}^{l} \left\langle l, m_l \left| \hat{l}_- \right| l, j \right\rangle \left\langle l, j \left| \hat{l}_+ \right| l, m_l \right\rangle$$

Since: $\hat{l}_- \, |l, j\rangle \propto |l, j-1\rangle$ and $\hat{l}_+ \left| l, m_l \right\rangle \propto \left| l, m_l + 1 \right\rangle$

⇒ the only nonvanishing term: $j = m_l + 1$

$$\left\langle l, m_l \left| \hat{l}_- \hat{l}_+ \right| l, m_l \right\rangle = \left\langle l, m_l \left| \hat{l}_- \right| l, m_l + 1 \right\rangle \left\langle l, m_l + 1 \left| \hat{l}_+ \right| l, m_l \right\rangle$$

$$\hat{l}_- \hat{l}_+ = \left(\hat{l}_x - \imath \hat{l}_y\right)\left(\hat{l}_x + \imath \hat{l}_y\right) = \hat{l}_x^2 + \hat{l}_y^2 + \imath\left[\hat{l}_x, \hat{l}_y\right]$$
$$= \hat{\mathbf{l}}^2 - \hat{l}_z^2 - \hat{l}_z,$$

$$\left\langle l, m_l \left| \hat{l}_- \hat{l}_+ \right| l, m_l \right\rangle = \left\langle l, m_l \left| \hat{\mathbf{l}}^2 - \hat{l}_z(\hat{l}_z + 1) \right| l, m_l \right\rangle$$

$$\hat{l}_- = \hat{l}_+^\dagger \quad \Rightarrow \quad \left| \left\langle l, m_l + 1 \middle| \hat{l}_+ \middle| l, m_l \right\rangle \right|^2 = l(l+1) - m_l(m_l+1)$$

$$\left\langle l, m_l + 1 \middle| \hat{l}_+ \middle| l, m_l \right\rangle = \sqrt{l(l+1) - m_l(m_l+1)}$$

$$\Rightarrow \quad \hat{l}_+ \left| l, m_l \right\rangle = \sqrt{l(l+1) - m_l(m_l+1)} \left| l, m_l + 1 \right\rangle$$

$$\hat{l}_- \left| l, m_l \right\rangle = \sqrt{l(l+1) - m_l(m_l-1)} \left| l, m_l - 1 \right\rangle$$

From these relations ⇒

$$\hat{l}_-\hat{l}_+ \left| l, m_l \right\rangle = (l - m_l)(l + m_l + 1) \left| l, m_l \right\rangle,$$

$$\hat{l}_+\hat{l}_- \left| l, m_l \right\rangle = (l + m_l)(l - m_l + 1) \left| l, m_l \right\rangle.$$

Example: $l = 1 \quad m_l = -1, 0, +1$

⇒ basis vectors: $|1,1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |1,-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$$\hat{l}_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \hat{l}_+ = \begin{bmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix}, \quad \hat{l}_- = \begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix}$$

$$\hat{l}_x = \frac{\hat{l}_+ + \hat{l}_-}{2} = \frac{1}{2} \begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix}$$

$$\hat{l}_y = \frac{\hat{l}_+ - \hat{l}_-}{2\imath} = \frac{1}{2\imath} \begin{bmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{bmatrix}$$

$$\hat{l}_z \psi(r,\theta,\phi) = -\imath \frac{\partial}{\partial \phi} \psi(r,\theta,\phi)$$

… expressing the partial derivatives in terms of the spherical coordinates:

$$\begin{aligned}
\frac{\partial}{\partial x} &= \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} \\
&= \sin\theta\cos\phi\frac{\partial}{\partial r} - \frac{1}{r}\frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial \phi} + \frac{1}{r}\cos\theta\cos\phi\frac{\partial}{\partial \theta}, \\
\frac{\partial}{\partial y} &= \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi} + \frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta} \\
&= \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{1}{r}\frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial \phi} + \frac{1}{r}\cos\theta\sin\phi\frac{\partial}{\partial \theta}, \\
\frac{\partial}{\partial z} &= \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial \phi}{\partial z}\frac{\partial}{\partial \phi} + \frac{\partial \theta}{\partial z}\frac{\partial}{\partial \theta} \\
&= \cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial \theta}.
\end{aligned}$$

$$\Rightarrow$$

$$\begin{aligned}
\hat{l}_x &= \imath\left(\sin\phi\frac{\partial}{\partial \theta} + \cos\phi\cot\theta\frac{\partial}{\partial \phi}\right), \\
\hat{l}_y &= -\imath\left(\cos\phi\frac{\partial}{\partial \theta} - \sin\phi\cot\theta\frac{\partial}{\partial \phi}\right)
\end{aligned}$$

$$\hat{l}_+ = e^{\imath\phi}\left(\frac{\partial}{\partial\theta} + \imath\cot\theta\frac{\partial}{\partial\phi}\right),$$
$$\hat{l}_- = e^{-\imath\phi}\left(\frac{\partial}{\partial\theta} - \imath\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$\hat{\mathbf{l}}^2 = \hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2$$
$$= -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2},$$

→ angular part of the Laplacian in spherical coordinates.

$$\hat{\mathbf{l}}^2\psi(r,\theta,\phi) = l(l+1)\psi(r,\theta,\phi)$$

∝ Laplace equation

⇒ separation of variables: $\psi(r,\theta,\phi) = \mathrm{R}(r)Y(\phi,\theta)$

$$\hat{\mathbf{l}}^2 Y_{lm}(\phi,\theta) = l(l+1)Y_{lm}(\phi,\theta),$$
$$\hat{l}_z Y_{lm}(\phi,\theta) = m_l Y_{lm}(\phi,\theta).$$

Normalization of spherical harmonics: $\int d\Omega Y^*_{l'm'}(\phi,\theta) Y_{lm}(\phi,\theta) = \delta_{ll'}\delta_{mm'}$

$$Y_{lm}(\phi,\theta) = \mathrm{F}_m(\phi)\Theta_{lm}(\theta) = \frac{e^{\imath m_l \phi}}{\sqrt{2\pi}}\Theta_{lm}(\theta)$$

$$Y_{lm}(\phi,\theta) = \frac{e^{\imath m_l \phi}}{\sqrt{2\pi}}(-\imath)^l \sqrt{\frac{(2l+1)(l+m_l)!}{2(l-m_l)!}} \frac{1}{2^l l!} \frac{1}{(\sin\theta)^{m_l}} \frac{d^{l-m_l}}{d\cos\theta^{l-m_l}} (\sin\theta)^{2l}$$

$$Y_{0,0}(\phi,\theta) = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,0}(\phi,\theta) = \imath\sqrt{\frac{3}{4\pi}}\cos\theta,$$

$$Y_{1,\pm 1}(\phi,\theta) = \pm\imath\sqrt{\frac{3}{8\pi}} e^{\pm\imath\phi}\sin\theta$$

$$Y_{2,0}(\phi,\theta) = -\sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right),$$

$$Y_{2,\pm 1}(\phi,\theta) = \pm\sqrt{\frac{15}{8\pi}} e^{\pm\imath\phi}\sin\theta\cos\theta,$$

$$Y_{2,\pm 2}(\phi,\theta) = \pm\sqrt{\frac{15}{32\pi}} e^{\pm 2\imath\phi}\sin^2\theta.$$

Spin

Spin 1/2 → wave function: $\psi(\mathbf{r}, s) = \psi_{\uparrow}(\mathbf{r}) + \psi_{\downarrow}(\mathbf{r}) = \psi(\mathbf{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi(\mathbf{r}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Spin 1/2 eigenbasis: $|\uparrow\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

⇨ $$\boxed{\psi(\mathbf{r}, s) = \langle \mathbf{r} \mid \psi \rangle \left(|\uparrow\rangle_z + |\downarrow\rangle_z \right)}$$

From the relations:

$\hat{s}_z |\uparrow\rangle_z = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \hat{s}_z |\downarrow\rangle_z = -\frac{1}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ ⇨ $\hat{s}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

Define the raising and lowering spin operators: $\hat{s}_{\pm} = \hat{s}_x \pm \imath \hat{s}_y$

$$\left[\hat{s}_z, \hat{s}_{\pm}\right] = \pm \hat{s}_{\pm}$$

$$\hat{s}_z\hat{s}_+ \,|\downarrow\rangle = \frac{1}{2}\hat{s}_+ \,|\downarrow\rangle \Rightarrow \hat{s}_+ \,|\downarrow\rangle = |\uparrow\rangle$$

$$\hat{s}_z\hat{s}_- \,|\uparrow\rangle = -\frac{1}{2}\hat{s}_- \,|\uparrow\rangle \Rightarrow \hat{s}_- \,|\uparrow\rangle = |\downarrow\rangle$$

$$\hat{s}_+ \,|\uparrow\rangle = 0, \quad \hat{s}_- \,|\downarrow\rangle = 0$$

$$\hat{s}_+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad \hat{s}_- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\hat{s}_x = \frac{\hat{s}_+ + \hat{s}_-}{2} \quad \text{and} \quad \hat{s}_y = \frac{\hat{s}_+ - \hat{s}_-}{2\imath}$$

$$\Rightarrow \hat{s}_x = \begin{bmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix} = \frac{1}{2}\hat{\sigma}_x, \quad \hat{s}_y = \begin{bmatrix} 0 & -\frac{\imath}{2} \\ \frac{\imath}{2} & 0 \end{bmatrix} = \frac{1}{2}\hat{\sigma}_y, \quad \hat{s}_z = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{bmatrix} = \frac{1}{2}\hat{\sigma}_z$$

The Pauli spin matrices: $\left[\hat{\sigma}_j, \hat{\sigma}_k\right] = 2\imath\epsilon_{jkn}\hat{\sigma}_n$ $\qquad \hat{\sigma}_x^2 = \hat{\sigma}_y^2 = \hat{\sigma}_z^2 = \hat{I}$

→ anticommutation relations: $\left[\hat{\sigma}_j, \hat{\sigma}_k\right]_+ = 2\hat{I}\delta_{jk}$

$$\hat{\sigma}_x \left| \uparrow \right\rangle_x = \left| \uparrow \right\rangle_x , \quad \hat{\sigma}_x \left| \downarrow \right\rangle_x = - \left| \downarrow \right\rangle_x$$

$$\hat{\sigma}_y \left| \uparrow \right\rangle_y = \left| \uparrow \right\rangle_y , \quad \hat{\sigma}_y \left| \downarrow \right\rangle_y = - \left| \downarrow \right\rangle_y$$

$$\left| \uparrow \right\rangle_x = \frac{1}{\sqrt{2}} \left(\left| \uparrow \right\rangle_z + \left| \downarrow \right\rangle_z \right), \quad \left| \downarrow \right\rangle_x = \frac{1}{\sqrt{2}} \left(\left| \uparrow \right\rangle_z - \left| \downarrow \right\rangle_z \right),$$

$$\left| \uparrow \right\rangle_y = \frac{1}{\sqrt{2}} \left(\left| \uparrow \right\rangle_z + \imath \left| \downarrow \right\rangle_z \right), \quad \left| \downarrow \right\rangle_y = \frac{1}{\sqrt{2}} \left(\left| \uparrow \right\rangle_z - \imath \left| \downarrow \right\rangle_z \right)$$

The Pauli matrices are simultaneously Hermitian and unitary. Together with the 2 × 2 identity matrix, they form an operatorial basis for the spin−1/2 Hilbert space: any operator in the spinor space can be written as a combination:

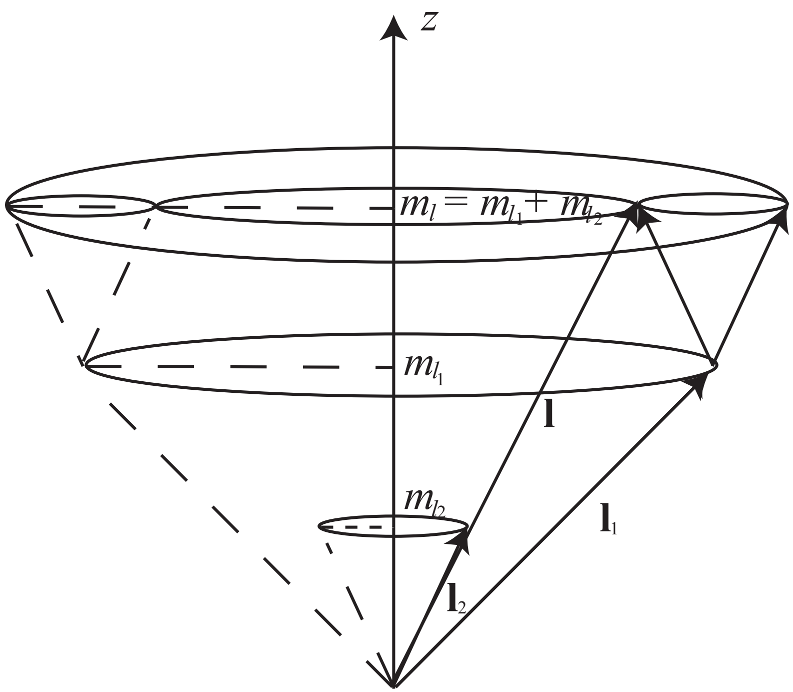
$$\hat{O} = \alpha \hat{I} + \boldsymbol{\beta} \cdot \hat{\boldsymbol{\sigma}} = \begin{bmatrix} \alpha + \beta_z & \beta_x - \imath \beta_y \\ \beta_x + \imath \beta_y & \alpha - \beta_z \end{bmatrix}$$

Angular momentum coupling

1. Independent orbital angular momenta

→ two particles S_1 and S_2 with independent angular momenta: $\left[\hat{\mathbf{l}}_1, \hat{\mathbf{l}}_2\right] = 0$

⇒ total angular momentum: $\hat{\mathbf{l}}_{1,2} = \hat{\mathbf{l}}_1 + \hat{\mathbf{l}}_2$



$$\left[\hat{l}_{1_j}, \quad \hat{l}_{1_k}\right] = \imath \epsilon_{jkn} \hat{l}_{1_n}, \quad \left[\hat{l}_{2_j}, \hat{l}_{2_k}\right] = \imath \epsilon_{jkn} \hat{l}_{2_n}$$

⇓

$$\left[\hat{l}_j, \hat{l}_k\right] = \left[\hat{l}_{1_j} + \hat{l}_{2_j}, \hat{l}_{1_k} + \hat{l}_{2_k}\right] = \imath \epsilon_{jkn} \hat{l}_n$$

The angular momenta of the two particles can be diagonalized simultaneously.

$$\left(\hat{\mathbf{l}}_{1,2}\right)^2 \left| l_{1,2}, m_{l_{1,2}} \right\rangle = l_{1,2}\left(l_{1,2}+1\right) \left| l_{1,2}, m_{l_{1,2}} \right\rangle ,$$
$$\hat{l}_{1,2_z} \left| l_{1,2}, m_{l_{1,2}} \right\rangle = m_{l_{1,2}} \left| l_{1,2}, m_{l_{1,2}} \right\rangle .$$

The basis of the product space: $\left\{ \left| l_1, m_{l_1}; l_2, m_{l_2} \right\rangle \right\} = \left\{ \left| l_1, m_{l_1} \right\rangle \otimes \left| l_2, m_{l_2} \right\rangle \right\}$

Example:

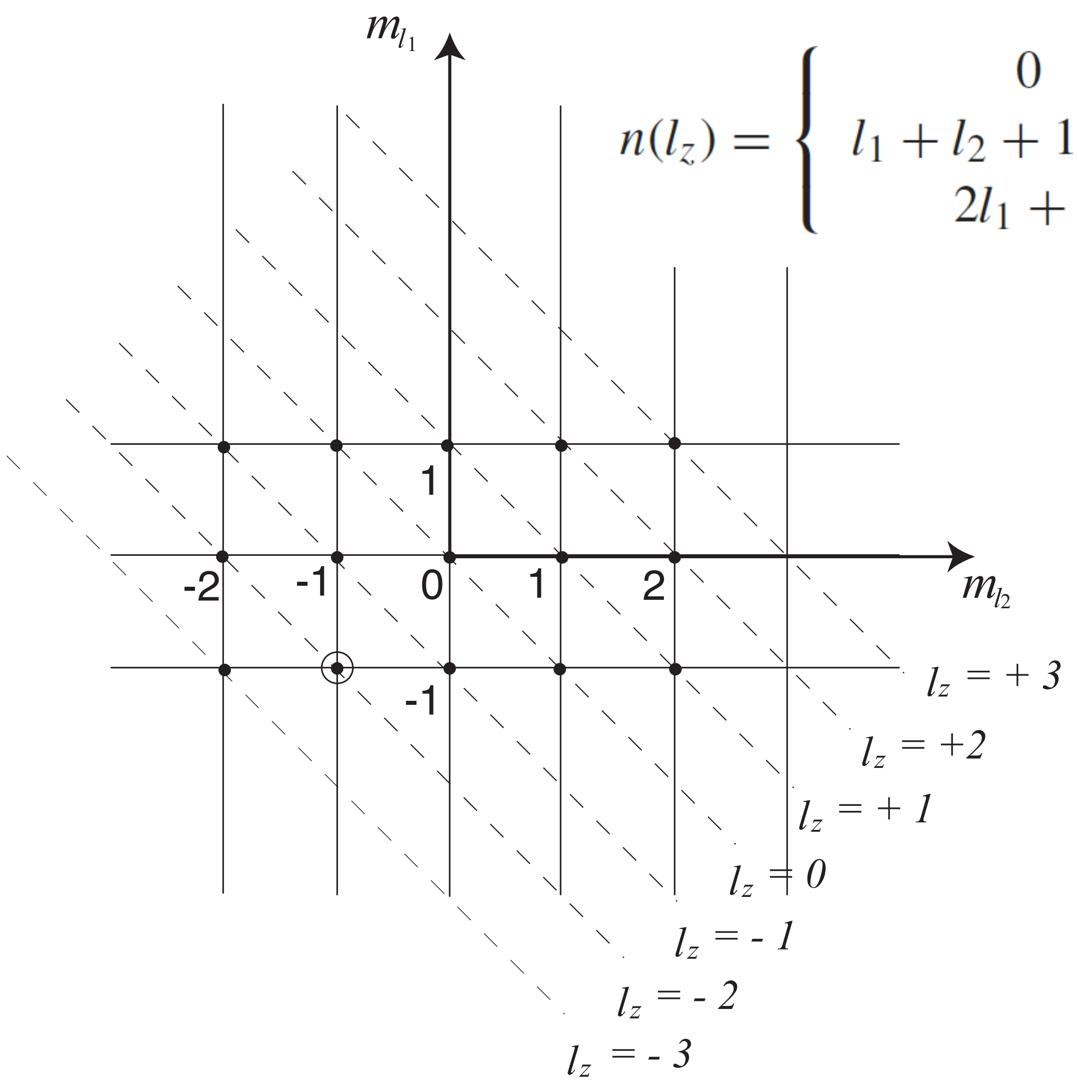
$$l_1 = 1 \qquad m_1 = -1, 0, +1$$
$$l_2 = 2 \qquad m_2 = -2, -1, 0, +1, +2$$

⇒ 3 × 5 = 15 possible states. The minimum value of the total angular momentum is l_{12} = 1 (l_1 and l_2 antiparallel), and the maximum value is l_{12} = 3 (l_1 and l_2 parallel). These 15 states can be arranged into multiplets:

$$l_{12} = 1 \qquad m_{12} = -1, 0, +1,$$
$$l_{12} = 2 \qquad m_{12} = -2, -1, 0, +1, +2$$
$$l_{12} = 3 \qquad m_{12} = -3, -2, -1, 0, +1, +2, +3$$

The projection of angular momentum is an additive quantum number:

$$\left(\hat{l}_{1_z} + \hat{l}_{2_z}\right)\left|l_1, m_{l_1}\right\rangle \otimes \left|l_2, m_{l_2}\right\rangle = \left(m_{l_1} + m_{l_2}\right)\left|l_1, m_{l_1}\right\rangle \otimes \left|l_2, m_{l_2}\right\rangle$$



$$n(l_z) = \begin{cases} 0 & \text{if} \quad |l_z| > l_1 + l_2 \\ l_1 + l_2 + 1 - |l_z| & \text{if} \quad l_1 + l_2 \geq |l_z| \geq |l_1 - l_2| \\ 2l_1 + 1 & \text{if} \quad |l_1 - l_2| \geq |l_z| \geq 0 \end{cases}$$

Theorem: $\vec{l} = \vec{l}_1 + \vec{l}_2$

⇒ allowed values:

$$|l_1 - l_2| \leq l \leq l_1 + l_2$$

To each value *l* correspond (2*l*+1) eigenvectors | *l*,m>.

2. Total angular momentum

→ sum of the orbital angular momentum and spin: $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ $\left[\hat{J}_k, \hat{J}_n\right] = \imath\hbar\epsilon_{knr}\hat{J}_r$

Example: $l = 1$ and $s = 1/2$

- $j = l - s = 1/2$

$$\hat{J}_x = \frac{1}{2}\hbar\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{J}_y = \frac{1}{2}\hbar\begin{bmatrix} 0 & -\imath \\ \imath & 0 \end{bmatrix},$$

$$\hat{J}_z = \frac{1}{2}\hbar\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \hat{\mathbf{J}}^2 = \frac{3}{4}\hbar^2\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

- and $j = l + s = 3/2$

$$\hat{J}_x = \frac{1}{2}\hbar\begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix}, \quad \hat{J}_y = \frac{1}{2}\hbar\begin{bmatrix} 0 & -\imath\sqrt{3} & 0 & 0 \\ \imath\sqrt{3} & 0 & -2\imath & 0 \\ 0 & -2\imath & 0 & -\imath\sqrt{3} \\ 0 & 0 & \imath\sqrt{3} & 0 \end{bmatrix}$$

$$\hat{J}_z = \frac{1}{2}\hbar\begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix}, \quad \hat{\mathbf{J}}^2 = \frac{15}{4}\hbar^2\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

3. Singlet and triplet states

$$s_1 = \frac{1}{2} \quad s_2 = \frac{1}{2} \quad \Rightarrow \quad \vec{s} = \vec{s}_1 + \vec{s}_2$$

Triplet:

$$|s=1, m_s=1\rangle_{12_z} = \left|s_1 = \frac{1}{2}, m_{s_1} = \frac{1}{2}\right\rangle_1 \left|s_2 = \frac{1}{2}, m_{s_2} = \frac{1}{2}\right\rangle_2$$
$$= |\uparrow\rangle_{1_z} |\uparrow\rangle_{2_z} ,$$

$$|s=1, m_s=-1\rangle_{12_z} = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle_1 \left|\frac{1}{2}, -\frac{1}{2}\right\rangle_2 = |\downarrow\rangle_{1_z} |\downarrow\rangle_{2_z} ,$$

$$|s=1, m_s=0\rangle_{12_z} = \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2}, \frac{1}{2}\right\rangle_1 \left|\frac{1}{2}, -\frac{1}{2}\right\rangle_2 + \left|\frac{1}{2}, -\frac{1}{2}\right\rangle_1 \left|\frac{1}{2}, \frac{1}{2}\right\rangle_2\right)$$
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{1_z} |\downarrow\rangle_{2_z} + |\downarrow\rangle_{1_z} |\uparrow\rangle_{2_z}\right),$$

Singlet:

$$|s=0, m_s=0\rangle_{12_z} = \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2}, \frac{1}{2}\right\rangle_1 \left|\frac{1}{2}, -\frac{1}{2}\right\rangle_2 - \left|\frac{1}{2}, -\frac{1}{2}\right\rangle_1 \left|\frac{1}{2}, \frac{1}{2}\right\rangle_2\right)$$
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{1_z} |\downarrow\rangle_{2_z} - |\downarrow\rangle_{1_z} |\uparrow\rangle_{2_z}\right).$$

The triplet states are symmetric with respect to $1 \leftrightarrow 2$, and the singlet state is antisymmetric.

4. Clebsch – Gordan coefficients

Two particles with angular momenta $\mathbf{j}_1$ and $\mathbf{j}_2$: $[\hat{\boldsymbol{j}}_1, \hat{\boldsymbol{j}}_2] = 0$

$$\hat{\boldsymbol{j}} = \hat{\boldsymbol{j}}_1 + \hat{\boldsymbol{j}}_2 \qquad \hat{\boldsymbol{j}}^2 = \hat{\boldsymbol{j}}_1^2 + \hat{\boldsymbol{j}}_2^2 + 2\hat{\boldsymbol{j}}_1 \cdot \hat{\boldsymbol{j}}_2 \qquad \hat{j}_z = \hat{j}_{1_z} + \hat{j}_{2_z}$$

Two different bases for the total Hilbert space:

1) The product eigenvectors of the operators: $\hat{\boldsymbol{j}}_1, \hat{j}_{1_z}$ and $\hat{\boldsymbol{j}}_2, \hat{j}_{2_z}$

$$\left| j_1, m_{j_1} \right\rangle \otimes \left| j_2, m_{j_2} \right\rangle = \left| j_1, j_2, m_{j_1}, m_{j_2} \right\rangle$$

2) Since: $\left[\hat{\boldsymbol{j}}^2, \hat{\boldsymbol{j}}_1^2\right] = \left[\hat{\boldsymbol{j}}^2, \hat{\boldsymbol{j}}_2^2\right] = 0$ ⇒ the eigenvectors: $\left| j_1, j_2; j, m_j \right\rangle$

The unitary transformation between the two bases:

$$\left| j_1, j_2; j, m_j \right\rangle = \sum_{m_{j_1}, m_{j_2}} \left| j_1, j_2, m_{j_1}, m_{j_2} \right\rangle \left\langle j_1, j_2, m_{j_1}, m_{j_2} \middle| j_1, j_2; j, m_j \right\rangle$$

The coefficients of the expansion:

$$\left\langle j_1, j_2, m_{j_1}, m_{j_2} \mid j_1, j_2; j, m_j \right\rangle$$

$$|j_1 - j_2| \le j \le j_1 + j_2$$

Clebsch – Gordan coefficients

$$\langle j_1, j_2, m_1, m_2 \mid j, m\rangle$$

Orthonormality relations:

$$\sum_{m_1, m_2} \langle j_1, j_2, m_1, m_2 \mid j, m\rangle \left\langle j_1, j_2, m_1, m_2 \mid j', m'\right\rangle = \delta_{jj'}\delta_{mm'},$$

$$\sum_{j, m} \langle j_1, j_2, m_1, m_2 \mid j, m\rangle \langle j_1, j_2, m_{1'}, m_{2'} \mid j, m\rangle = \delta_{m_1 m_{1'}}\delta_{m_2 m_{2'}}.$$

Table 6.3 Values of j and m and the corresponding number of possible states in the case of the addition of angular momenta $j_1 = j_2 = 1$

j	m	Number of possible states
2	$-2 \le m \le +2$	5
1	$-1 \le m \le +1$	3
0	0	1
Total number of states		9

Case $j = 2$

- $j = 2, m = 2$ $\quad |1,1;2,2\rangle = \langle 1,1,1,1\,|\,2,2\rangle\,|1,1,1,1\rangle$

$$\Rightarrow \quad \langle 1,1,1,1\,|\,2,2\rangle = 1$$

- $j = 2, m = -2$

$$|1,1;2,-2\rangle = \langle 1,1,-1,-1\,|\,2,-2\rangle\,|1,1,-1,-1\rangle$$

$$\Rightarrow \quad \langle 1,1,-1,-1\,|\,2,-2\rangle = 1$$

$$\hat{j}_{\pm}\,|j_1, j_2; j, m\rangle = \sqrt{(j \pm m + 1)\,(j \mp m)}\,|j_1, j_2; j, m \pm 1\rangle$$

$$(\hat{j}_{1\pm} + \hat{j}_{2\pm})\,|j_1, j_2, m_1, m_2\rangle = \sqrt{(j_1 \pm m_1 + 1)\,(j_1 \mp m_1)}\,|j_1 j_2, m_1 \pm 1, m_2\rangle + \sqrt{(j_2 \pm m_2 + 1)\,(j_2 \mp m_2)}\,|j_1, j_2, m_1, m_2 \pm 1\rangle$$

- $j = 2, m = 1$ Two possibilities: $(m_1, m_2) = (1, 0)$ $(m_1, m_2) = (0, 1)$

$$|1, 1; 2, 1\rangle = \langle 1, 1, 1, 0 \mid 2, 1\rangle \,|1, 1, 1, 0\rangle + \langle 1, 1, 0, 1 \mid 2, 1\rangle \,|1, 1, 0, 1\rangle$$

$$|1, 1; 2, 2\rangle = \langle 1, 1, 1, 1 \mid 2, 2\rangle \,|1, 1, 1, 1\rangle$$

The CG coefficient = 1. By acting on both sides with the operator $j_- = j_{1-} + j_{2-}$

$$2\,|1, 1; 2, 1\rangle = \sqrt{2}\,|1, 1, 0, 1\rangle + \sqrt{2}\,|1, 1, 1, 0\rangle$$

$$\Rightarrow \quad \langle 1, 1, 1, 0 \mid 2, 1\rangle = \frac{1}{\sqrt{2}}, \quad \langle 1, 1, 0, 1 \mid 2, 1\rangle = \frac{1}{\sqrt{2}}.$$

- $j = 2, m = 0$ Three possibilities for m_1 i m_2: $(+1, -1)$, $(0, 0)$ $(-1, +1)$

$$|1, 1; 2, 0\rangle = \langle 1, 1, 1, -1 \mid 2, 0\rangle \,|1, 1, 1, -1\rangle + \langle 1, 1, 0, 0 \mid 2, 0\rangle \,|1, 1, 0, 0\rangle + \langle 1, 1, -1, 1 \mid 2, 0\rangle \,|1, 1, -1, 1\rangle$$

etc.