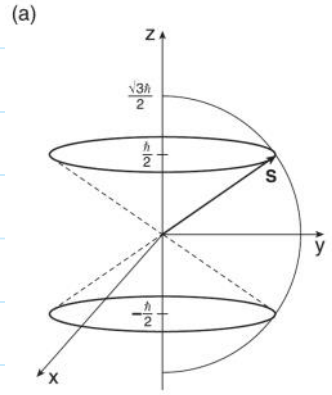
Spin 1/2

Reference: Griffiths 4.4.1
McIntyre 2.1, 2.2, 3.2

We know now that an electron (or any particle with spin $\frac{1}{2}$) has two simultaneous eigenstates of $\hat{S}^2$ and $\hat{S}_z$

$$\begin{array}{ll} & \quad\;\; s \quad m \\ |\uparrow\rangle = & \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle \\ |\downarrow\rangle = & \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle \end{array} \qquad \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



We represent these states in the z-basis as "spinors", (column vectors) χ_+, χ_-. Any general spin state is

$$\begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_- \quad \text{or,} \quad |\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$$

Question: What are the matrix representations of the operators $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$ in this basis? $\hat{S}_z$ and $\hat{S}^2$ are easy:

We know

$$\hat{S}^2|\uparrow\rangle = \hbar^2 \cdot \tfrac{1}{2}\left(\tfrac{1}{2}+1\right)|\uparrow\rangle = \frac{3\hbar^2}{4}|\uparrow\rangle$$

$$\hat{S}^2|\downarrow\rangle = \hbar^2\, \tfrac{1}{2}\left(\tfrac{1}{2}+1\right)|\downarrow\rangle = \frac{3\hbar^2}{4}|\downarrow\rangle$$

matrix elements:

$$(S^2)_{11} = \langle\uparrow|\hat{S}^2|\uparrow\rangle = \tfrac{3}{4}\hbar^2\langle\uparrow|\uparrow\rangle = \tfrac{3}{4}\hbar^2$$

$$(S^2)_{12} = \langle\uparrow|\hat{S}^2|\downarrow\rangle$$
$$\tfrac{3}{4}\hbar^2\langle\uparrow|\downarrow\rangle = 0$$

similarly

$$(S^2)_{21} = 0$$
$$(S^2)_{22} = \tfrac{3}{4}\hbar^2$$

$$\boxed{S^2 = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}$$

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Similarly,
$$\hat{S}_z \left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle = \hat{S}_z|\uparrow\rangle = \tfrac{1}{2}\hbar|\uparrow\rangle$$
$$\hat{S}_z \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = \hat{S}_z|\downarrow\rangle = \tfrac{1}{2}\hbar|\downarrow\rangle$$

So the matrix elements are easily calculated:

$$(S_z)_{11} = \langle\uparrow|S_z|\uparrow\rangle = \tfrac{\hbar}{2}\langle\uparrow|\uparrow\rangle = \hbar/2$$
$$(S_z)_{12} = \langle\uparrow|S_z|\downarrow\rangle = -\tfrac{\hbar}{2}\langle\uparrow|\downarrow\rangle = 0$$
$$(S_z)_{21} = \langle\downarrow|S_z|\uparrow\rangle = \tfrac{\hbar}{2}\langle\downarrow|\uparrow\rangle = 0$$
$$(S_z)_{22} = \langle\downarrow|S_z|\downarrow\rangle = -\hbar/2\,\langle\downarrow|\downarrow\rangle = -\hbar/2$$

$$\boxed{S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

Now, the elements of S_x and S_y are a bit trickier... after all $|\uparrow\rangle$ is an eigenstate of $\hat{S}_z$. But $\hat{S}_x$ and $\hat{S}_y$ do not commute with $\hat{S}_z$, so they don't share eigenstates. It's not so obvious what $\hat{S}_x|\uparrow\rangle$ is...

<u>Review of Ladder Operators</u>

The combination $\hat{S}_+ \equiv \hat{S}_x + i\hat{S}_y$ and $\hat{S}_- = \hat{S}_x - i\hat{S}_y$ are the raising / lowering operators.

$$[\hat{S}^2, \hat{S}_+] = [\hat{S}^2, \hat{S}_x] + i[\hat{S}^2, \hat{S}_y] = 0$$

$$\hat{S}_+|s,m\rangle = \hbar\sqrt{s(s+1) - m(m+1)}\;|s, m+1\rangle$$
$$\hat{S}_-|s,m\rangle = \hbar\sqrt{s(s+1) - m(m-1)}\;|s, m-1\rangle$$

If you need a refresher of where these come from, see the appendix of this section.

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Poll Q: Matrix Elements of S_+.

What is $\langle \uparrow | \hat{S}_+ | \downarrow \rangle = ?$

A.) Zero B.) Not Zero

Poll Q: Matrix Elements of S_+.

What is $\langle \uparrow | \hat{S}_+ | \downarrow \rangle = ?$

A.) Zero B.) Not Zero

In the case of spin ½:

$$\hat{S}_+ |\tfrac{1}{2}, -\tfrac{1}{2}\rangle = \hat{S}_+ |\downarrow\rangle = \hbar \sqrt{\tfrac{1}{2}(\tfrac{1}{2}+1) - (-\tfrac{1}{2})(-\tfrac{1}{2}+1)} \, |\uparrow\rangle$$
$$= \hbar \sqrt{\tfrac{3}{4} - (-\tfrac{1}{4})} = \hbar |\downarrow\rangle$$

$$\hat{S}_- |\tfrac{1}{2}, +\tfrac{1}{2}\rangle = \hat{S}_- |\uparrow\rangle = \hbar \sqrt{\tfrac{1}{2}(\tfrac{1}{2}+1) - \tfrac{1}{2}(\tfrac{1}{2}-1)} \, |\downarrow\rangle$$
$$= \hbar \sqrt{\tfrac{3}{4} + \tfrac{1}{4}} \, |\downarrow\rangle$$

Summary:

$$\underbrace{\begin{aligned} \hat{S}_+ |\uparrow\rangle &= 0 \\ \hat{S}_- |\downarrow\rangle &= 0 \end{aligned}} \qquad \begin{aligned} \hat{S}_+ |\downarrow\rangle &= \hbar |\uparrow\rangle \\ \hat{S}_- |\uparrow\rangle &= \hbar |\downarrow\rangle \end{aligned}$$

You can't lower the lowest S_z state any further
" " raise the highest S_z " " ".

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So, the matrix elements of these operators are:

$$\hat{S}_+ = \begin{pmatrix} \langle \uparrow | \hat{S}_+ | \uparrow \rangle & \langle \uparrow | \hat{S}_+ | \downarrow \rangle \\ \langle \downarrow | \hat{S}_+ | \uparrow \rangle & \langle \downarrow | \hat{S}_+ | \downarrow \rangle \end{pmatrix} = \begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix}$$

$$\hat{S}_- = \begin{pmatrix} \langle \uparrow | \hat{S}_- | \uparrow \rangle & \langle \uparrow | S_- | \downarrow \rangle \\ \langle \downarrow | \hat{S}_- | \uparrow \rangle & \langle \downarrow | \hat{S}_- | \downarrow \rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}$$

Now we're getting somewhere!

$$\left.\begin{aligned} \hat{S}_+ &= \hat{S}_x + i\hat{S}_y \\ \hat{S}_- &= \hat{S}_x - i\hat{S}_y \end{aligned}\right\}$$

add $\hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-)$

subtract $\hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-)$

So:

$$\hat{S}_x = \frac{1}{2}\left\{\begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}\right\} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\hat{S}_y = \frac{1}{2i}\left\{\begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}\right\} = \frac{\hbar}{2i}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

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

Pauli Matrices - since all operators have a factor of $\frac{\hbar}{2}$, we usually write, for the matrix representation of spin operators (in the z-basis).

$$S_x = (\hbar/2)\sigma_x \qquad S_y = (\hbar/2)\sigma_y \qquad S_z = (\hbar/2)\sigma_z$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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Example: Griffiths Example 4.2

Suppose an electron is in state $|\chi\rangle = \frac{1}{\sqrt{6}}\left[(1+i)|\uparrow\rangle + 2|\downarrow\rangle\right]$ where we're using the z-basis.

a.) What are the probabilities of getting $\hbar/2$ and $-\hbar/2$ if you measure S_z?

$$P(\hbar/2)_z = |\langle\uparrow|\chi\rangle|^2 = \left|\frac{1}{\sqrt{6}}(1+i)\overset{1}{\cancel{\langle\uparrow|\uparrow\rangle}} + \frac{2}{\sqrt{6}}\overset{0}{\cancel{\langle\uparrow|\downarrow\rangle}}\right|^2$$

$$= \frac{1}{6}\left[1^2 + 1^2\right] = \underline{\underline{\frac{1}{3}}}$$

$$P(-\hbar/2)_z = |\langle\downarrow|\chi\rangle|^2 = \left|\frac{1}{\sqrt{6}}(1+i)\langle\downarrow|\uparrow\rangle + \frac{2}{\sqrt{6}}\langle\downarrow|\downarrow\rangle\right|^2$$
$$= \left|\frac{2}{\sqrt{6}}\right|^2 = \frac{4}{6} = \underline{\underline{\frac{2}{3}}}$$

b.) What are the probabilities of measuring $\pm\hbar/2$ if I measure S_x?

$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ we need the eigenvectors and eigenvalues!

eigenvalues: $\begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda^2 - \frac{\hbar^2}{4} = 0$

$\lambda = \pm\hbar/2$ (no surprise)

eigenvectors: Let's call them $|+\rangle_x$ and $|-\rangle_x$

$$\hat{S}_x|+\rangle_x = \frac{\hbar}{2}|+\rangle_x \qquad \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

$$\boxed{a = b}$$

$|+\rangle_x \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ the other one must be orthogonal

$|-\rangle_x \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

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So, what's the probability I'll collapse to $|+\rangle_x$ if I measure S_x?

$$P(\hbar/2)_x = |{}_x\langle +|\chi\rangle|^2$$

$$= \left| \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \end{pmatrix} \cdot \frac{1}{\sqrt{6}} \begin{pmatrix} 1+i \\ 2 \end{pmatrix} \right|^2$$

$$= \left| \frac{1}{\sqrt{12}} [1+i+2] \right|^2 = \left| \frac{3+i}{\sqrt{12}} \right|^2 = \frac{1}{12}(3^2+1^2) = \frac{10}{12} = \underline{\underline{\frac{5}{6}}}$$

and, similarly:

$$P(-\hbar/2)_x = |{}_x\langle -|\chi\rangle|^2$$

$$= \left| \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \end{pmatrix} \cdot \frac{1}{\sqrt{6}} \begin{pmatrix} 1+i \\ 2 \end{pmatrix} \right|^2 = \left| \frac{1}{\sqrt{12}} (1+i-2) \right|^2$$

$$= \frac{1}{12} |i-1|^2 = \frac{1}{12}[1^2+1^2] = \frac{2}{12} = \underline{\underline{1/6}}$$

c.) What is $\langle S_x \rangle = ?$

Recall how to calculate expectation values:

$$\langle S_x \rangle = \sum_i (s_{x,i}) \cdot P(s_{x,i}) = \frac{\hbar}{2} \cdot \frac{5}{6} + \left(-\frac{\hbar}{2}\right)\frac{1}{6} = \underline{\underline{\frac{\hbar}{3}}}$$

<u>Calculating expectation values with matrices:</u>

Here is a nice way to calculate expectation values using matrices: Suppose you're in state $|\psi\rangle$ and you want $\langle Q \rangle$ for some operator: $|\psi\rangle = \sum_i c_i |q_i\rangle$ $|\psi\rangle$ is a combo of $\hat{Q}$'s eigenvectors.

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$$|\psi\rangle = \sum_i c_i |q_i\rangle$$

act — eigenvalue for $|q_i\rangle$

$$\hat{Q}|\psi\rangle = \sum_i c_i \hat{Q}|q_i\rangle = \sum_i c_i q_i |q_i\rangle$$

$$\langle\psi| = \sum_j c_j^* \langle q_j|$$

multiply $\hat{Q}|\psi\rangle$ on the left by $\langle\psi|$

$$\langle\psi|\hat{Q}|\psi\rangle = \left(\sum_j c_j^* \langle q_j|\right)\left(\sum_i c_i q_i |q_i\rangle\right)$$

$$= \sum_i \sum_j q_i c_j^* c_i \underbrace{\langle q_i|q_j\rangle}_{\delta_{ij}}$$

δ_{ij} only non-zero if $i=j$

$$= \sum_i q_i c_i^* c_i = \sum_i q_i |c_i|^2 = \sum_i q_i P(q_i) = \langle Q\rangle \,!$$

So, $\langle Q\rangle = \langle\psi|\hat{Q}|\psi\rangle$, which can be written as a matrix multiplication

$= \psi^\dagger Q \psi$

row — matrix — column

Check for the problem at hand: $\chi = \frac{1}{\sqrt{6}}\begin{pmatrix}1+i\\2\end{pmatrix}$

$$\langle S_x\rangle = \chi^\dagger S_x \chi$$

$$= \frac{1}{\sqrt{6}}\begin{pmatrix}1-i & 2\end{pmatrix}\cdot\frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}\cdot\frac{1}{\sqrt{6}}\begin{pmatrix}1+i\\2\end{pmatrix}$$

$$= \frac{\hbar}{12}\begin{pmatrix}1-i & 2\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1+i\\2\end{pmatrix} = \frac{\hbar}{12}\begin{pmatrix}1-i & 2\end{pmatrix}\begin{pmatrix}2\\1+i\end{pmatrix}$$

$$= \frac{\hbar}{12}\left[2(1-i)+2(1+i)\right] = \underline{\underline{\hbar/3}}\ \checkmark$$

Spin 1/2 - Appendix

<u>More Details on Ladder operators</u>

We start from $[\hat{S}^2, \hat{S}_+] = 0$

$$\hat{S}^2 \underbrace{\left(\hat{S}_+ |s,m\rangle\right)} = \hat{S}_+ \hat{S}^2 |s,m\rangle = \Big[\hat{S}_+ \cdot \hbar^2 s(s+1) |s,m\rangle\Big]$$

$|\psi\rangle$

call this $|\psi\rangle$ $\quad \therefore \quad \hat{S}^2 |\psi\rangle = \hbar^2 s(s+1) |\psi\rangle$.

so, if $|s,m\rangle$ is an eigenstate of $\hat{S}^2$, $\hat{S}_+ |s,m\rangle$ is also an eigenstate with the same total spin angular momentum

And, $$[\hat{S}_z, \hat{S}_+] = [\hat{S}_z, \hat{S}_x] + i[\hat{S}_z, \hat{S}_y]$$
$$= i\hbar \hat{S}_y + i(-i\hbar)\hat{S}_x$$
$$= \hbar[\hat{S}_x + i\hat{S}_y] = \hbar \hat{S}_+$$

So, $$\hat{S}_z \hat{S}_+ |s,m\rangle = (\hat{S}_+ \hat{S}_z + \hbar \hat{S}_+)|s,m\rangle$$

$$= \hat{S}_+ \Big[\hat{S}_z |s,m\rangle + \hbar |s,m\rangle\Big]$$
$$= \hat{S}_+ (m\hbar + \hbar)|s,m\rangle$$

So $$\hat{S}_z \Big[\underbrace{\hat{S}_+ |s,m\rangle}_{|\psi\rangle}\Big] = (m+1)\hbar \underbrace{\hat{S}_+ |s,m\rangle}_{|\psi\rangle}$$

$|\psi\rangle = \hat{S}_+ |s,m\rangle$ is an eigenfunction of $\hat{S}_z$ with eigenvalue $(m+1)\hbar$.

So, $|\psi\rangle = \hat{S}_+ |s,m\rangle$ is an eigenfunction of both $\hat{S}^2$ and $\hat{S}_z$, with eigenvalues $s(s+1)\hbar^2$ and $(m+1)\hbar$ respectively.

proportional to.

$\therefore \; |\psi\rangle \propto |s, m+1\rangle \quad$ and $\quad \hat{S}_+ \propto |s, m+1\rangle$

The same arguments give $\quad \hat{S}_- \propto |s, m-1\rangle$

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For the spin $\frac{1}{2}$ case, we know that $\hat{S}_+|\downarrow\rangle = C_+|\uparrow\rangle$
$\hat{S}_-|\uparrow\rangle = C_-|\downarrow\rangle$

Now let's determine these constants. We'll need the relation
$\hat{S}_+\hat{S}_- = \hat{S}^2 - \hat{S}_z^2 - \hbar\hat{S}_z$

<u>proof</u>:

$$\begin{aligned}\hat{S}_+\hat{S}_- &= (\hat{S}_x + i\hat{S}_y)(\hat{S}_x - i\hat{S}_y) \\ &= \hat{S}_x^2 + \hat{S}_y^2 + i\hat{S}_y\hat{S}_x - i\hat{S}_x\hat{S}_y \\ &= \hat{S}_x^2 + \hat{S}_y^2 - i[\hat{S}_x, \hat{S}_y] = \hat{S}_x^2 + \hat{S}_y^2 - i(i\hbar\hat{S}_z) \\ &= \hat{S}_x^2 + \hat{S}_y^2 + \hbar\hat{S}_z\end{aligned}$$

and

$$\hat{S}_+\hat{S}_- + \hat{S}_z^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 + \hbar\hat{S}_z$$
$$\hat{S}_+\hat{S}_- = \hat{S}^2 - \hat{S}_z^2 + \hbar\hat{S}_z \qquad \text{QED}$$

We also need to know that $\hat{S}_+^\dagger = \hat{S}_-$ this is hopefully obvious since $\hat{S}_+ = \hat{S}_x + i\hat{S}_y$

$\hat{S}_+^\dagger = \hat{S}_x^\dagger - i\hat{S}_y^\dagger$ but $\hat{S}_x = \hat{S}_x^\dagger$ $\hat{S}_y = \hat{S}_y^\dagger$
(Hermitian <u>Observables</u>).

Now to determine C_+ :

① $\hat{S}_-|\uparrow\rangle = C_-|\downarrow\rangle$ take the Hermitian conjugate $\longrightarrow$ $\langle\uparrow|\hat{S}_-^\dagger = C_-^*\langle\downarrow|$

② $\langle\uparrow|\hat{S}_+ = C_-^*\langle\downarrow|$

Now multiply ① on left by ② $\langle\uparrow|\hat{S}_+\hat{S}_-|\uparrow\rangle = C_-C_-^*\cancel{\langle\downarrow|\downarrow\rangle}^{1}$

So, $|C_-|^2 = \langle\uparrow|\hat{S}_+\hat{S}_-|\uparrow\rangle$ now use the identity above

$$= \langle\uparrow|\hat{S}^2 - \hat{S}_z^2 + \hbar\hat{S}_z|\uparrow\rangle = \frac{3}{4}\hbar^2\langle\uparrow|\uparrow\rangle - \left(\frac{1}{2}\hbar\right)^2\langle\uparrow|\uparrow\rangle + \frac{\hbar^2}{2}\langle\uparrow|\uparrow\rangle \Rightarrow \boxed{|C_-|^2 = \hbar^2}$$

$\therefore\ C_- = \hbar$

The proof of $C_+ = \hbar$ is almost the same.

So, $\boxed{\hat{S}_-|\uparrow\rangle = \hbar|\downarrow\rangle \quad \text{and} \quad \hat{S}_+|\downarrow\rangle = \hbar|\uparrow\rangle}$