Using matrices and vectors for spin operators and wave functions.

A general form of a wave function of a spin-½ state can be written as follows: $\Psi = b_1\alpha + b_2\beta$. Recall that because functions α and β form a complete set, any function describing a spin-1/2 system can be written as a linear combination/superposition of α and β, with b_1 and b_2 being "projection coefficients". Because the eigenfunctions α and β are the same for the various wave functions Ψ, the wave function Ψ is fully defined by the projection coefficients b_1 and b_2. Thus it can simply be represented as a list of values: $\{b_1\ \ b_2\}$ which can also be presented as a 2-element vector: $\Psi = b_1\alpha + b_2\beta = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$. It could be a row-vector or a column-vector. For convenience of using matrix multiplications (see below), a column-vector is typically used.

For example, the eigenfunctions of the $\hat{S}_z$ operator can be represented as column-vectors:

$$\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix};\ \ \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Complex conjugates of these functions are represented as row-vectors:

$$\alpha^* = \begin{pmatrix} 1 & 0 \end{pmatrix};\ \ \beta^* = \begin{pmatrix} 0 & 1 \end{pmatrix};\ \Psi^* = \begin{pmatrix} b_1 & b_2 \end{pmatrix}.$$

(Strictly speaking, for matrices and vectors we have to make them not only complex conjugate but also transpose; these conjugate transpose are called *adjoint* matrices or vectors and typically designated as $\alpha^\dagger=(\alpha^*)^T$, but I will only the asterisk here, for simplicity.)

So, an integral of two wave functions, for example, $\Psi = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$ and $\Phi = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$, can be represented simply as a vector multiplication:

$\int \Psi^* \Phi\, d\sigma = \begin{pmatrix} b_1 & b_2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = b_1 c_1 + b_2 c_2$. Recall we discussed that this integral in QM has the meaning of a projection of function Ψ onto Φ (and vice versa) and is analogous to a dot-product of two vectors -- here it is actually a dot product!

For example, using these rules you can verify that the vectors representing the functions α and β are orthonormal:

$$\int \alpha^*\alpha\ d\sigma = \begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1;\ \int \beta^*\beta\ d\sigma = \begin{pmatrix} 0 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 1;\ \ \int \alpha^*\beta\ d\sigma = \begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0; \int \beta^*\alpha\ d\sigma = \begin{pmatrix} 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0;$$

In the same spirit, spin-1/2 operators are the conveniently represented by 2x2 matrices:

$$\hat{S}_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix};\ \hat{S}_y = \frac{i\hbar}{2}\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix};\ \ \hat{S}_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix};\ \hat{S}^2 = \hat{S}_x^{\ 2} + \hat{S}_y^{\ 2} + \hat{S}_z^{\ 2} = \frac{3\hbar^2}{4}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

You can easily derive these matrices using the following equations that define how the spin-1/2 operators act on the functions α and β.

$$\hat{S}_z\alpha = \frac{\hbar}{2}\alpha\,;\ \hat{S}_z\beta = -\frac{\hbar}{2}\beta\,;\ \hat{S}_x\alpha = \frac{\hbar}{2}\beta\,;\ \hat{S}_x\beta = \frac{\hbar}{2}\alpha\,;\ \hat{S}_y\alpha = i\frac{\hbar}{2}\beta\,;\ \hat{S}_y\beta = -i\frac{\hbar}{2}\alpha$$

$$\int \alpha^*\alpha\, d\sigma = 1\,;\ \int \beta^*\beta\, d\sigma = 1\,;\ \int \beta^*\alpha\, d\sigma = 0\,;\ \int \alpha^*\beta\, d\sigma = 0$$

For example, let's derive a matrix representation for $\hat{S}_z$. We start with a general form of a 2x2 matrix:

$\hat{S}_z = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$; where *a*,*b*,*c*,*d* are the unknowns that we need to determine. First let's substitute the vector form or α and the matrix form of $\hat{S}_z$ into the equation: $\hat{S}_z\alpha = \frac{\hbar}{2}\alpha$, which now reads $\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$. The multiplication in the left-hand-side of this equation gives $\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ c \end{pmatrix}$, and we get $\begin{pmatrix} a \\ c \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$. This immediately gives ➔ $a = \frac{\hbar}{2}$ and $c = 0$.

Likewise, using the equation $\hat{S}_z\beta = -\frac{\hbar}{2}\beta$, we get $\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} b \\ d \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, ➔ $b = 0$ and $d = -\frac{\hbar}{2}$. Finally, after putting these values of *a*,*b*,*c*,*d* into the matrix expression for $\hat{S}_z$ we get

$\hat{S}_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$. (Q.E.D.)

Here I considered the case of spin S=½. The same approach can be used for other spin values, just the vectors will be of length 2S+1, and the matrices will be of size (2S+1)x(2S+1). Because spin is an angular momentum, the same concept applies to the general case of the angular momentum operator $\hat{\vec{l}}$ and its components: $(\hat{l}_x, \hat{l}_y, \hat{l}_z)$, and the wave functions corresponding to various states of the angular momentum – just the size of such vectors representing wave functions will be 2*l*+1 and the matrices will be of size (2*l*+1)x(2*l*+1). Furthermore, a similar representation can be used for any countable/denumerable set of wave functions (for example, representing discrete states of a Q.M. system) and the corresponding operators.