

Using matrices and vectors for spin operators and wavefunctions.

Consider spin $S=\frac{1}{2}$. Eigenfunctions of the \hat{S}_z operator can be represented as column-vectors:

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

A general form of a wavefunction of a spin- $\frac{1}{2}$ state: $\Psi = b_1\alpha + b_2\beta = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$. (Recall that because 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).

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

$$\alpha^* = (1 \ 0); \quad \beta^* = (0 \ 1); \quad \Psi^* = (b_1 \ b_2).$$

(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 $\alpha^\dagger = (\alpha^*)^\top$, but I will only use the asterisk, for simplicity.)

So, an integral of two wavefunctions, 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:

$$\int \Psi^* \Phi d\sigma = (b_1 \ b_2) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = b_1 c_1 + b_2 c_2. \text{ Recall we discussed that this integral in QM has the meaning}$$

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:

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

Spin-1/2 operators are conveniently represented by 2x2 matrices:

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

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 .

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

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

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 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 $\rightarrow a = \frac{\hbar}{2}$ and $c = 0$.

Likewise, using the equation $\hat{S}_z \beta = -\frac{\hbar}{2} \beta$, we get $\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} b \\ d \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $\rightarrow b = 0$ 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

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

Here I considered the case of spin $S = \frac{1}{2}$. 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 $(2S+1) \times (2S+1)$. Furthermore, a similar representation can be used for any countable/denumerable set of wavefunctions (for example, representing discrete states of a Q.M. system) and the corresponding operators.