Pauli Two-Component Formalism

Manipulations with the state kets of spin ½ systems can be conveniently carried out using the two-component spinor formalism introduced by W. Pauli in 1926.

In Section 1.3 we learned how a ket (bra) can be represented by a column (row) matrix; all we have to do is arrange the expansion coefficients in terms of a certain specified set of base kets into a column (row) matrix.

In the spin ½ case we have for the base kets and bras

$$|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv \chi_+ \qquad |-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \chi_-$$

$$\langle +| \doteq (1,0) = \chi_+^\dagger \qquad \langle -| \doteq (0,1) = \chi_-^\dagger$$

and we have for an arbitrary state ket and the corresponding state bra.

$$|\alpha\rangle = |+\rangle\langle +|\alpha\rangle + |-\rangle\langle -|\alpha\rangle \doteq \begin{pmatrix} \langle +|\alpha\rangle \\ \langle -|\alpha\rangle \end{pmatrix}$$

$$\langle\alpha| = \langle\alpha|+\rangle\langle +| + \langle\alpha|-\rangle\langle -| \doteq (\langle\alpha|+\rangle, \langle\alpha|-\rangle)$$

Column matrix $|\alpha>$ is referred to as a two-component spinor and is written as

$$\chi = \begin{pmatrix} \langle + | \alpha \rangle \\ \langle - | \alpha \rangle \end{pmatrix} \equiv \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

$$= c_+ \chi_+ + c_- \chi_-,$$

where c_+ and c_- are, in general, complex numbers.

For $\chi^\dagger$ we have

$$\chi^\dagger = (\langle \alpha | + \rangle, \langle \alpha | - \rangle) = (c_+^*, c_-^*)$$

The matrix elements $< \pm|S_k| +>$ and $< \pm|S_k| ->$, apart from $\frac{\hbar}{2}$ are to be set equal to those of 2×2 matrices σ_k known as the **Pauli matrices**. We identify

$$\langle \pm|S_k|+\rangle \equiv \left(\frac{\hbar}{2}\right)(\sigma_k)_{\pm,+}, \qquad \langle \pm|S_k|-\rangle \equiv \left(\frac{\hbar}{2}\right)(\sigma_k)_{\pm,-}$$

We can now write the expectation value $<S_k>$ in terms of χ and σ_k:

$$\langle S_k\rangle = \langle\alpha|S_k|\alpha\rangle = \sum_{a'=+,-}\sum_{a''=+,-}\langle\alpha|a'\rangle\langle a'|S_k|a''\rangle\langle a''|\alpha\rangle$$

$$= \left(\frac{\hbar}{2}\right)\chi^\dagger\sigma_k\chi$$

where the usual rule of matrix multiplication is used in the last line.

Explicitly, we see from

$$S_x = \left(\frac{\hbar}{2}\right)\{(|+\rangle\langle -|) + (|-\rangle\langle +|)\},$$

$$S_y = \left(\frac{i\hbar}{2}\right)\{-(|+\rangle\langle -|) + (|-\rangle\langle +|)\},$$

$$S_z = \left(\frac{\hbar}{2}\right)\{(|+\rangle\langle +|) - (|-\rangle\langle -|)\}$$

together with

$$\langle \pm|S_k|+\rangle \equiv \left(\frac{\hbar}{2}\right)(\sigma_k)_{\pm,+}, \qquad \langle \pm|S_k|-\rangle \equiv \left(\frac{\hbar}{2}\right)(\sigma_k)_{\pm,-}$$

that

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where the subscripts 1, 2, and 3 refer to x, y, and z, respectively.

We record some properties of the Pauli matrices.

First,

$$\sigma_i^2 = 1$$

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 0, \quad \text{for } i \neq j.$$

where the right-hand side of the first equation is to be understood as the 2×2 identity matrix.

These two relations are, of course, equivalent to the anticommutation relations

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

We also have the commutation relations

$$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k$$

which we see to be the explicit 2x2 matrix realizations of the angular-momentum commutation relations $[J_i, J_j]$.

Combining $\{\sigma_i, \sigma_j\}$ and $[\sigma_i, \sigma_j]$, we can obtain

$$\sigma_1\sigma_2 = -\sigma_2\sigma_1 = i\sigma_3 \ldots .$$

Notice also that

$$\sigma_i^\dagger = \sigma_i ,$$
$$\det(\sigma_i) = -1,$$
$$\mathrm{Tr}(\sigma_i) = 0.$$

We now consider $\boldsymbol{\sigma}.\mathbf{a}$, where $\mathbf{a}$ is a vector in three dimensions.

This is actually to be understood as a 2×2 matrix.

Thus

$$\boldsymbol{\sigma}\cdot\mathbf{a} \equiv \sum_k a_k \sigma_k = \begin{pmatrix} +a_3 & a_1 - ia_2 \\ a_1 + ia_2 & -a_3 \end{pmatrix}$$

There is also a very important identity,

$$(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + i\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b})$$

To prove this all we need are the anticommutation and commutation relations, $\{\sigma_i, \sigma_j\}$ and $[\sigma_i, \sigma_j]$, respectively:

$$(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \sum_j \sigma_j a_j \sum_k \sigma_k b_k$$

$$= \sum_j \sum_k \left(\frac{1}{2}\{\sigma_j, \sigma_k\} + \frac{1}{2}[\sigma_j, \sigma_k] \right) a_j b_k$$

$$= \sum_j \sum_k \left(\delta_{jk} + i\varepsilon_{jkl}\sigma_l \right) a_j b_k$$

$$= \mathbf{a}\cdot\mathbf{b} + i\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b})$$

If the components of **a** are real, we have

$$(\boldsymbol{\sigma}\cdot\mathbf{a})^2 = |\mathbf{a}|^2$$

where |**a**| is the magnitude of the vector **a**.

Rotations in the Two-Component Formalism

Let us now study the 2×2 matrix representation of the rotation operator $\mathscr{D}(\hat{\boldsymbol{n}},\phi)$.

We have

$$\exp\left(\frac{-i\mathbf{S}\cdot\hat{\mathbf{n}}\phi}{\hbar}\right) \doteq \exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right)$$

Using

$$(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^n = \begin{cases} 1 & \text{for } n \text{ even,} \\ \boldsymbol{\sigma}\cdot\hat{\mathbf{n}} & \text{for } n \text{ odd,} \end{cases}$$

which follows from

$$(\boldsymbol{\sigma}\cdot\mathbf{a})^2 = |\mathbf{a}|^2$$

We can write

Explicitly, in 2×2 form we have

$$\exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right) = \left[1 - \frac{(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^2}{2!}\left(\frac{\phi}{2}\right)^2 + \frac{(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^4}{4!}\left(\frac{\phi}{2}\right)^4 - \cdots\right]$$

$$- i\left[(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})\frac{\phi}{2} - \frac{(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^3}{3!}\left(\frac{\phi}{2}\right)^3 + \cdots\right]$$

$$= \mathbf{1}\cos\left(\frac{\phi}{2}\right) - i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\sin\left(\frac{\phi}{2}\right).$$

$$\exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right) = \begin{pmatrix} \cos\left(\frac{\phi}{2}\right) - in_z\sin\left(\frac{\phi}{2}\right) & (-in_x - n_y)\sin\left(\frac{\phi}{2}\right) \\ (-in_x + n_y)\sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right) + in_z\sin\left(\frac{\phi}{2}\right) \end{pmatrix}$$

Just as the operator $\exp(\frac{-iS.\hat{n}\phi}{\hbar})$ acts on a state ket |α>, the 2×2 matrix $\exp(\frac{-i\sigma.\hat{n}\phi}{\hbar})$ acts on a two-component spinor χ.

Under rotations we change χ as follows:

$$\chi \rightarrow \exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right)\chi$$

On the other hand, the σ_i's themselves are to remain unchanged under rotations.

So strictly speaking, despite its appearance, σ is not to be regarded as a vector; rather, it is $\chi^\dagger\sigma\chi$ which obeys the transformation property of a vector:

$$\chi^\dagger\sigma_k\chi \rightarrow \sum_l R_{kl}\chi^\dagger\sigma_l\chi$$

An explicit proof of this may be given using

$$\exp\left(\frac{i\sigma_3\phi}{2}\right)\sigma_1\exp\left(\frac{-i\sigma_3\phi}{2}\right) = \sigma_1\cos\phi - \sigma_2\sin\phi$$

and so on, which is the 2×2 matrix analogue of:

$$\exp\left(\frac{iS_z\phi}{\hbar}\right)S_x\exp\left(\frac{-iS_z\phi}{\hbar}\right) = S_x\cos\phi - S_y\sin\phi$$

In discussing a 2π rotation using the ket formalism, we have seen that a spin ½ ket |α> goes into -|α>.

The 2×2 analogue of this statement is

$$\exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right)\bigg|_{\phi=2\pi} = -1, \quad \text{for any } \hat{\mathbf{n}}$$

which is evident from:

$$\exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right)=\mathbf{1}\cos\left(\frac{\phi}{2}\right)-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\sin\left(\frac{\phi}{2}\right)$$

As an instructive application of rotation matrix

$$\exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right)=\begin{pmatrix}\cos\left(\frac{\phi}{2}\right)-in_z\sin\left(\frac{\phi}{2}\right) & (-in_x-n_y)\sin\left(\frac{\phi}{2}\right)\\ (-in_x+n_y)\sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right)+in_z\sin\left(\frac{\phi}{2}\right)\end{pmatrix}$$

let us see how we can construct an eigenspinor of $\boldsymbol{\sigma}.\hat{\boldsymbol{n}}$ with eigenvalue +1, where $\hat{\boldsymbol{n}}$ is a unit vector in some specified direction.

Our object is to construct χ satisfying

$$\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\chi = \chi$$

In other words, we look for the two-component column matrix representation of $|\boldsymbol{S}.\hat{\boldsymbol{n}}\rangle$ defined by

$$\mathbf{S}\cdot\hat{\mathbf{n}}|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle = \left(\frac{\hbar}{2}\right)|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle$$

Actually this can be solved as a straightforward eigenvalue problem (see Problem 9 in Chapter 1), but here we present an alternative method based on rotation matrix:

$$\exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right) = \begin{pmatrix} \cos\left(\frac{\phi}{2}\right) - in_z\sin\left(\frac{\phi}{2}\right) & (-in_x - n_y)\sin\left(\frac{\phi}{2}\right) \\ (-in_x + n_y)\sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right) + in_z\sin\left(\frac{\phi}{2}\right) \end{pmatrix}$$

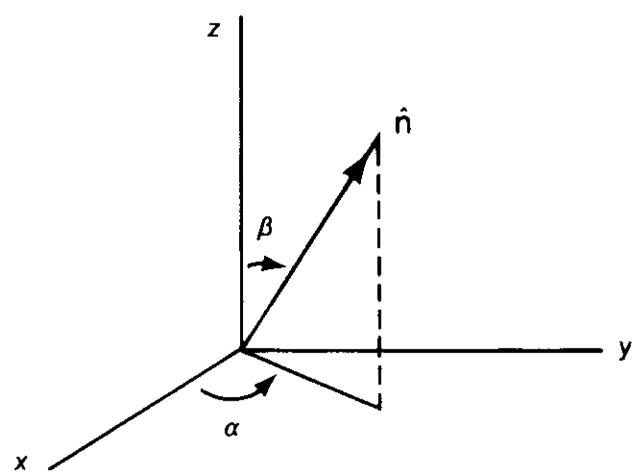
9. Construct $|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle$ such that

$$\mathbf{S}\cdot\hat{\mathbf{n}}|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle = \left(\frac{\hbar}{2}\right)|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle$$

where $\hat{\mathbf{n}}$ is characterized by the angles shown in the figure. Express your answer as a linear combination of $|+\rangle$ and $|-\rangle$. [*Note*: The answer is

$$\cos\left(\frac{\beta}{2}\right)|+\rangle + \sin\left(\frac{\beta}{2}\right)e^{i\alpha}|-\rangle.$$

But do not just verify that this answer satisfies the above eigenvalue equation. Rather, treat the problem as a straightforward eigenvalue problem. Also do not use rotation operators, which we will introduce later in this book.]

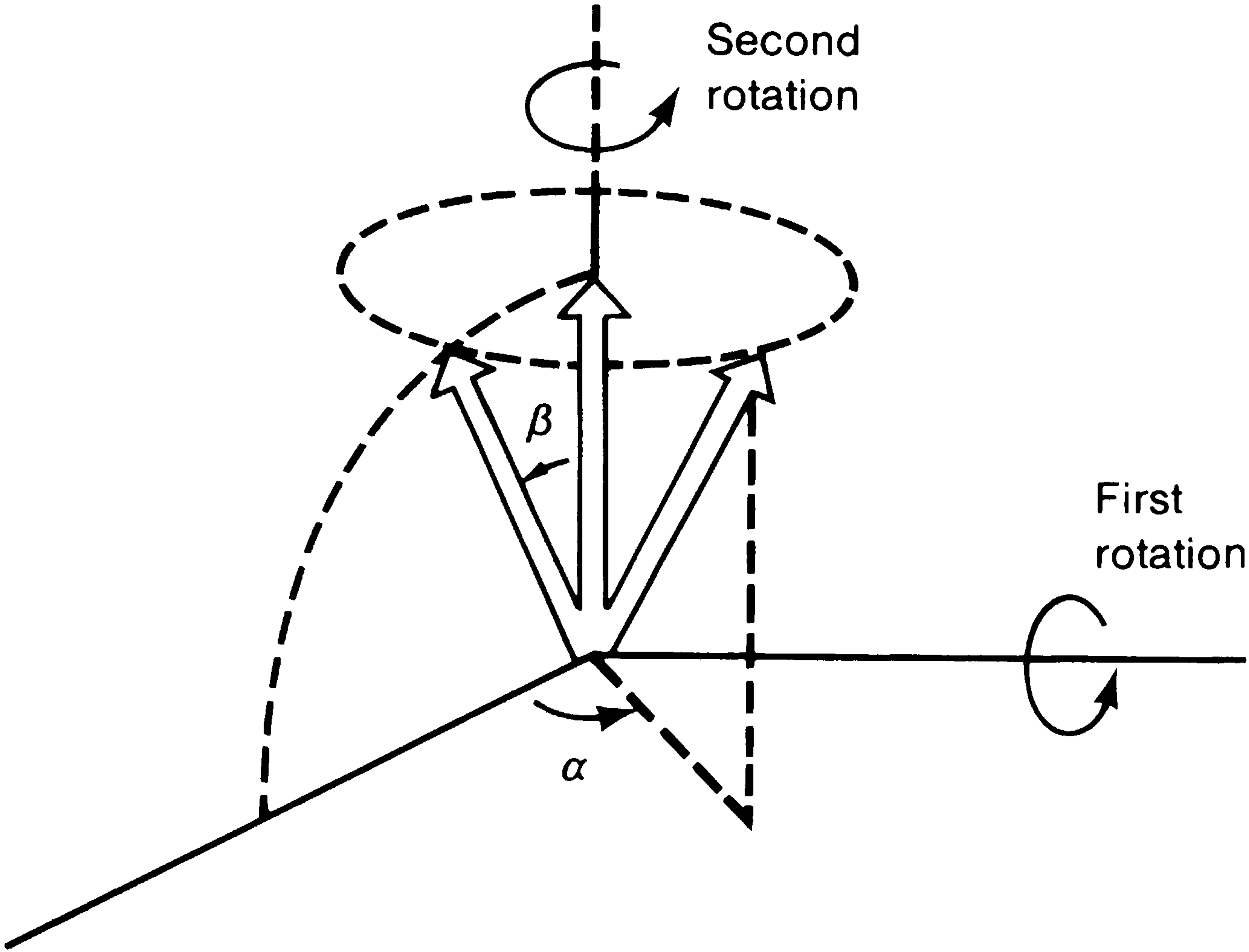


Let the polar and the azimuthal angles that characterize $\hat{n}$ be β and α, respectively.

We start with $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, the two-component spinor that represents the spin-up state.

Given this, we first rotate about the y-axis by angle β; we subsequently rotate by angle α about the z-axis.

We see that the desired spin state is then obtained; see Figure 3.3.


Second rotation
First rotation
β
α

In the Pauli spinor language this sequence of operations is equivalent to applying $\exp(\frac{-i\sigma_2\beta}{2})$ to followed by an application of $\exp(\frac{-i\sigma_3\alpha}{2})$.

The net result is

$$\chi = \left[\cos\left(\frac{\alpha}{2}\right) - i\sigma_3 \sin\left(\frac{\alpha}{2}\right)\right]\left[\cos\left(\frac{\beta}{2}\right) - i\sigma_2 \sin\left(\frac{\beta}{2}\right)\right]\begin{pmatrix}1\\0\end{pmatrix}$$

$$= \begin{pmatrix} \cos\left(\frac{\alpha}{2}\right) - i\sin\left(\frac{\alpha}{2}\right) & 0 \\ 0 & \cos\left(\frac{\alpha}{2}\right) + i\sin\left(\frac{\alpha}{2}\right) \end{pmatrix}\begin{pmatrix} \cos\left(\frac{\beta}{2}\right) & -\sin\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right) & \cos\left(\frac{\beta}{2}\right) \end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}$$

$$= \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) e^{-i\alpha/2} \\ \sin\left(\frac{\beta}{2}\right) e^{i\alpha/2} \end{pmatrix}$$

in complete agreement with Problem 9 of Chapter 1 if we realize that a phase common to both the upper and lower components is devoid of physical significance.