TOTAL-S MATRIX AND EIGENSTATES IN PRODUCT BASIS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 15.1.1.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Although we've looked at the addition of two spins while working through Griffiths's book, this problem from Shankar is a nice exercise in dealing with a direct product of two vector spaces, so we'll analyze it that way.

The problem is to find the spin operator **S** obtained by adding two spin-$\frac{1}{2}$ systems. Each spin comprises a vector space of dimension 2, and the components can be written using the spin matrices

$$S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1}$$

Each spin resides in its own 2-dim vector space, so the vector space for the combined system is formed by taking the direct product of the two spin spaces. We can write the matrices for the combined space by following the formulas we gave earlier. The notation we'll use is to add a subscript 1 or 2 to indicate which particle we're considering. In the product space, for particle 1 we have

$$S_{1x} = S_x^{(1)} \otimes I^{(2)} \tag{2}$$

$$= \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{3}$$

$$= \frac{\hbar}{2}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{4}$$

$$S_{1y} = S_y^{(1)} \otimes I^{(2)} \tag{5}$$

$$= \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{6}$$

$$= \frac{\hbar}{2}\begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix} \tag{7}$$

$$S_{1z} = S_z^{(1)} \otimes I^{(2)} \tag{8}$$

$$= \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{9}$$

$$= \frac{\hbar}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{10}$$

For particle 2, we have

$$S_{2x} = I^{(1)} \otimes S_x^{(2)} \tag{11}$$
$$= \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{12}$$
$$= \frac{\hbar}{2}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{13}$$
$$S_{2y} = I^{(1)} \otimes S_y^{(2)} \tag{14}$$
$$= \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{15}$$
$$= \frac{\hbar}{2}\begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix} \tag{16}$$
$$S_{2z} = I^{(1)} \otimes S_z^{(2)} \tag{17}$$
$$= \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{18}$$
$$= \frac{\hbar}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{19}$$

Given these matrices, it's just a matter of matrix multiplication and addition to obtain the overall operators. For the overall z component we have

$$S_z = S_{1z} + S_{2z} = \hbar\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{20}$$

We can get S^2 from the above components

$$S^2 = (\mathbf{S}_1 + \mathbf{S}_2) \cdot (\mathbf{S}_1 + \mathbf{S}_2) \tag{21}$$
$$= S_1^2 + S_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{22}$$

We could just use brute force and calculate these by multiplying out the matrices above. For example

$$S_1^2 = S_{1x}^2 + S_{1y}^2 + S_{1z}^2 \tag{23}$$

and so on. However, if we use Shankar's suggestion and remember that $S_1^2 = S_2^2 = \frac{3}{4}\hbar^2 I$ (where I refers to the identity matrix within the appropriate vector space), then we need to work out the last term in 22. Using the raising and lowering operators for spin

$$S_\pm = S_x \pm i S_y \tag{24}$$

we have

$$S_{1+}S_{2-} + S_{1-}S_{2+} = S_{1x}S_{2x} + S_{1y}S_{2y} + i\left(-S_{1x}S_{2y} + S_{1y}S_{2x}\right) + \tag{25}$$

$$S_{1x}S_{2x} + S_{1y}S_{2y} - i\left(-S_{1x}S_{2y} + S_{1y}S_{2x}\right) \tag{26}$$

$$= 2\left(S_{1x}S_{2x} + S_{1y}S_{2y}\right) \tag{27}$$

We therefore get

$$2\mathbf{S}_1 \cdot \mathbf{S}_2 = S_{1+}S_{2-} + S_{1-}S_{2+} + 2S_{1z}S_{2z} \tag{28}$$

We can work out the matrix forms of the raising and lowering operators from the above matrices, and we have

$$S_{1+} = S_{1x} + iS_{1y} \tag{29}$$

$$= \hbar \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{30}$$

$$S_{1-} = S_{1x} - iS_{1y} \tag{31}$$

$$= \hbar \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{32}$$

$$S_{2+} = S_{2x} + iS_{2y} \tag{33}$$

$$= \hbar \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{34}$$

$$S_{2-} = S_{2x} - iS_{2y} \tag{35}$$

$$= \hbar \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{36}$$

For the products, we have

$$S_{1+}S_{2-} = \hbar^2 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{37}$$

$$S_{1-}S_{2+} = \hbar^2 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{38}$$

$$2S_{1z}S_{2z} = \frac{\hbar^2}{2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{39}$$

For the total, we have

$$S^2 = 2\times\frac{3\hbar^2}{4}\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix}+\hbar^2\begin{bmatrix}0&0&0&0\\0&0&1&0\\0&0&0&0\\0&0&0&0\end{bmatrix}+ \tag{40}$$

$$\hbar^2\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&1&0&0\\0&0&0&0\end{bmatrix}+\frac{\hbar^2}{2}\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{bmatrix} \tag{41}$$

$$=\hbar^2\begin{bmatrix}2&0&0&0\\0&1&1&0\\0&1&1&0\\0&0&0&2\end{bmatrix}\equiv\hbar^2\Lambda \tag{42}$$

The eigenvalues and eigenvectors of the matrix in 42 are found in the usual way, by calculating the characteristic determinant:

$$|\Lambda-\lambda I| = \begin{vmatrix}2-\lambda&0&0&0\\0&1-\lambda&1&0\\0&1&1-\lambda&0\\0&0&0&2-\lambda\end{vmatrix}=0 \tag{43}$$

This gives the polynomial

$$(2-\lambda)^2\left[(1-\lambda)^2-1\right]=0 \tag{44}$$

The roots (eigenvalues) are 0 (once) and 2 (3 times). The corresponding normalized eigenvectors can be found from solving the equations:

For the eigenvalue $\lambda=0$, we have for the eigenvector $v_0=\begin{bmatrix}a&b&c&d\end{bmatrix}^T$

$$\Lambda v_0 = 0 \tag{45}$$

$$a = d=0 \tag{46}$$

$$b = -c \tag{47}$$

Thus the normalized eigenvector is

$$v_0=\frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\-1\\0\end{bmatrix} \tag{48}$$

This is the singlet state with $s=0$, $m=0$.

For the triply degenerate eigenvalue $\lambda = 2$, we have

$$\Lambda v_2 = 2v_2 \tag{49}$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{50}$$

The normalized eigenvectors are then

$$v_{2a} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{51}$$

$$v_{2b} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{52}$$

$$v_{2c} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} \tag{53}$$

This gives us the triplet state, with $s = 1$ and $m = 1, 0, -1$.

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