ADDING TWO SPIN-1/2 SYSTEMS - PRODUCT AND TOTAL-S BASES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.1.

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When adding two spins we can work in the product basis, which is the vector space formed by the direct product of the two vector spaces which correspond to the two spins, taken separately. For spin-$\frac{1}{2}$, the single-spin basis consists of two spinors

$$\chi_{\uparrow} = \frac{\hbar}{2}\begin{bmatrix}1\\0\end{bmatrix} \tag{1}$$

$$\chi_{\downarrow} = \frac{\hbar}{2}\begin{bmatrix}0\\1\end{bmatrix} \tag{2}$$

In this basis, the spin operator $\mathbf{S}$ is formed from the 3 Pauli matrices as

$$\mathbf{S}_i = \frac{\hbar}{2}\sigma \tag{3}$$

$$\sigma_x = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} \tag{4}$$

$$\sigma_y = \begin{bmatrix}0 & -i\\i & 0\end{bmatrix} \tag{5}$$

$$\sigma_z = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix} \tag{6}$$

where the subscript i labels which particle we're considering.

When we add two independent spins, we get a total spin operator $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$. However, if we use the product basis, the vector space in which $\mathbf{S}$ resides is the direct product of the two vector spaces for the individual spins:

$$\mathbb{V}_{tot} = \mathbb{V}^{(1)} \otimes \mathbb{V}^{(2)} \tag{7}$$

where $\mathbb{V}^{(i)}$ is the 2-d vector space corresponding to spin i. We've seen in an earlier post how to construct the components of $\mathbf{S}$ in this vector space, so we'll quote the results:

$$S_x = S_{1x} + S_{2x} = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \tag{8}$$

$$S_y = S_{1y} + S_{2y} = \frac{\hbar}{2}\begin{bmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{bmatrix} \tag{9}$$

$$S_z = S_{1z} + S_{2z} = \hbar\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{10}$$

We also have, again working directly from the earlier results in the product basis

$$S_1^2 = S_2^2 = \frac{3\hbar^2}{4}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \frac{3\hbar^2}{4} I \tag{11}$$

The square of the total spin operator in the product basis comes out to

$$S^2 = \hbar^2\begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \tag{12}$$

From these results, we see that (since S_1^2 and S_2^2 are multiplies of the identity matrix) both S_z and S^2 commute with S_1^2 and S_2^2. We can also see by direct calculation that $\left[S^2, S_z\right] = 0$, so S^2, S_z, S_1^2 and S_2^2 form a set of 4 mutually commuting matrices. Since the matrices are all hermitian (they represent observable quantities), it must be possible to find a basis in which all 4 are diagonal. The problem in this case is fairly simple, since in the product basis, only S^2 is not diagonal, so if we can find the unitary transformation that diagonalizes S^2, we should have our new basis. The desired unitary transformation matrix is the matrix whose columns are the normalized eigenvectors of S^2. In the previous post we found these eigenvectors to be

$$v_0 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix} \tag{13}$$

$$v_{2a} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{14}$$

$$v_{2b} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{15}$$

$$v_{2c} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} \tag{16}$$

The first eigenvector v_0 corresponds to eigenvalue 0, and the other 3 to eigenvalue 2. The unitary transformation matrix is then

$$U = \begin{bmatrix} 0 & 1 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{17}$$

By direct multiplication, we find that S^2 in what Shankar calls the total-s basis is

$$U^T S^2 U = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \tag{18}$$

The normalized eigenvectors are

$$u_i = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{19}$$

The first eigenvector corresponds to the singlet state and the last 3 to the triplet state. We can verify by direct calculation that S_z, S_1^2 and S_2^2 are unchanged by this transformation, remaining as given in 10 and 11.

The basis is related to the product basis by (using the notation $|ss_z s_1 s_2\rangle$ for the vectors in the total-s basis):

$$\left|00\frac{1}{2}\frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{20}$$

$$\left|11\frac{1}{2}\frac{1}{2}\right\rangle = |\uparrow\uparrow\rangle \tag{21}$$

$$\left|10\frac{1}{2}\frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \tag{22}$$

$$\left|1-1\frac{1}{2}\frac{1}{2}\right\rangle = |\downarrow\downarrow\rangle \tag{23}$$

We can use either basis in practical calculations. The choice depends on the form of the Hamiltonian: if it can be expressed entirely in terms of S^2,S_z, S_1^2 and S_2^2 then it makes sense to use the total-s basis.

PINGBACKS

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