KINEMATICS OF SPIN: HILBERT SPACE FOR AN ELECTRON

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 14.3.

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

We've looked at quantum mechanical spin before but Shankar's treatment is quite different to that of Griffiths, so it's worth another look. Shankar begins with a thought experiment in which an electron is prepared (don't ask how!) in a state with zero momentum. Since its momentum is known precisely, its position is completely uncertain, so we can take the wave function in position space to be a constant, independent of position. Since the angular momentum operator $\mathbf{L}$ that we've met before is defined by replacing classical quantities by quantum operators in the classical relation $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, an electron in this state must have $\mathbf{L} = 0$. (We can see this also from the relation $L_z = -i\hbar \frac{\partial}{\partial \phi}$ which gives zero since the wave function is independent of position.) However, if we measure the angular momentum along some direction such as z of an electron in such a state, we find that it always has the values $\pm \frac{\hbar}{2}$.

If we want to construct a wave function that describes the electron, we therefore need to consider a function that has a component that is independent of position, but which has eigenvalues $\pm \frac{\hbar}{2}$ when operated on by some operator with the properties of an angular momentum operator. The key to finding such a wave function is given by our example of a vector wave function. In that example, which considered the behaviour of a 2-d vector valued function under an infinitesimal rotation, we found that there were two effects of such a rotation. (It might help the reader to refer back to our earlier discussion at this point.) First, the rotation carries a vector $\mathbf{V}$ from its initial location A to some other point B. Second, the original vector $\mathbf{V}$ also gets rotated through the infinitesimal angle so that it now points in a slightly different direction, giving the rotated vector $\mathbf{V}'$. The components of $\mathbf{V}'$ are linear combinations of the components of the unrotated vector $\mathbf{V}$.

The first effect (that of rotating the function at A into the new position B) is generated by the original angular momentum operator $\mathbf{L}$. This rotation depends on the position coordinates, since we must know the coordinates

of the two points A and B to calculate the effect of the rotation. The second effect (that of rotating the vector so it points in a different direction) does not depend on the positions; rather, it depends only on the angle of rotation. As we showed in the previous example (working in 2-d), the second effect is generated by a 2×2 matrix S_z. We need a matrix rather than just a single number since we need to form a linear combination of the two components of the original vector to get the rotated vector.

In the special case of the 2-d rotation, the combined effect of these two types of rotation are given by

$$J_z = L_z + S_z \tag{1}$$

$$= \begin{bmatrix} L_z & 0 \\ 0 & L_z \end{bmatrix} + \begin{bmatrix} 0 & -i\hbar \\ i\hbar & 0 \end{bmatrix} \tag{2}$$

The transformation then becomes

$$\begin{bmatrix} V_1' \\ V_2' \end{bmatrix} = \left[I - \frac{i\varepsilon_z}{\hbar} J_z \right] \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} \tag{3}$$

This equation is valid for the rotation of a vector wave function with two components through an angle ε_z about the z axis, in two dimensions.

At this point, we can generalize this result to 3-d, and also to a wave function with some arbitrary number n components. The dimension of the matrix is determined by n, so if we again consider a rotation about the z axis by some angle ε, we get

$$\begin{bmatrix} \psi_1' \\ \vdots \\ \psi_n' \end{bmatrix} = \left[I - \frac{i\varepsilon_z}{\hbar} J_z \right] \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} \tag{4}$$

$$= \left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{i\varepsilon_z}{\hbar} \begin{bmatrix} -i\hbar\frac{\partial}{\partial\phi} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & -i\hbar\frac{\partial}{\partial\phi} \end{bmatrix} - \frac{i\varepsilon_z}{\hbar} S_z \right) \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} \tag{5}$$

Here, the actual form of S_z is yet to be determined.

Although we worked out this for the special case of a rotation about the z axis, we can generalize it to a rotation about an arbitrary axis, and thus get a vector operator:

$$\mathbf{J} = \mathbf{L} + \mathbf{S} \tag{6}$$

The orbital angular momentum operator $\mathbf{L}$ operates on spatial coordinates (and is the same operator on each of the n components), while the spin operator $\mathbf{S}$ mixes the n components of the wave function (and not on the spatial coordinates). As these two operators operate on different quantities, they commute, which leads to the commutation relation

$$\left[J_i, J_j\right] = i\hbar \sum_k \varepsilon_{ijk} J_k \tag{7}$$

which separates into the same commutation relations for each component of $\mathbf{J}$ so we have

$$\left[L_i, L_j\right] = i\hbar \sum_k \varepsilon_{ijk} L_k \tag{8}$$

$$\left[S_i, S_j\right] = i\hbar \sum_k \varepsilon_{ijk} S_k \tag{9}$$

Shankar worked out the matrices that satisfy 7 in his equations 12.5.22 to 12.5.24 so we won't go through that again here. What's important to remember is that these matrices are block diagonal matrices consisting of a series of blocks of dimension $(2j+1)\times(2j+1)$ for $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. Each of these blocks satisfies 7 on its own, so we can pick the block with the right dimension to satisfy the experimental result that the electron has two spin states: $\pm\frac{\hbar}{2}$. That is, for the electron, we have the number of components in the wave $n = 2$, so we choose $j = \frac{1}{2}$ for the spin operators, which turn out to be the familiar ones we've met before:

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

$$S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{11}$$

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{12}$$

The complete wave function of an electron is therefore the product of a function of position with a two-component vector, called a *spinor*, which represents the spin state. That is, we can write, in the position-spin basis

$$|\psi\rangle = \psi_+(\mathbf{r})\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \psi_-(\mathbf{r})\begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{13}$$

In terms of Hilbert space, the spatial components are essentially the infinite-dimensional vectors ψ_+ and ψ_- which have values defined at each point in

3-d space, while the spinor components are 2-d vectors. Thus the complete Hilbert space $\mathbb{V}_e$ of an electron is defined as

$$\mathbb{V}_e = \mathbb{V}_0 \otimes \mathbb{V}_s \tag{14}$$

where $\mathbb{V}_0$ is the infinite-dimensional spatial component and $\mathbb{V}_s$ is the 2-d spinor component. In terms of this space, we can create a unit operator as a sum over a complete set of states:

$$\mathbf{1} = \sum_{s_z} \int |xyzs_z\rangle \langle xyzs_z| \, dx \, dy \, dz \tag{15}$$

The normalization condition for a wave function thus becomes

$$1 = \langle \psi | \psi \rangle = \sum_{s_z} \int \langle \psi | xyzs_z \rangle \langle xyzs_z | \psi \rangle \, dx \, dy \, dz \tag{16}$$

$$= \int \left(|\psi_+|^2 + |\psi_-|^2 \right) dx \, dy \, dz \tag{17}$$

where we get the last line by substituting 13. The term

$$\int |\psi_+|^2 \, dx \, dy \, dz \tag{18}$$

represents the probability that the electron will be found in the spin state $+\frac{\hbar}{2}$ anywhere in space.

The important point to remember from this derivation is that spin is an essentially new phenomenon with no classical analogue. Thus the wave function for a particle that has spin is necessarily an expanded Hilbert space where the extra subspace $\mathbb{V}_s$ is introduced to allow the extra spin states. The two spaces $\mathbb{V}_0$ and $\mathbb{V}_s$ are completely separate from each other, with each possessing its own operators, eigenstates and eigenvalues. Of course, it's possible to construct operators that are composed of other operators from both spaces, but we'll leave that until later.

One final point is worth making. The above derivation of the Hilbert space for an electron relied on the experimental result that the electron has exactly two spin states, thus leading to the 2×2 spin matrices. This is the best we can do in non-relativistic quantum theory. Shankar promises us that when we study the Dirac equation, which arose out of the need to introduce special relativity, the two spin states of the electron can actually be derived.