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# Applying classical geometry intuition to quantum spin

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## Abstract

Using concepts of geometric orthogonality and linear independence, we logically deduce the form of the Pauli spin matrices and the relationships between the three spatially orthogonal basis sets of the spin-1/2 system. Rather than a mathematically rigorous derivation, the relationships are found by forcing expectation values of the different basis states to have the properties we expect of a classical, geometric coordinate system. The process highlights the correspondence of quantum angular momentum with classical notions of geometric orthogonality, even for the inherently non-classical spin-1/2 system. In the process, differences in and connections between geometrical space and Hilbert space are illustrated.

Keywords: spin, quantum mechanics, orthogonality

(Some figures may appear in colour only in the online journal)

## 1. Introduction

It is possible to find the Pauli spin matrices and the corresponding geometrically orthogonal basis sets for the spin-1/2 system using arguments from classical geometry. Like the vector model [1, 2], this undertaking leverages classical understanding to build intuition for quantum angular momentum. But rather than using a semi-classical model, our approach uses completely quantum spin states. It involves the application of classical principles to expectation

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values, in a manner similar to Ehrenfest's theorem [3, 4]. The technique can provide valuable insight for anyone with an advanced undergraduate or introductory graduate understanding of quantum mechanics.

This method illuminates the correspondence between Hilbert space, which is used to mathematically describe quantum states, and the geometrical space we use in classical descriptions of angular momentum. It makes connections between the parameters used to define a Cartesian coordinate system and the free parameters selected when defining geometrically orthogonal sets of basis states to describe a quantum spin-1/2 particle. The procedure clarifies some common misconceptions about the quantum picture of angular momentum, in particular the confusion students often have distinguishing between geometric and Hilbert space, discussed in [5]. It does not explain the *why* of quantum spin, but focuses on how we *work with* quantum angular momentum states.

There are several rigorous ways to derive the well-known relationships between the  $x$ ,  $y$ , and  $z$  basis sets of the spin-1/2 system and the corresponding Pauli matrices. These include the use of rotation operations [6, 7], ladder operators [8], direct diagonalization [9], or symmetry arguments [10, 11]. Here we *deduce*, rather than *derive*, the relationships.

We limit our discussion to a spin-1/2 system for simplicity and clarity. This also avoids dealing with different types of unbiased states [12]. For example, as discussed later, for a spin-1/2 particle described using the  $z$  basis, the only states with a zero expectation value of the  $z$  component of angular momentum are ones made of an equal superposition of spin up and spin down. For a spin-1 particle, this is not only achieved with an equal superposition of  $m = -1$  and  $m = 1$ , but also with the  $m = 0$  basis state, or any combination of all states for which the  $-1$  and  $1$  basis states have amplitudes of equal size.

The canonical spin-1/2 system illustrates the universality of the core principle behind Ehrenfest's theorem, even in systems with no classical analogue [13, 14]; even though you cannot explain an electron's intrinsic angular momentum as the result of physical rotation in the classical sense, the expectation values of a spin-1/2 system do obey principles of classical geometry. While the *origin* of spin cannot be described semi-classically, classical intuition *can* be applied to better understand the *consequences* of spin.

## 2. Quantum spin-1/2 formalism

It is common to describe spin-1/2 particles using a basis consisting of the two eigenstates of the  $z$ -component of angular momentum,  $|\uparrow_z\rangle$  and  $|\downarrow_z\rangle$ . In vector notation, we can write these states as

$$|\uparrow_z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |\downarrow_z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1)$$

We will use the  $z$  basis as our starting point to deduce the form of the Pauli spin matrices and find the relationships between the  $x$ ,  $y$ , and  $z$  basis states.

We assume that the  $z$  basis exists and that every possible state of our particle can be expressed as a sum of these two states in the form

$$|\psi\rangle = a |\uparrow_z\rangle + b |\downarrow_z\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \quad (2)$$

where  $a$  and  $b$  are scalar, potentially complex, constants.

In matrix notation, the operators that yield information about the  $x$ ,  $y$ , and  $z$  components of spin can be written as  $\hbar/2$  times the Pauli spin matrices. The Pauli spin matrix  $\sigma_z$  can be easily found by noting that it is the matrix for which  $|\uparrow_z\rangle$  and  $|\downarrow_z\rangle$  are the eigenvectors with

eigenvalues of  $+1$  and  $-1$ . This gives us the matrix

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3)$$

If we measure the  $z$ -component of angular momentum for a spin-1/2 particle in an arbitrary state, we will always get either plus or minus  $\hbar/2$ , with probabilities of  $a^*a$  and  $b^*b$  if the state is normalised. To predict the outcome of a measurement along a *different* axis, we can write our quantum state in terms of the eigenstates of the component of angular momentum we plan to measure. Since the  $z$  axis is chosen arbitrarily, we know that a pair of eigenstates of *any* component of angular momentum along *any* axis must exist and have similar properties to the  $z$  basis states.

Two special basis sets are made up of the eigenstates of angular momentum along the  $x$  and  $y$  axes, respectively. Because the  $z$  basis forms a complete set, we should be able to write these basis states in terms of the  $z$  states<sup>2</sup>. We will start by writing the  $x$  basis states as

$$|\uparrow_x\rangle = A|\uparrow_z\rangle + B|\downarrow_z\rangle \quad \text{and} \quad (4)$$

$$|\downarrow_x\rangle = C|\uparrow_z\rangle + D|\downarrow_z\rangle, \quad (5)$$

where  $A$ ,  $B$ ,  $C$ , and  $D$  are constants. We can deduce what these constants must be simply by considering what properties these states should have. In the process, we will see connections between physical (geometric) space and Hilbert space.

### 3. Orthogonality

To find  $A$  and  $B$  in equation (4) we note that a classical particle with its angular momentum in the  $x$  direction will have no component of angular momentum in the  $z$  direction. For a quantum spin-1/2 particle we will *always* measure the  $z$  component to be  $\pm\hbar/2$ , never zero, regardless of the particle's state. So rather than mapping our intuition of geometrical orthogonality onto possible measurement outcomes, we will make our  $x$  basis states geometrically orthogonal to  $z$  by setting the *expectation value* of the  $z$  component of angular momentum to zero.

For the expectation value to be zero, it must be exactly as likely to measure the  $z$  component of spin to be  $-\hbar/2$  as it is to measure  $+\hbar/2$ , such that the two possibilities cancel each other out. As such, we intuitively expect that  $|\uparrow_x\rangle$  should be an equal superposition of  $|\uparrow_z\rangle$  and  $|\downarrow_z\rangle$ .

To show this more rigorously, we use the operator

$$S_z = \frac{\hbar}{2}(|\uparrow_z\rangle\langle\uparrow_z| - |\downarrow_z\rangle\langle\downarrow_z|) = \frac{\hbar}{2}\sigma_z \quad (6)$$

to find the expectation value of the  $z$  component of angular momentum. Using this operator, we get

$$\langle\uparrow_x|S_z|\uparrow_x\rangle = \frac{\hbar}{2}(A^*A - B^*B). \quad (7)$$

We require that this expectation value be zero, such that

$$A^*A - B^*B = |A|^2 - |B|^2 = 0. \quad (8)$$

<sup>2</sup> And, likewise, since the  $x$  and  $y$  basis sets will be complete, we should be able to write the  $z$  basis states in terms of the  $x$  or  $y$  basis states.

As we expected,  $A$  and  $B$  must have the same magnitude, giving an equal superposition of  $|\uparrow_z\rangle$  and  $|\downarrow_z\rangle$ . But the complex phases of  $A$  and  $B$  are unrestricted. So the most general form for  $|\uparrow_x\rangle$ , subject only to the limitation that it be normalised and geometrically orthogonal to the  $z$  basis states, is

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}[e^{i\phi_1}|\uparrow_z\rangle + e^{i\phi_2}|\downarrow_z\rangle], \quad (9)$$

where  $\phi_1$  and  $\phi_2$  are arbitrary real constants.

It makes sense that we get one arbitrary phase angle, since quantum mechanics always allows us an arbitrary overall phase factor. But why two? There's a geometric explanation for this freedom. After defining the  $z$  axis of a Cartesian coordinate system, the  $x$  axis can point in any one of an infinite number of directions which are orthogonal to  $z$ . These choices can be parametrised by an angle relative to some reference direction, as shown in figure 1.

We will set  $\phi_1$  and  $\phi_2$  to zero—both for simplicity and because it gives us the conventional form of the basis state

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}[|\uparrow_z\rangle + |\downarrow_z\rangle]. \quad (10)$$

#### 4. Linear independence

To find  $|\downarrow_x\rangle$  we note that it, too, must be geometrically orthogonal to the  $z$  basis. So it must have the form

$$|\downarrow_x\rangle = \frac{1}{\sqrt{2}}[e^{i\phi_3}|\uparrow_z\rangle + e^{i\phi_4}|\downarrow_z\rangle]. \quad (11)$$

We find an additional constraint when we consider that the  $x$  basis states *could* have been the  $z$  basis states had we simply chosen a different direction for our  $z$  axis. As such, since our  $z$  basis states are orthogonal to each other, we expect the two states in the  $x$  basis to be orthogonal to each other as well.

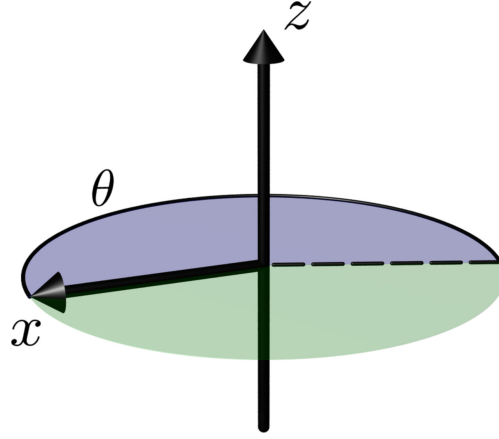
As is often done, we have unfortunately used the word ‘orthogonal’ to mean two different things. When we say that the  $x$  states must be orthogonal to the  $z$  states, we are referring to geometric orthogonality. But when we say that the  $x$  states must be orthogonal to each other, we refer to *orthogonality in Hilbert space* or *linear independence*. Just as a dot product of zero assures geometric orthogonality, an inner product  $\langle\uparrow_x|\downarrow_x\rangle = 0$  guarantees that  $|\uparrow_x\rangle$  and  $|\downarrow_x\rangle$  are linearly independent, such that one cannot be written in terms of the other.

The inner product of the  $x$  basis states is

$$\begin{aligned} \langle\uparrow_x|\downarrow_x\rangle &= \frac{1}{2}[\langle\uparrow_z| + \langle\downarrow_z|][e^{i\phi_3}|\uparrow_z\rangle + e^{i\phi_4}|\downarrow_z\rangle] \\ &= \frac{1}{2}(e^{i\phi_3} + e^{i\phi_4}). \end{aligned} \quad (12)$$

For this to be zero, the two phases must differ by  $\pi$  radians. If we choose the arbitrary global quantum phase of this state such that  $\phi_3 = 0$ , both for simplicity and by convention, we find that  $e^{i\phi_4} = -1$  and

$$|\downarrow_x\rangle = \frac{1}{\sqrt{2}}[|\uparrow_z\rangle - |\downarrow_z\rangle]. \quad (13)$$



**Figure 1.** Once the  $z$  axis of a Cartesian coordinate system is selected, there are still an infinite number of possible choices for the  $x$  axis which are all orthogonal to  $z$ . These choices are parametrised by the variable  $\theta$  in the figure.

Knowing the form of  $|\uparrow_x\rangle$  and  $|\downarrow_x\rangle$ , it is simple to show that the Pauli spin matrix  $\sigma_x$  is given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (14)$$

## 5. The $y$ basis

Just as we saw for the  $x$  basis states, for the  $y$  basis states to be normalised and geometrically orthogonal to the  $z$  axis, they must have the form

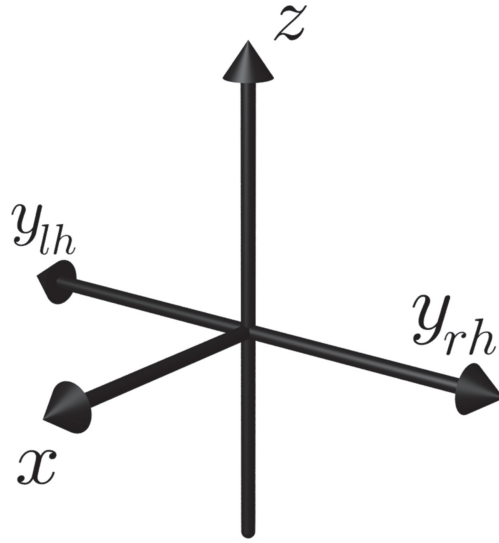
$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}}[e^{i\phi_5}|\uparrow_z\rangle + e^{i\phi_6}|\downarrow_z\rangle], \quad (15)$$

$$|\downarrow_y\rangle = \frac{1}{\sqrt{2}}[e^{i\phi_7}|\uparrow_z\rangle + e^{i\phi_8}|\downarrow_z\rangle]. \quad (16)$$

Since we have the freedom to multiply each state by an arbitrary overall phase factor, for simplicity (and to arrive at the canonical form of the states), we can set  $\phi_5$  and  $\phi_7$  to zero. The other phase angles are constrained by that fact that, in addition to being geometrically orthogonal to  $z$ , these states must also be geometrically orthogonal to the  $x$  axis we have defined.

The operator which gives us information about the  $x$  component of spin can be found by noting that, when written in the  $x$  basis, this operator should look similar to  $S_z$  represented in the  $z$  basis:

$$S_x = \frac{\hbar}{2}(|\uparrow_x\rangle\langle\uparrow_x| - |\downarrow_x\rangle\langle\downarrow_x|). \quad (17)$$



**Figure 2.** Once the  $x$  and  $z$  axes are selected, there are still two possible choices for the  $y$  direction. One choice, labelled  $y_{lh}$  in the figure, will result in a left-handed coordinate system. The other choice results in a right-handed coordinate system.

To write this in the  $z$  basis we plug in equations (10) and (13) to get

$$S_x = \frac{\hbar}{2} (| \uparrow_z \rangle \langle \downarrow_z | + | \downarrow_z \rangle \langle \uparrow_z | ) = \frac{\hbar}{2} \sigma_x. \quad (18)$$

We can use  $S_x$  to find the expectation value of the  $x$  component of angular momentum for a particle in the state  $| \uparrow_y \rangle$ :

$$\langle \uparrow_y | S_x | \uparrow_y \rangle = \frac{\hbar}{4} (e^{i\phi_6} + e^{-i\phi_6}) = \frac{\hbar}{2} \cos(\phi_6). \quad (19)$$

If we want  $| \uparrow_y \rangle$  to be geometrically orthogonal to the  $x$  states then this must be zero, implying that  $\phi_6 = \pm\pi/2$  and giving us only two unique possibilities:

$$| \uparrow_y \rangle = \frac{1}{\sqrt{2}} [ | \uparrow_z \rangle \pm i | \downarrow_z \rangle ]. \quad (20)$$

As we discuss in the next section, the choice of whether to use the upper or lower sign is not arbitrary, so we will not select one over the other just yet.

Applying the same condition to  $| \downarrow_y \rangle$  and forcing the inner product  $\langle \uparrow_y | \downarrow_y \rangle$  to be zero gives us

$$| \downarrow_y \rangle = \frac{1}{\sqrt{2}} [ | \uparrow_z \rangle \mp i | \downarrow_z \rangle ]. \quad (21)$$

## 6. Coordinate system handedness

There is a geometric explanation for the two possible choices in equations (20) and (21). In a Cartesian coordinate system, once the  $z$  and  $x$  axes have been selected, there are still two

possible directions for  $y$ . As illustrated in figure 2, one direction results in a right-handed and the other in a left-handed coordinate system.

We can find the handedness of a geometric coordinate system with cross products. For example, if  $\hat{n}_j$  is a unit vector along the  $j$ th axis, then for a right-handed coordinate system using a right-handed cross product,  $\hat{n}_x \times \hat{n}_y = \hat{n}_z$ . For a left-handed coordinate system we get a minus sign:  $\hat{n}_x \times \hat{n}_y = -\hat{n}_z$ .

Similarly, we can find the ‘handedness’ of the Pauli spin matrices by noting that the Pauli matrices, multiplied by a constant and combined with the  $(2 \times 2)$  identity matrix, form the basis of the  $SU(2)$  Lie group [15]. Then we can evaluate Lie brackets, which are analogous to cross products. If we evaluate the Lie bracket of  $\sigma_z/2$  with  $\sigma_x/2$ , we get

$$\left[ \frac{1}{2}\sigma_z, \frac{1}{2}\sigma_x \right] = \frac{i}{2}\sigma_{y+} = -\frac{i}{2}\sigma_{y-}, \quad (22)$$

where  $\sigma_{y+}/\sigma_{y-}$  is the Pauli spin matrix we get if we choose the upper/lower sign for equations (20) and (21). The change in sign in equation (22) is just what we would expect when going from a right- to a left-handed coordinate system.

Similarly, there is a link between the Pauli matrices and quaternions [16–18], and between cross products and commutators in quaternion algebra [19]. This suggests a connection between cross products in geometric space and commutators in Hilbert space.

Because there is no spatial representation of the spin-1/2 particle’s angular momentum operator, we will make an analogy with the orbital angular momentum operator [20]:

$$\vec{L} = \vec{r} \times \vec{p}. \quad (23)$$

Here  $\vec{r}$  is the position and  $\vec{p}$  the momentum operator. Assuming a right-handed coordinate system, the components of  $\vec{L}$  are

$$L_x = yp_z - zp_y, \quad (24)$$

$$L_y = zp_x - xp_z, \quad (25)$$

$$L_z = xp_y - yp_x. \quad (26)$$

We can use these components to calculate the commutator of  $L_x$  with  $L_y$ . Noting that position and linear momentum operators commute with operators for orthogonal spatial dimensions and that  $[z, p_z] = i\hbar$ , it is easy to show that  $[L_x, L_y] = i\hbar L_z$ . If we had chosen a left-handed coordinate system (but still used a right-handed cross product), we would have gotten the same result but with a minus sign.

By analogy, we may suppose that a right-handed coordinate system for a spin-1/2 particle is the one that results in the commutation relation

$$[S_x, S_y] = i\hbar S_z, \quad (27)$$

while a left-handed coordinate system would result in a minus sign in the commutation relation. We get the commutation relation in equation (27) if we choose the upper sign in equations (20) and (21):

$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}}[|\uparrow_z\rangle + i|\downarrow_z\rangle], \quad (28)$$

$$|\downarrow_y\rangle = \frac{1}{\sqrt{2}}[|\uparrow_z\rangle - i|\downarrow_z\rangle]. \quad (29)$$

From these, the Pauli matrix  $\sigma_y$  can be found:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (30)$$

This is the last piece of the puzzle, and we have now ‘deduced’ the relationships between the  $x$ ,  $y$ , and  $z$  basis states as well as the Pauli matrices for the spin-1/2 system.

## 7. Conclusion

We deduced the Pauli matrices and the relationships between the  $x$ ,  $y$ , and  $z$  basis states for a spin-1/2 particle using the concepts of geometric orthogonality and linear independence. By insisting that the two states in the  $x$  basis be normalized, geometrically orthogonal to the  $z$  states, and orthogonal to each other in Hilbert space (linearly independent), we arrived at expressions which were completely specified except for three arbitrary phase angles—two due to arbitrary overall phase factors, and a third related to choosing the direction for the  $x$  axis for a given selection of  $z$  axis direction in a Cartesian coordinate system.

With the  $y$  basis we had less freedom because the states had to be geometrically orthogonal to both the  $z$  and the  $x$  basis states. We again had an arbitrary overall phase factor for each basis state. But we only had two possible choices for the remaining phase factors, similar to the choice of handedness in a Cartesian coordinate system. We determined handedness by making a connection between cross products and commutators.

This intuitive exercise illustrates the connection between classical geometric space and quantum Hilbert space, even for spin-1/2 systems, which are intrinsically not classical.

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