VIB. Simulating Spin Operators and Spin Space

LibreTexts: *Introductory Quantum Mechanics - Spin Operators*

The basic principles of quantum theory can be demonstrated very simply by exploring the properties of electron spin using Heisenberg's formulation of quantum mechanics which is usually referred to as matrix mechanics. The matrix formulation provides clear illustrations of the following essential quantum mechanical concepts: eigenvector, operator, eigenvalue, expectation value, the linear superposition, and the commutation relations.

Four quantum numbers are required to describe an electron in quantum mechanics. The last of these is the spin quantum number, s. The electron has a spin component in the x-, y-, and z-directions and for each of these directions the electron can have a value of ↑ spin-up or ↓ spin-down, or +1 and -1 in units of h/4π.
These six spin states, $S_{\alpha\beta}$, are represented by vectors as is shown below.

XY Z Axes Spin States (Up and Down) and Operators: Math

Transpose of Complex Conjugate (Shift")^T

$$S_{xu} := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\1\end{pmatrix} \qquad S_{xd} := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-1\end{pmatrix} \qquad \left(\overline{S_{xu}}\right)^T = (0.707 \quad 0.707) \qquad \left(\overline{S_{xd}}\right)^T = (0.707 \quad -0.707)$$

$$S_{yu} := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\i\end{pmatrix} \qquad S_{yd} := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-i\end{pmatrix} \qquad \left(\overline{S_{yu}}\right)^T = (0.707 \quad -0.707i) \qquad \left(\overline{S_{yd}}\right)^T = (0.707 \quad 0.707i)$$

$$S_{zu} := \begin{pmatrix}1\\0\end{pmatrix} \qquad S_{zd} := \begin{pmatrix}0\\1\end{pmatrix} \qquad \left(\overline{S_{zu}}\right)^T = (1 \quad 0) \qquad \left(\overline{S_{zd}}\right)^T = (0 \quad 1)$$

Let's look at the the **y-direction spin states because they are complex**, and therefore are slightly more difficult to deal with. In Dirac notation these four bra and ket ***y*** vectors are written as $|S_{yu}\rangle$, $|S_{yd}\rangle$, $\langle S_{yu}|$, and $\langle S_{yd}|$. Note that the **bra-vectors are the transpose of the complex conjugate of the ket-vectors**. It is also easy to show that these spin vectors in the x-, y-, and z-directions form orthonormal basis sets. That means they are normalized and orthogonal to each other.

$$\left(\overline{S_{xu}}\right)^T\cdot S_{xu} = 1 \qquad \left(\overline{S_{xd}}\right)^T\cdot S_{xd} = 1 \qquad \left(\overline{S_{xu}}\right)^T\cdot S_{xd} = 0$$

$$\left(\overline{S_{yu}}\right)^T\cdot S_{yu} = 1 \qquad \left(\overline{S_{yd}}\right)^T\cdot S_{yd} = 1 \qquad \left(\overline{S_{yu}}\right)^T\cdot S_{yd} = 0$$

$$\left(\overline{S_{zu}}\right)^T\cdot S_{zu} = 1 \qquad \left(\overline{S_{zd}}\right)^T\cdot S_{zd} = 1 \qquad \left(\overline{S_{zu}}\right)^T\cdot S_{zd} = 0$$

In Dirac notation we would write the first row as: $\langle S_{xu}|S_{xu}\rangle = \langle S_{xd}|S_{xd}\rangle = 1$, $\langle S_{xu}|S_{xd}\rangle = 0$. In other words the **projection of the spin states onto themselves is 1** (normalized) and the projection onto the other state is zero (orthogonal). Momentum is only in one direction. Spin can only be ↑ or ↓.

The calculations above for the y-direction spin vectors are shown explicitly below.

$$(0.707 \quad -.707i)\cdot\begin{pmatrix}.707\\.707i\end{pmatrix} = 1 \qquad (0.707 \quad .707i)\cdot\begin{pmatrix}.707\\-.707i\end{pmatrix} = 1 \qquad (0.707 \quad -.707i)\cdot\begin{pmatrix}.707\\-.707i\end{pmatrix} = 0$$

It is easy to show that **x- and z-spin states are not orthogonal** to one another. Any two different spin directions are not orthogonal. $\langle S_{xu}|S_{zu}\rangle = 0.707$, for example. **This is a 45° angle.**

$$\left(\overline{S_{xu}}\right)^T \cdot S_{zu} = 0.707 \quad \left(\overline{S_{xu}}\right)^T \cdot S_{zd} = 0.707 \quad \left(\overline{S_{xd}}\right)^T \cdot S_{zu} = 0.707 \quad \left(\overline{S_{xd}}\right)^T \cdot S_{zd} = -0.707$$

This of course means that, for example, $|S_{xu}\rangle$ and $|S_{xd}\rangle$ can be written as linear superpositions of $|S_{zu}\rangle$ and $|S_{zd}\rangle$, and $|S_{zu}\rangle$ and $|S_{zd}\rangle$ can be written as linear superpositions of $|S_{xu}\rangle$ and $|S_{xd}\rangle$.

$$S_{xu} = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{zu} + \frac{1}{\sqrt{2}} \cdot S_{zd} = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \quad S_{xd} = \begin{pmatrix} 0.707 \\ -0.707 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{zu} - \frac{1}{\sqrt{2}} \cdot S_{zd} = \begin{pmatrix} 0.707 \\ -0.707 \end{pmatrix}$$

$$S_{zu} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{xu} + \frac{1}{\sqrt{2}} \cdot S_{xd} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad S_{zd} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{xu} - \frac{1}{\sqrt{2}} \cdot S_{xd} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The concept of the linear superposition is central in quantum theory and has no classical analog. For example, if by measurement an electron is found to have spin-up in the z-direction, this means that the electron does not have a definite spin in either the x- or the y-direction because $|S_{zu}\rangle$ is a linear superposition of the x- and y-direction spin states.

$$S_{zu} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{xu} + \frac{1}{\sqrt{2}} \cdot S_{xd} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{yu} + \frac{1}{\sqrt{2}} \cdot S_{yd} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

In spite of its appearance, **a linear superposition is not a mixture**. In other words $|S_{zu}\rangle$ is not 50% $|S_{xu}\rangle$ and 50% $|S_{xd}\rangle$, or 50% $|S_{yu}\rangle$ and 50% $|S_{yd}\rangle$.

Another central dogma of quantum theory is that the wavefunction or state vector contains all the physical information available for the system. Quantum mechanics therefore consists, in large part, of extracting physical information from the wavefunction or state vector. Quantum mechanics consists of a small set of rules for carrying this procedure out mathematically.

For every observable of the system there is an operator. Since electrons can spin in the x-, y-, or z-directions, there are spin operators in those directions, or for that matter in any other arbitrary direction you might think of. In quantum mechanics **states are vectors and operators are matrices.** The spin operators in units of $h/4\pi$ are shown below. Note that squaring these operators gives the identity operator.

$$S_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$S_x^{\,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad S_y^{\,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad S_z^{\,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

For example, the square of the total spin operator in units of $h/4\pi$ is

$$S_{xyz} := S_x^{\,2} + S_y^{\,2} + S_z^{\,2} \qquad S_{xyz} = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}$$

A measurement operator extracts information about the system by operating on the wavefunction or state vector. One possible outcome is that the operation returns the state vector multiplied by a numerical constant. For example,

$$S_x \cdot S_{xu} = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \qquad S_x \cdot S_{xd} = \begin{pmatrix} -0.707 \\ 0.707 \end{pmatrix} \qquad S_y \cdot S_{yu} = \begin{pmatrix} 0.707 \\ 0.707i \end{pmatrix} \qquad S_y \cdot S_{yd} = \begin{pmatrix} -0.707 \\ 0.707i \end{pmatrix}$$

$$S_z \cdot S_{zu} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad S_z \cdot S_{zd} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} \qquad \text{or, for example:} \qquad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

In Dirac notation we would summarize these calculations as follows: $\mathbf{S_x}|S_{xu}\rangle = +1|S_{xu}\rangle$, $\mathbf{S_x}|S_{xd}\rangle = -1|S_{xd}\rangle$, $\mathbf{S_y}|S_{yu}\rangle = +1|S_{yu}\rangle$, $\mathbf{S_y}|S_{yd}\rangle = -1|S_{yd}\rangle$, $\mathbf{S_z}|S_{zu}\rangle = +1|S_{zu}\rangle$, $\mathbf{S_z}|S_{zd}\rangle = -1|S_{zd}\rangle$. In each of these cases, the state vector is an eigenfunction of the measurement operator with eigenvalue of either +1 or -1 (in units of $h/4\pi$). We say, for example, that $|S_{xu}\rangle$ is an eigenfunction of $\mathbf{S_x}$ with eigenvalue +1. The electron has a well-defined value for spin in the x-direction (spin-up) and subsequent measurements of the x-direction spin will yield the value of +1 as long as no intervening measurements in another spin direction are made.

The other possible outcome of the measurement operation is that it yields another state vector.

$$S_x \cdot S_{yu} = \begin{pmatrix} 0.707i \\ 0.707 \end{pmatrix} \qquad S_x \cdot S_{yd} = \begin{pmatrix} -0.707i \\ 0.707 \end{pmatrix} \qquad S_x \cdot S_{zu} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad S_x \cdot S_{zd} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$S_y \cdot S_{xu} = \begin{pmatrix} -0.707i \\ 0.707i \end{pmatrix} \qquad S_y \cdot S_{xd} = \begin{pmatrix} 0.707i \\ 0.707i \end{pmatrix} \qquad S_y \cdot S_{zu} = \begin{pmatrix} 0 \\ i \end{pmatrix} \qquad S_y \cdot S_{zd} = \begin{pmatrix} -i \\ 0 \end{pmatrix}$$

$$S_z \cdot S_{xu} = \begin{pmatrix} 0.707 \\ -0.707 \end{pmatrix} \qquad S_z \cdot S_{xd} = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \qquad S_z \cdot S_{yu} = \begin{pmatrix} 0.707 \\ -0.707i \end{pmatrix} \qquad S_z \cdot S_{yd} = \begin{pmatrix} 0.707 \\ 0.707i \end{pmatrix}$$

In Dirac notation these operations appear as: $\mathbf{S_x}|S_{yu}\rangle = i|S_{yd}\rangle$, $\mathbf{S_x}|S_{yd}\rangle = -i|S_{yu}\rangle$, $\mathbf{S_x}|S_{zu}\rangle = |S_{zd}\rangle$, $\mathbf{S_x}|S_{zd}\rangle = |S_{zu}\rangle$, etc. In each case the resulting vector is different than the vector operated on. We say, for example, $|S_{yu}\rangle$ is not an eigenfunction of $\mathbf{S_x}$, and therefore an electron in this state does not have a definite value for spin in the x-direction. X-direction spin measurements on a system known to be in state $|S_{yu}\rangle$ will yield completely random results.

To put it another way, quantum mechanical principles state that a system can be in a well-defined state, $|S_{yu}\rangle$, and yet the outcome of all experiments are not uniquely determined. While a measurement of spin in the y-direction will yield a predictable result, +1, measurement of spin in the x- or z-direction is completely unpredictable and all we can calculate is the average value, or expectation value for a large number of measurements. This is completely different than classical physics where if you know the state of the system, you know the values of all physical observables.

Let's review these concepts by taking a specific example. The electron is in the state $|S_{xu}>$ and we wish to measure $\mathbf{S_z}$. According to quantum mechanical procedures the average value for a statistically meaningful number of measurements is zero - $<S_{xu}|\mathbf{S_z}|S_{xu}> = 0$. The eigenstates (eigenfunctions) for $\mathbf{S_z}$ are $|S_{zu}>$ and $|S_{zd}>$ with eigenvalues +1 and -1, respectively. As the first two entries above show, the probability that an electron in state $|S_{xu}>$ will be found in $|S_{zu}>$ with eigenvalue +1 is 0.5, and the probability that it will be found in state $|S_{zd}>$ with eigenvalue -1 is 0.5. Thus, the **average value** is **expected** to be zero, and the two ways of determining the average or expectation value of a measurement are consistent and equivalent.

There is yet another way to look at this issue. In quantum mechanics for most pairs of observables the order of measurement is important. Quantum mechanical operators don't generally commute. For example, as shown below, $\mathbf{S_xS_y}|S_{zu}>$ does not equal $\mathbf{S_yS_x}|S_{zu}>$. This means that if the electron is in the state $|S_{zu}>$ the combined operators $\mathbf{S_xS_y}$ and $\mathbf{S_yS_x}$ yield different measurement results.

$$S_x \cdot S_y \cdot S_{zu} = \begin{pmatrix} i \\ 0 \end{pmatrix} \qquad S_y \cdot S_x \cdot S_{zu} = \begin{pmatrix} -i \\ 0 \end{pmatrix} \qquad \left(S_x \cdot S_y - S_y \cdot S_x\right) \cdot S_{zu} = \begin{pmatrix} 2i \\ 0 \end{pmatrix}$$

Operators that do not commute have incompatible eigenstates. If a state vector is an eigenstate of one of the operators, it is not an eigenstate of the other. The fact that **Sx** and **Sy** do not commute means that an electron cannot simultaneously have well-defined values for S_x and S_y. It is not surprising that there is a **deep connection between these properties of operators** and **the Uncertainty Principle**.

The commutators for the spin operators are shown below.

$$S_x \cdot S_y - S_y \cdot S_x = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} \qquad 2 \cdot i \cdot S_z = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} \qquad S_z \cdot S_x - S_x \cdot S_z = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}$$

$$S_y \cdot S_z - S_z \cdot S_y = \begin{pmatrix} 0 & 2i \\ 2i & 0 \end{pmatrix} \qquad 2 \cdot i \cdot S_x = \begin{pmatrix} 0 & 2i \\ 2i & 0 \end{pmatrix} \qquad 2 \cdot i \cdot S_y = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}$$

T**he Uncertainty Principle can also be illustrated** by calculating ΔSx and ΔSy for an electron known to be in the Szu state. Since we are working in units of h/4π, the uncertainty relation is: $\Delta S_x \cdot \Delta S_y \geq 1$.

$$\sqrt{S_{zu}{}^T \cdot S_x \cdot S_x \cdot S_{zu} - \left(S_{zu}{}^T \cdot S_x \cdot S_{zu}\right)^2} \cdot \sqrt{S_{zu}{}^T \cdot S_y \cdot S_y \cdot S_{zu} - \left(S_{zu}{}^T \cdot S_y \cdot S_{zu}\right)^2} = 1$$

We have been dealing with matrix operators and their associated eigenvectors and eigenvalues.

The eigenvectors and eigenvalues can be obtained:

from the matrix operators with the Math **eigenvecs** and **eigenvals** commands as is shown below.

$$eigenvals\left(S_x\right) = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad eigenvec\left(S_x, 1\right) = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \qquad eigenvec\left(S_x, -1\right) = \begin{pmatrix} -0.707 \\ 0.707 \end{pmatrix}$$

$$eigenvals\left(S_y\right) = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad eigenvecs\left(S_y\right) = \begin{pmatrix} -0.707i & 0.707 \\ 0.707 & -0.707i \end{pmatrix}$$

$$eigenvals\left(S_z\right) = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad eigenvecs\left(S_z\right) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$