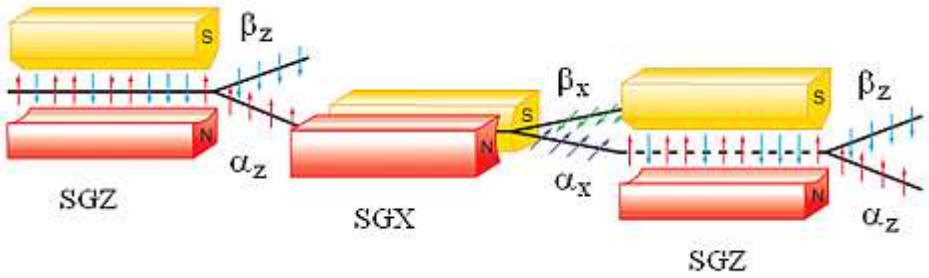
Analysis of the Stern-Gerlach Experiment - Discovery of Electron Spin, 1922

Quantum Chemistry, Thomas Engel



Quantum Computing, Jozef Gruska

The quantum theory explanation is the following one: Passing an atom through a magnetic field amounts to a measurement of its magnetic alignment, and until you make such a measurement there is no sense in saying what the atom's magnetic alignment might be only when you make a measurement do you obtain one of only two possible outcomes, with equal probability, and those two possibilities are defined by the direction of the magnetic field that you use to make the measurement.

Actually, no matter how the magnetic field was lined up, it always splits the beam of atoms into two. (An exception to this is, as a result of interference, is shown on page 23.) As if each atom was forced somehow to take up either one or the other of just two possible orientations, dictated by the alignment of the magnets.

Silver atoms are deflected by an inhomogeneous magnetic field because of the two-valued magnetic moment associated with their unpaired 5s electron ($[Kr]5s^1 4d^{10}$). The beam of silver atoms entering the Stern-Gerlach magnet oriented in the z-direction (SGZ) on the left is unpolarized. This means it is a **mixture** of randomly spin-polarized Ag atoms. As such, it is **impossible to write a quantum mechanical wavefunctio**n for this initial state. It was only after modern quantum mechanics was founded, beginning in 1925, that physicists realized that the silver atom's magnetism is produced not by the orbit of its outermost electron but by that **electron's intrinsic spin**, which makes it act like a tiny bar magnet.

This situation is exactly analogous to the **Three-Polarizer "Paradox"** demonstration described in a previous section. Light emerging from an incandescent light bulb is unpolarized, a mixture of all possible polarization angles, so we can't write a wave function for it. The first Stern-Gerlach magnet plays the same role as the first polarizer, it forces the Ag atoms into one of measurement eigenstates - spin-up or spin-down in the z-direction. The only difference is that in the three-polarizer demonstration only one state was created - vertical polarization. Both demonstrations illustrate an important quantum mechanical postulate - the only values that are observed in a measurement are the eigenvalues of the measurement operator.

To continue with the analysis of the Stern-Gerlach demonstration we need vectors to represent the various spin states of the Ag atoms. We will restrict our attention to the x- and z- spin directions, although the spin states for the y-direction are also available.

Spin Eigenfunctions

Spin-up in the z-direction: $\alpha_z := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ Spin-down in the z-direction: $\beta_z := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Spin-up in the x-direction: $\alpha_x := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ Spin-down in the x-direction: $\beta_x := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

After the SGZ magnet, the spin-up beam (deflected toward the magnet's north pole) enters a magnet oriented in the x-direction, SGX. The α_z beam splits into α_x and β_x beams of equal intensity. This is because it is a **superposition of the x-direction spin eigenstate**s as shown below.

$$\frac{1}{\sqrt{2}}\cdot\left[\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\1\end{pmatrix}+\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-1\end{pmatrix}\right]=\begin{pmatrix}1\\0\end{pmatrix}\qquad\frac{1}{\sqrt{2}}\cdot\left(\alpha_x+\beta_x\right)=\begin{pmatrix}1\\0\end{pmatrix}$$

Next the a_x beam is directed toward a second SGZ magnet and splits into two equal a_z and b_z beams. This happens because a_x is a superposition of the a_z and b_z spin states.

$$\frac{1}{\sqrt{2}}\cdot\left[\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right]=\begin{pmatrix}0.707\\0.707\end{pmatrix}\qquad\frac{1}{\sqrt{2}}\cdot\left(\alpha_z+\beta_z\right)=\begin{pmatrix}0.707\\0.707\end{pmatrix}$$

Operators (Pauli)

We can also **use the Pauli operators** (in units of h/4π) to analyze this experiment. The matrix operators associated with the two Stern-Gelach magnets are shown below.

SGZ operator: $SGZ:=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ SGX operator: $SGX:=\begin{pmatrix}0&1\\1&0\end{pmatrix}$

NOTE: SGY operator: $SGY:=\begin{pmatrix}0&-i\\i&0\end{pmatrix}$

The spin states **a_z and b_z** are **eigenfunction**s of the SGZ operator with **eigenvalues +1 and -1**, respectively:

$$SGZ\cdot\alpha_z=\alpha_z\quad SGZ\cdot\alpha_z=\begin{pmatrix}1\\0\end{pmatrix}\quad\alpha_z=\begin{pmatrix}1\\0\end{pmatrix}\qquad SGZ\cdot\beta_z=-\beta_z\quad SGZ\cdot\beta_z=\begin{pmatrix}0\\-1\end{pmatrix}\quad-\beta_z=\begin{pmatrix}0\\-1\end{pmatrix}$$

The spin states **a_x and b_x** are **eigenfunction**s of the SGX operator with **eigenvalues +1 and -1**, respectively:

$$SGX\cdot\alpha_x=\alpha_x\quad SGX\cdot\alpha_x=\begin{pmatrix}0.707\\0.707\end{pmatrix}\quad\alpha_x=\begin{pmatrix}0.707\\0.707\end{pmatrix}\quad SGX\cdot\beta_x=-\beta_x\quad SGX\cdot\beta_x=\begin{pmatrix}-0.707\\0.707\end{pmatrix}$$

The spin states a_x and b_x are **not eigenfunctions of the SGZ operator** as is shown below.

$$SGZ\cdot\alpha_x=\beta_x\qquad SGZ\cdot\alpha_x=\begin{pmatrix}0.707\\-0.707\end{pmatrix}\qquad SGZ\cdot\beta_x=\alpha_x\qquad SGZ\cdot\beta_x=\begin{pmatrix}0.707\\0.707\end{pmatrix}\qquad\beta_x=\begin{pmatrix}0.707\\-0.707\end{pmatrix}$$

And, of course, the spin states a_z and b_z are **not eigenfunctions** of the SGX operator as is shown below.

$$SGX\cdot\alpha_z=\beta_z\qquad SGX\cdot\alpha_z=\begin{pmatrix}0\\1\end{pmatrix}\qquad\alpha_z=\begin{pmatrix}1\\0\end{pmatrix}\qquad SGX\cdot\beta_z=\alpha_z\quad SGX\cdot\beta_z=\begin{pmatrix}1\\0\end{pmatrix}\qquad\beta_z=\begin{pmatrix}0\\1\end{pmatrix}$$

The Predicted Results After the SGX Magnet

The probability that an a_z Ag atom will emerge spin-up after passing through a SGX magnet:

Note: *The **arrow symbol** → below is used to indicate evaluating an expression symbolically. Math returns the result as another expression in terms of the variable and symbols in the original problem.*

$$\left|\langle \alpha_x | SGX | \alpha_z \rangle\right|^2 = ½ \qquad \left(\left|\alpha_x{}^T \cdot SGX \cdot \alpha_z\right|\right)^2 \to \frac{1}{2}$$

The probability that an a_z Ag atom will emerge spin-down after passing through a SGX magnet:

$$\left|\langle \beta_x | SGX | \alpha_z \rangle\right|^2 = ½ \qquad \left(\left|\beta_x{}^T \cdot SGX \cdot \alpha_z\right|\right)^2 \to \frac{1}{2}$$

The Predicted Results After the Final SGZ Magnet

The probability that an a_x Ag atom will emerge spin-up after passing through a SGZ magnet:

$$\left|\langle \alpha_z | SGZ | \alpha_x \rangle\right|^2 = ½ \qquad \left(\left|\alpha_z{}^T \cdot SGZ \cdot \alpha_x\right|\right)^2 \to \frac{1}{2}$$

The probability that an a_x Ag atom will emerge spin-down after passing through a SGZ magnet:

$$\left|\langle \beta_z | SGZ | \alpha_x \rangle\right|^2 = ½ \qquad \left(\left|\beta_z{}^T \cdot SGZ \cdot \alpha_x\right|\right)^2 \to \frac{1}{2}$$

The Predicted Results for the First SGZ Magnet

Now we deal with the most difficult part of the analysis. How does quantum mechanics predict what will happen when an unpolarized spin beam encounters the initial SGZ magnet. As mention earlier, an unpolarized spin beam is a **mixture** of all possible spin polarizations. We proceed by introducing the density operator, which is a more general quantum mechanical construct that can be used to represent both pure states and mixtures, as shown below.

$$\hat{\rho}_{pure} = |\Psi\rangle\langle\Psi| \qquad \hat{\rho}_{mixed} = \sum p_i |\Psi_i\rangle\langle\Psi_i|$$

In the equation on the right, p_i is the fraction of the mixture in the state Y_i. It is not difficult to elucidate the origin of the density operator and its utility in quantum mechanical calculations. The expectation value for a pure state Y for the measurement operator A is traditionally written as follows.

$$\langle A \rangle = \langle \Psi | \hat{A} | \Psi \rangle$$

Expansion of Y in the eigenfunctions of the measurement operator, followed by rearrangement of the brackets yields the calculation of the expectation value of A in terms of the product of density operator and the measurement operator, A.

$$\langle A \rangle = \langle \Psi | \hat{A} | \Psi \rangle = \sum_a \langle \Psi | \hat{A} | a \rangle \langle a | \Psi \rangle = \sum_a \langle a | \Psi \rangle \langle \Psi | \hat{A} | a \rangle = \sum_a \langle a | \hat{\rho} \hat{A} | a \rangle = Trace\left(\hat{\rho} \hat{A}\right)$$

We now show that the traditional method and the method using the trace function give the same result for the z-direction spin eigenfunctions.

$$\alpha_z^T \cdot SGZ \cdot \alpha_z = 1 \qquad tr\left(\alpha_z \cdot \alpha_z^T \cdot SGZ\right) = 1$$

$$\beta_z^T \cdot SGZ \cdot \beta_z = -1 \qquad tr\left(\beta_z \cdot \beta_z^T \cdot SGZ\right) = -1$$

An unpolarized beam can be written as a 50-50 mixture of any of the orthogonal spin eigenfunctions - α_z and β_z, or α_x and β_x, or α_y and β_y. Thus, according to the previous definition the density operator for an unpolarized spin beam is as follows.

$$\hat{\rho}_{mix} = \frac{1}{2}|\alpha_z\rangle\langle\alpha_z| + \frac{1}{2}|\beta_z\rangle\langle\beta_z| = \frac{1}{2}|\alpha_x\rangle\langle\alpha_x| + \frac{1}{2}|\beta_x\rangle\langle\beta_x| = \frac{1}{2}|\alpha_y\rangle\langle\alpha_y| + \frac{1}{2}|\beta_y\rangle\langle\beta_y|$$

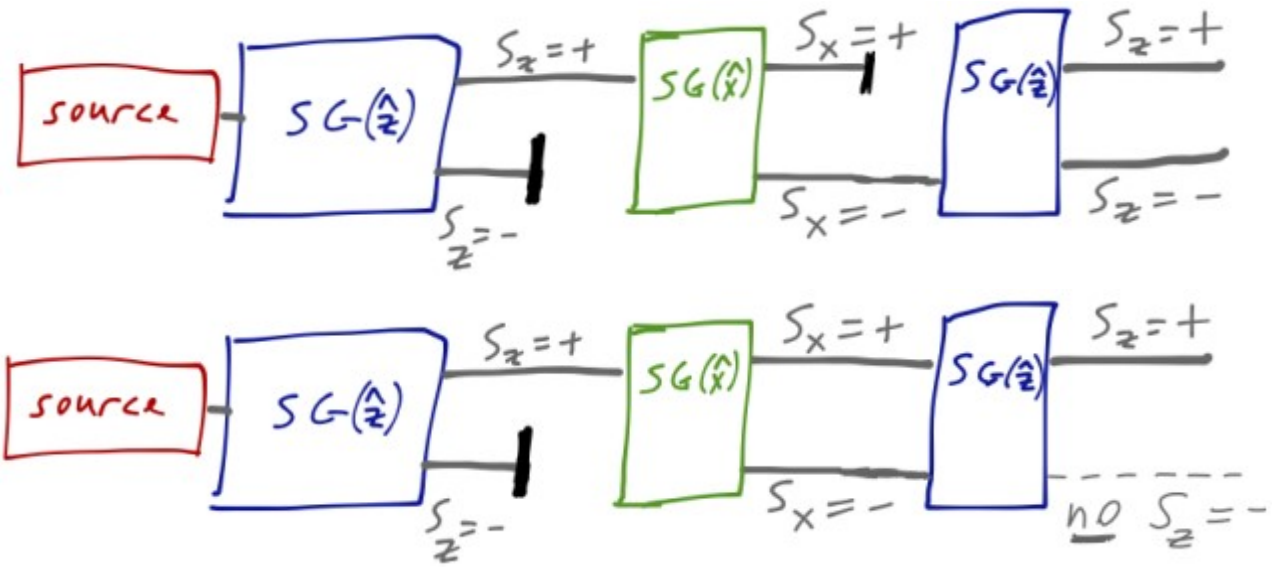
Fifty percent of the silver atoms are deflected toward the north pole (a_z, eigenvalue +1) and fifty percent toward the south pole (b_z, eigenvalue -1). Therefore, the expectation value should be zero as is calculated below using both z- and x- spin directions.

$$tr\left[\left(\frac{1}{2}\cdot\alpha_z\cdot\alpha_z^T + \frac{1}{2}\cdot\beta_z\cdot\beta_z^T\right)\cdot SGZ\right] = 0 \qquad tr\left[\left(\frac{1}{2}\cdot\alpha_x\cdot\alpha_x^T + \frac{1}{2}\cdot\beta_x\cdot\beta_x^T\right)\cdot SGZ\right] = 0$$

An equivalent method of obtaining the same result is shown below.

$$\frac{1}{2}\cdot\alpha_z^T\cdot SGZ\cdot\alpha_z + \frac{1}{2}\cdot\beta_z^T\cdot SGZ\cdot\beta_z = 0 \qquad \frac{1}{2}\cdot\alpha_z^T\cdot SGZ\cdot\alpha_z + \frac{1}{2}\cdot\beta_z^T\cdot SGZ\cdot\beta_z = 0$$

Superposition effects are evident when we start chaining them together:



The *disappearance* of the $S_z = -\hbar/2$ component when we *unblock* the $S_x = +\hbar/2$ output of the middle Stern-Gerlach analyzer is a signature interference effect. Since all of the outputs of this experiment are probabilistic, the statement that the probability observed is different in the "combined" experiment with both outputs unblocked is best written as

$$p(S_z = -|S_x = + \text{ or } S_x = -) \neq p(S_z = -|S_x = +) + p(S_z = -|S_x = -).$$

this is *suggestive* of superposition, because for any two events A and B in classical probability theory, we have

$$p(A \text{ or } B) = p(A) + p(B) - p(A \text{ and } B).$$

so we can get destructive contributions if we allow the last term. The actual equations that I wrote out last time playing off this relation were not formulated very well, and in particular ignored the very important fact that the state was $S_z = +$ *before* we went through the $SG(\hat{x})$ analyzer - which would lead to some very unwieldy compound conditional probabilities. Besides, we know that in quantum mechanics we work with *probability amplitudes* ψ, which we have to square to get probabilities, schematically

$$p(A) = |\psi(A)|^2$$

so the correct, quantum version of the superposition statement above is

$$p_{\text{quantum}}(A \text{ or } B) = |\psi(A) + \psi(B)|^2 = p(A) + p(B) + 2\text{Re}(\psi^*(A)\psi(B)),$$

In this abstract vector space, passing our beam through a Stern-Gerlach device and blocking one of the output components is exactly a projection along the given direction. It's easy to see in these terms that even after projecting only the $S_z = +\hbar/2$ component out, the subsequent projection on the $S_x = +\hbar/2$ direction will have *both* $\hat{z}$ spin components present.

We've been forgetting about the third direction, S_y. There should be nothing special about the $\hat{x}$ direction versus $\hat{y}$, of course - and indeed if we run the experiment above using $\hat{y}$ instead of $\hat{x}$, we get the same results. But it seems like we've used up our mathematical freedom in defining the S_x states! Moreover, we know that S_x and S_y have to be distinct, since obviously we expect the same results yet again if we run the sequential S-G experiment in the $\hat{x}$ and $\hat{y}$ directions.

The only way out is to enlarge the space by allowing the vector components to be *complex*; then

$$S_y = \pm\hbar/2 \Rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix}.$$