

Memorandum M-1950

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SUBJECT: GROUP 63 SEMINAR ON MAGNETISM, XLV

To: Group 63 Engineers

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Before going further into current literature let us return to fundamental concepts and consider the angular momentum and spin operators. This is important in our work in establishing a more basic understanding of the principles involved in the spin reversal of electrons. At meeting XXIX the spin functions ψ were introduced and expressed in terms of α and β . At that time only electrostatic perturbations were considered, and the result of the perturbation Hamiltonian operating on the spin functions was zero. However, there are other perturbing functions, such as an externally applied magnetic field, which interact strongly with the spin functions; and calculation of this type of perturbation requires a more extensive definition of the spin operator than we have used to date.

In classical mechanics the angular momentum \vec{M} is defined by

$$\vec{M} = \vec{r} \times \vec{p}$$

where \vec{r} is a radius vector to moving particle
 \vec{p} is the linear momentum of particle

Expressed in cartesian coordinates

$$\vec{M} = \hat{i}(y p_z - z p_y) + \hat{j}(z p_x - x p_z) + \hat{k}(x p_y - y p_x) \quad \text{XLV-1}$$

In meeting XXI we defined the linear momentum operator

$$P = -i\hbar \nabla$$

with components $P_x = -i\hbar \frac{\partial}{\partial x}$

$$P_y = -i\hbar \frac{\partial}{\partial y}$$

$$P_z = -i\hbar \frac{\partial}{\partial z}$$

XLV-2

If we substitute XLV-2 into XLV-1 to obtain the angular momentum operator, we have

$$\vec{M} = -i\hbar \left[\hat{i} \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) + \hat{j} \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) + \hat{k} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right]$$

with components $M_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$

$$M_y = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

XLV-4

$$M_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

We are interested in the commutation relationships of the angular momentum vectors. Let us consider two operators, A and B. Let B operate on a function ϕ , and A operate on the resultant. Reverse the order of the operations, and if the same result is obtained in both cases the operators are said to commute. Expressed mathematically,

$$\text{If } A [B \phi] = B [A \phi]$$

A and B commute.

The angular momentum components do not commute. To show this, let us determine the commutation relationship of the operators M_x and M_y .

$$M_x M_y = -\hbar^2 \left[y \frac{\partial}{\partial x} + y \frac{\partial^2}{\partial z \partial x} - xy \frac{\partial^2}{\partial z^2} - z^2 \frac{\partial^2}{\partial x \partial y} + xz \frac{\partial^2}{\partial y \partial z} \right]$$

$$M_y M_x = -\hbar^2 \left[yz \frac{\partial^2}{\partial x \partial z} - y^2 \frac{\partial^2}{\partial x \partial z} - xy \frac{\partial^2}{\partial z^2} + x \frac{\partial}{\partial y} + xz \frac{\partial^2}{\partial y \partial z} \right]$$

Therefore

$$M_x M_y - M_y M_x = -i\hbar^2 \left[y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right] = i\hbar M_z \neq 0 \quad \text{XLV-5}$$

The commutation of two operators, $AB-BA$ is generally expressed by the commutation bracket $[AB]$. Using this notation, XLV-5 may be rewritten

$$[M_x M_y] = i\hbar M_z \quad \text{XLV-6}$$

Similar commutation relations can be found for the other angular momentum components. The commutation relationships can be taken as the fundamental equations from which matrix mechanics can be built. This matrix mechanics is completely equivalent to the Schrodinger wave mechanics with which we have dealt.

As an example of this equivalence, consider the commutation relationship of the energy and time operators acting on a function $\varphi(t)$ and the commutation relationship of linear momentum and displacement operating on a function $\varphi(x)$.

$$E = i\hbar \frac{\partial}{\partial t}$$

$$t = t$$

Therefore

$$\begin{aligned} (Et - tE) \varphi(t) &= i\hbar \left[\frac{\partial}{\partial t} (t\varphi(t)) - t \frac{\partial}{\partial t} \varphi(t) \right] \\ &= i\hbar \varphi(t) \end{aligned}$$

$$\therefore Et - tE = i\hbar$$

$$\text{i.e. } [Et] = i\hbar$$

XLV-7

and,

$$P_x = -i\hbar \frac{\partial}{\partial x}$$

$$x = x$$

$$\begin{aligned}
 (Px - xP)\psi(x) &= -i\hbar \left[\frac{d}{dx}(x\psi(x)) - x \frac{d}{dx}\psi(x) \right] \\
 &= i\hbar \psi(x)
 \end{aligned}$$

$$[Px] = -i\hbar$$

XLV-8

Equations XLV-7 and XLV-8 represent the uncertainty principle expressed in operator form. When two operators do not commute their corresponding eigenvalues **cannot** be accurately known simultaneously. However, when they do commute, it is possible to find a set of **functions** which are **simultaneously eigenfunctions** of both operators.

Despite the **equivalence** of wave and matrix mechanics, wave mechanics has been used **exclusively** in this seminar up to the present, appearing to be the more convenient approach. However, matrix mechanics leads to a more explicit definition of the spin functions, and is therefore being used in this instance.

A matrix is an ordered array of numbers in two or more dimensions. The components are placed in rows, characterized by the first subscript, and columns, characterized by the second subscript. Matrices can be manipulated algebraically. Matrices may be added to one another by adding the corresponding components. Thus:

$$\begin{aligned}
 &\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \end{pmatrix} + \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \end{pmatrix} \\
 &= \begin{pmatrix} (a_{11} + b_{11}) & (a_{12} + b_{12}) & (a_{13} + b_{13}) & (a_{14} + b_{14}) \\ (a_{21} + b_{21}) & (a_{22} + b_{22}) & (a_{23} + b_{23}) & (a_{24} + b_{24}) \\ (a_{31} + b_{31}) & (a_{32} + b_{32}) & (a_{33} + b_{33}) & (a_{34} + b_{34}) \end{pmatrix}
 \end{aligned}$$

Matrix multiplication is carried out in the following manner:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \end{pmatrix} \times \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \\ b_{41} & b_{42} & b_{43} \end{pmatrix}$$

$$= \begin{pmatrix} (a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} + a_{14}b_{41}) & (a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} + a_{14}b_{42}) & (a_{11}b_{13} + a_{12}b_{23} + a_{13}b_{33} + a_{14}b_{43}) \\ (a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} + a_{24}b_{41}) & (a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} + a_{24}b_{42}) & (a_{21}b_{13} + a_{22}b_{23} + a_{23}b_{33} + a_{24}b_{43}) \\ (a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31} + a_{34}b_{41}) & (a_{31}b_{12} + a_{32}b_{22} + a_{33}b_{32} + a_{34}b_{42}) & (a_{31}b_{13} + a_{32}b_{23} + a_{33}b_{33} + a_{34}b_{43}) \end{pmatrix}$$

The spin operators should obey the same commutation relations as those given for the angular momentum operators in equation XLV-6. The spin operators are:

$$\sigma_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

XLV-9

We shall not prove the uniqueness of these solutions, but show below that they obey the angular momentum commutation relations.

$$\begin{aligned}\sigma_x \sigma_y &= \frac{\hbar^2}{4} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \left(\frac{i\hbar}{2}\right) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \frac{i\hbar}{2} \sigma_z\end{aligned}$$

$$\begin{aligned}\sigma_x \sigma_y &= \frac{\hbar^2}{4} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \left(-\frac{i\hbar}{2}\right) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= -\frac{i\hbar}{2} \sigma_z\end{aligned}$$

Therefore

$$\sigma_x \sigma_y - \sigma_y \sigma_x = i\hbar \sigma_z$$

$$[\sigma_x, \sigma_y] = i\hbar \sigma_z$$

XLV-10

Comparison of the above with XLV-6 shows the spin operators commute properly.

Further investigation shows

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\hbar^2}{4}$$

Therefore

$$\sigma^2 = \frac{3\hbar^2}{4}$$

It may be recalled that at meeting XXIX the functions α and β were defined. α was taken as zero everywhere except at a particular positive value of the spin coordinate, and β was zero everywhere except at a particular negative value of the spin coordinate (see figure 53). These functions can be expressed in terms of the single column matrices

$$\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

In that case, a linear combination of α and β may be taken as

$$x\alpha + y\beta = \begin{pmatrix} x \\ y \end{pmatrix}$$

Let us now find the eigenvalues of the components of σ :

$$\sigma_z \begin{pmatrix} x \\ y \end{pmatrix} = K \begin{pmatrix} x \\ y \end{pmatrix}$$

where K is an eigenvalue of σ_z .

$$\begin{aligned} \sigma_z \begin{pmatrix} x \\ y \end{pmatrix} &= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} x \\ -y \end{pmatrix}. \end{aligned}$$

Therefore

$$Kx = \frac{\hbar}{2} x$$

$$Ky = -\frac{\hbar}{2} y$$

These two equations cannot be satisfied simultaneously unless x or y equals zero.

$$\text{If } x = 0, \quad K = -\frac{\hbar}{2}, \quad y = 1$$

$$\text{If } y = 0, \quad K = \frac{\hbar}{2}, \quad x = 1$$

There are thus two eigenfunctions of σ_z , $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, with eigenvalues $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ respectively. These eigenfunctions correspond to the spin functions α and β .

$$\begin{aligned} \sigma_y \begin{pmatrix} x \\ y \end{pmatrix} &= \frac{\hbar}{2} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} -iy \\ ix \end{pmatrix} = K' \begin{pmatrix} x \\ y \end{pmatrix} \end{aligned}$$

Therefore

$$K'x = -\frac{iy\hbar}{2}$$

$$K'y = \frac{ix\hbar}{2}$$

so

$$\frac{x}{y} = -\frac{y}{x} \quad \text{and } x = \pm iy,$$

$$\text{when } x = iy, \quad K' = -\frac{\hbar}{2}$$

$$x = -iy, \quad K' = \frac{\hbar}{2}$$

The two eigenfunctions of σ_y are therefore $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ with eigenvalues of $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ respectively.

$$\sigma_x \begin{pmatrix} x \\ y \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} y \\ x \end{pmatrix} = K'' \begin{pmatrix} x \\ y \end{pmatrix}$$

Therefore $K'' x = \frac{\hbar}{2} y$

$$K'' y = \frac{\hbar}{2} x$$

so

$$\frac{x}{y} = \frac{y}{x} \quad \text{and} \quad x = \pm y$$

when $x = y, K'' = \frac{\hbar}{2}$

$$x = -y, K'' = -\frac{\hbar}{2}$$

The eigenfunctions of σ_x are therefore $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, with eigenvalues $-\frac{\hbar}{2}$ and $\frac{\hbar}{2}$ respectively.

The eigenvalues of all the spin components are therefore $\pm \frac{\hbar}{2}$; the total spin is therefore $\frac{\sqrt{3}}{2}$, in agreement with the eigenvalue of S^2 operator, which is $\frac{3}{4}$.

Signed

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