SPIN 1/2 PARTICLE
Stern-Gerlach experiment

The experiment consists of studying the deflection of a beam of neutral ground state paramagnetic atoms (silver) in inhomogeneous magnetic field:

A silver atom emitted from high temperature furnace E and collimated by F is deflected by the gradient of the magnetic field created by an electromagnet A and then condenses at N on plate P.

Result expected from classical mechanics

Silver atoms are neutral but possess a permanent magnetic moment $\mathcal{M}$ which comes from their intrinsic angular momentum, or spin $\mathcal{S}$

$$\mathcal{M} = \gamma \mathcal{S}$$

This interacts with the magnetic field $\mathbf{B}$ leading to the potential

$$W = -\mathcal{M} \, . \, \mathbf{B}$$

and thus also the force

$$\mathbf{F} = \nabla \, (\mathcal{M} \, . \, \mathbf{B}) = \mathcal{M}_z \, \nabla B_z = \mathcal{M} \, \frac{\partial B_z}{\partial z}$$

Since the magnetic moments of the emitted silver atoms are distributed randomly in all directions in space, classical mechanics predicts that a measurement of $\mathcal{M}_z$ can yield with equal probability all values included between $\pm \, |\mathcal{M}|$.

Results of the Stern-Gerlach experiment contradict classical prediction

If we measure the component $\mathcal{S}_z$ of the intrinsic angular momentum of a silver atom in its ground state, we can find only one or the other of two values, corresponding to the deflections HN_1 and HN_2.

We have to reject the classical picture and have to conclude that:

$\mathcal{S}_z$ is a quantized physical quantity whose discrete spectrum includes only two eigenvalues, $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$.

Theoretical description

We associate an observable $\hat{S}_z$ with $\mathcal{S}_z$. According to the experiment it has to satisfy the eigenvalue equations:

$$
\begin{aligned}
\hat{S}_z \left|+\right\rangle &= +\frac{\hbar}{2} \left|+\right\rangle \\
\hat{S}_z \left|-\right\rangle &= -\frac{\hbar}{2} \left|-\right\rangle
\end{aligned}
$$

where $|+\rangle$ and $|-\rangle$ are normalized and orthogonal and thus form a basis of the two-dimensional Hilbert space of one spin 1/2 particle

$$
|+\rangle\langle+| + |-\rangle\langle-| = \hat{1}
$$

The spin observables:

$$(S_x) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad (S_y) = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad (S_z) = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The spin component along the direction of a unit vector $\vec{u}$:

$$\begin{aligned} (S_u) = \hat{\vec{S}}\,.\,\vec{u} &= (S_x)\sin\theta\cos\phi + (S_y)\sin\theta\sin\phi + (S_z)\cos\theta \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{pmatrix} \end{aligned}$$

The eigenvectors of S_x, S_y and S_u:

$$
\begin{aligned}
|\pm\rangle_x &= \frac{1}{\sqrt{2}}\left(|+\rangle \pm |-\rangle\right) \\
|\pm\rangle_y &= \frac{1}{\sqrt{2}}\left(|+\rangle \pm i|-\rangle\right) \\
|+\rangle_u &= \cos\frac{\theta}{2}e^{-i\phi/2}|+\rangle + \sin\frac{\theta}{2}e^{i\phi/2}|-\rangle \\
|-\rangle_u &= -\sin\frac{\theta}{2}e^{-i\phi/2}|+\rangle + \cos\frac{\theta}{2}e^{i\phi/2}|-\rangle
\end{aligned}
$$

Preparation of the states $|+\rangle$ and $|-\rangle$

Each of the atoms of the beam which propagates to the right of the plate P is a physical system on which we have just performed a measurement of the observable S_z with the result $+\hbar/2$.

Preparation of the states $|\pm\rangle_x$, $|\pm\rangle_y$ and $|\pm\rangle_u$

To prepare one of the eigenstates of S_x, for example, we must select, after a measurement of S_x, the atoms for which this measurement has yielded the corresponding eigenvalue.

By placing the Stern-Gerlach apparatus so that the axis of the magnetic field is parallel to an arbitrary unit vector $\vec{u}$ and piercing the plate either at N_1 or at N_2, we can prepare silver atoms in the spin state $|+\rangle_u$ or $|-\rangle_u$ respectively.

Spin measurements

First experiment

Measurement of the observable S_z on the system prepared in the state $|+\rangle$ yields with certainty the eigenvalue $+\hbar/2$.

Second experiment

We place the apparatus along the unit vecotr $\vec{u}$, with polar angles θ and $\phi = 0$. The spin state of the atoms when they leave the ”polarizer” is

$$|\psi\rangle = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle$$

The second apparatus, the ”analyzer”, measures S_z. We find that, even though all atoms are prepared in the same state, certain atoms condensed at N_1 and others at N_2, thus always giving either $+\hbar/2$ or $-\hbar/2$. The corresponding probabilities are respectively $\cos^2\frac{\theta}{2}$ and $\sin^2\frac{\theta}{2}$.

Third experiment

We take the same polarizer as in the previous example and prepare the atoms in the state

$$|\psi\rangle = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle$$

We rotate the analyzer, so that it measures the component S_x of the spin angular momentum.

To calculate the predictions, we must expand the state in terms of the eigenstate of the observable S_x

$$\begin{aligned} {}_x\langle+|\psi\rangle &= \frac{1}{\sqrt{2}}\left(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}\right) = \cos\left(\frac{\pi}{4} - \frac{\theta}{2}\right) \\ {}_x\langle-|\psi\rangle &= \frac{1}{\sqrt{2}}\left(\cos\frac{\theta}{2} - \sin\frac{\theta}{2}\right) = \sin\left(\frac{\pi}{4} - \frac{\theta}{2}\right) \end{aligned}$$

The probability of finding the corresponding eigenvalues are

$$+\hbar/2 \qquad \cos^2\left(\frac{\pi}{4} - \frac{\theta}{2}\right)$$

$$-\hbar/2 \qquad \sin^2\left(\frac{\pi}{4} - \frac{\theta}{2}\right)$$

CHAPTER 3: ELECTRON SPIN

(From Cohen-Tannoudji, Chapter IX)

Spin is an intrinsic property of quantum particles which comes naturally out of relativistic description of particles and specifically from the structure of the Lorentz group.

Spin of electron can be incorporated into non-relativistic quantum mechanics through the addition of several postulates. This is known as **Pauli theory of electron spin**.

Pauli theory will allows us to incorporate relativistic corrections (relativistic kinematics, magnetic effects) into our theory of the hydrogen atom.

A. INTRODUCTION OF ELECTRON SPIN

1. Experimental evidence

a. FINE STRUCTURE OF SPECTRAL LINES

Each spectral line is made of several distinguishable components having nearly identical frequencies. This structure comes from relativistic effects related to interaction between the various angular momenta of constituent particles of an atom.

b. ANOMALOUS ZEEMAN EFFECT

In a uniform magnetic field, each of the spectral lines, i.e. each component of the fine structure, of an atom, splits into a certain number of equidistant lines. This is called **the Zeeman effect**. The theory predicts the magnetic moment to be proportional to the orbital angular momentum

$$\hat{\vec{M}} = \frac{\mu_{\mathrm{B}}}{\hbar}\hat{\vec{L}} \tag{3.1}$$

where μ_{B} is the Bohr magneton

$$\mu_{\mathrm{B}} = \frac{q\hbar}{2m_e} \tag{3.2}$$

This theory of the Zeeman effect is confirmed in some experiments (”normal” Zeeman effect) but it is contradicted in other ones (”anomalous”). For example, for hydrogen and the atoms with odd atomic number Z, the energy levels are divided into an even number of Zeeman sub-levels though it should be an odd number $(2l + 1)$.

C. EXISTENCE OF HALF-INTEGRAL ANGULAR MOMENTA

In the Stern-Gerlach experiment, the ground state neutral atoms are deflected by a perpendicular magnetic field according to their value of spin. For example Ag atoms are deflected in such a way that they split symmetrically into two beams. This shows, as through 2s+1=2, that the atoms have only two possible values of the magnetic quantum number $m_z = \pm\frac{1}{2}$ and are characterized by the azimuthal quantum number $s = \frac{1}{2}$ in this case.

2. Quantum description: postulates of the Pauli theory

Uhlenbeck and Goudsmit hypothesis (1925)

electron ”spins” and that gives it an intrinsic angular momentum called **spin**. To interpret the experimental observations, we assume the magnetic moment is associated with the spin angular momentum

$$\hat{\vec{M}}_S = 2\frac{\mu_{\mathrm{B}}}{\hbar}\hat{\vec{S}} \tag{3.3}$$

where the spin gyromagnetic ratio is twice the orbital gyromagnetic ratio.

Pauli stated this hypothesis more precisely and formulated description of spin in a non-relativistic limit.

Spin postulates:

(i) The spin is characterized by the spin operator $\hat{\vec{S}}$ which is an angular momentum, that is, it satisfies the angular momentum commutation relations

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z \tag{3.4}$$

$$\left[\hat{S}_y, \hat{S}_z\right] = i\hbar\hat{S}_x \tag{3.5}$$

$$\left[\hat{S}_z, \hat{S}_x\right] = i\hbar\hat{S}_y \tag{3.6}$$

(ii) $\hat{\vec{S}}$ acts in a new space, spin state space $\mathcal{E}_s$ where $\hat{S}^2$ and $\hat{S}_z$ constitute C.S.C.O. The space $\mathcal{E}_s$ is spanned by eigenvectors of $\hat{S}^2$ and $\hat{S}_z$ (and is $(2s+1)$ dimensional):

$$\hat{S}^2|s,m\rangle = s(s+1)\hbar^2|s,m\rangle \tag{3.7}$$

$$\hat{S}_z|s,m\rangle = m\hbar|s,m\rangle \tag{3.8}$$

From general theory of angular momentum we know that s is either integral or half-integral and $m = s, s-1, ..., -s+1, -s$.

A particle characterized by a unique value of s is said to have spin s.

(iii) The state space of the particle $\mathcal{E}$ represents both the orbital and spin angular momentum d.o.f. and since all the spin observables commute with all orbital observables, the state space factorizes into a tensor product as follows

$$\mathcal{E} = \mathcal{E}_{\vec{r}} \otimes \mathcal{E}_s \qquad (3.9)$$

C.S.C.O. of the whole system consists of the spin C.S.C.O. (whose eigenvectors span $\mathcal{E}_s$), and the orbital C.S.C.O. ($\mathcal{E}_{\vec{r}}$). For example, $\mathcal{E}$ is spanned by $\{|x, y, z, s, m\rangle\}$.

The electron is a spin-1/2 particle ($s = 1/2$) and its intrinsic magnetic moment is given by

$$\hat{\vec{M}}_S = 2\frac{\mu_B}{\hbar}\hat{\vec{S}} \tag{3.10}$$

$\mathcal{E}_s$ is two-dimensional with the standard basis vectors $|\frac{1}{2}, +\frac{1}{2}\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle$.

Remarks:
Proton and neutron are also spin-1/2 particles but with a different gyromagnetic ratios.

Spin has no classical analog.

B. SPECIAL PROPERTIES OF AN ANGULAR MOMENTUM 1/2

Electron:

$$s = \frac{1}{2}$$

$$dim(\mathcal{E}_s) = 2$$

basis $\mathcal{B} = \left\{|\frac{1}{2}, +\frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle\right\} = \{|+\rangle, |-\rangle\}$

- the eigenvalue equations:

$$\hat{S}^2|\pm\rangle = \frac{3}{4}\hbar^2|\pm\rangle \tag{3.11}$$

$$\hat{S}_z|\pm\rangle = \pm\frac{1}{2}\hbar|\pm\rangle \tag{3.12}$$

- properties of the basis vectors and the completeness relation

$$\langle +|-\rangle = 0 \tag{3.13}$$

$$\langle +|+\rangle = \langle -|-\rangle = 1 \tag{3.14}$$

$$|+\rangle\langle +| + |-\rangle\langle -| = \hat{1} \tag{3.15}$$

- a general spin state of an electron

$$|\chi\rangle \quad = \quad c_+|+\rangle + c_-|-\rangle \tag{3.16}$$

- the action of rising and lowering operators:

$$\hat{S}_\pm \quad = \quad \hat{S}_x \pm i\hat{S}_y \tag{3.17}$$

$$\hat{S}_+|+\rangle = 0 \qquad \hat{S}_+|-\rangle = \hbar|+\rangle \tag{3.18}$$

$$\hat{S}_-|+\rangle = \hbar|-\rangle \qquad \hat{S}_-|-\rangle = 0 \tag{3.19}$$

All operators acting in $\mathcal{E}_s$ can in the standard basis be represented by 2×2 matrices:

$$\left(\hat{\vec{S}}\right) = \frac{\hbar}{2}\vec{\sigma} \tag{3.20}$$

where

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.21}$$

are the **Pauli matrices**.

Any 2×2 matrix can be written as a linear combination of the matrices $\{I, \sigma_x, \sigma_y, \sigma_z\}$.

The properties of the Pauli matrices are

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \hat{1} \tag{3.22}$$

$$\{\sigma_x, \sigma_y\} = \sigma_x\sigma_y + \sigma_y\sigma_x = \{\sigma_y, \sigma_z\} = \{\sigma_z, \sigma_x\} = 0 \tag{3.23}$$

$$\left[\sigma_x, \sigma_y\right] = 2i\sigma_z \qquad \left[\sigma_y, \sigma_z\right] = 2i\sigma_x \qquad [\sigma_z, \sigma_x] = 2i\sigma_y \tag{3.24}$$

$$\sigma_x\sigma_y = i\sigma_z \qquad \sigma_y\sigma_z = i\sigma_x \qquad \sigma_z\sigma_x = i\sigma_y \tag{3.25}$$

$$\operatorname{tr}\sigma_x = \operatorname{tr}\sigma_y = \operatorname{tr}\sigma_z = 0 \tag{3.26}$$

$$\det\sigma_x = \det\sigma_y = \det\sigma_x = -1 \tag{3.27}$$

$$\left(\vec{\sigma}\cdot\vec{A}\right)\left(\vec{\sigma}\cdot\vec{B}\right) = \vec{A}\cdot\vec{B} + i\vec{\sigma}\cdot\left(\vec{A}\times\vec{B}\right) \tag{3.28}$$

The properties of electron spin operators (from the general theory of angular momentum):

$$\hat{S}_x^2 = \hat{S}_y^2 = \hat{S}_z^2 = \frac{\hbar^2}{4}\,\hat{1} \tag{3.29}$$

$$\hat{S}_x\hat{S}_y + \hat{S}_y\hat{S}_x = 0 \quad \ldots \tag{3.30}$$

$$\hat{S}_x\hat{S}_y = \frac{i}{2}\hbar\hat{S}_z \quad \ldots \tag{3.31}$$

$$\hat{S}_+^2 = \hat{S}_-^2 = 0 \tag{3.32}$$

(dots mean that similar relations hold for the other components)

C. NON-RELATIVISTIC DESCRIPTION OF A SPIN 1/2 PARTICLE

1. Observables and state space

a. STATE SPACE

$$\mathcal{E} = \mathcal{E}_{\vec{r}} \otimes \mathcal{E}_s \tag{3.33}$$

The possible C.S.C.O. are for example:

$$\left\{\hat{X}, \hat{Y}, \hat{Z}, \hat{S}^2, \hat{S}_z\right\} \tag{3.34}$$

$$\left\{\hat{P}_x, \hat{P}_y, \hat{P}_z, \hat{S}^2, \hat{S}_z\right\} \tag{3.35}$$

$$\left\{\hat{H}, \hat{L}^2, \hat{L}_z, \hat{S}^2, \hat{S}_z\right\} \tag{3.36}$$

Let us choose the C.S.C.O. $\left\{\hat{X}, \hat{Y}, \hat{Z}, \hat{S}^2, \hat{S}_z\right\}$

$$|\vec{r}, \varepsilon\rangle \equiv |x, y, z, \varepsilon\rangle = |\vec{r}\rangle \otimes |\varepsilon\rangle \tag{3.37}$$

where $|\vec{r}\rangle \in \mathcal{E}_r$ and $|\epsilon\rangle \in \mathcal{E}_s$ with $\epsilon = +$ or $-$.

The eigenvalue equations are

$$\hat{X}|\vec{r}, \varepsilon\rangle = x|\vec{r}, \varepsilon\rangle \tag{3.38}$$

$$\hat{Y}|\vec{r}, \varepsilon\rangle = y|\vec{r}, \varepsilon\rangle \tag{3.39}$$

$$\hat{Z}|\vec{r}, \varepsilon\rangle = z|\vec{r}, \varepsilon\rangle \tag{3.40}$$

$$\hat{S}^2|\vec{r}, \varepsilon\rangle = \frac{3}{4}\hbar^2|\vec{r}, \varepsilon\rangle \tag{3.41}$$

$$\hat{S}_z|\vec{r}, \varepsilon\rangle = \varepsilon\frac{\hbar}{2}|\vec{r}, \varepsilon\rangle \tag{3.42}$$

$\{|\vec{r},\epsilon\rangle\}$ form an orthonormal system

$$\langle\vec{r}',\varepsilon'|\vec{r},\varepsilon\rangle = \delta_{\varepsilon'\varepsilon}\delta\left(\vec{r}'-\vec{r}\right) \tag{3.43}$$

The completeness relation is

$$\sum_{\varepsilon}\int \mathrm{d}^3r|\vec{r},\varepsilon\rangle\langle\vec{r},\varepsilon| = \int \mathrm{d}^3r|\vec{r},+\rangle\langle\vec{r},+| + \int \mathrm{d}^3r|\vec{r},-\rangle\langle\vec{r},-| = \hat{1} \tag{3.44}$$

The basis set $\{|\vec{r},\epsilon\rangle\}$ offers the $\{|\vec{r},\epsilon\rangle\}$ representation which we will now define.

b. $\{|\vec{r},\varepsilon\rangle\}$ REPRESENTATION

α. State vectors

$$|\psi\rangle = \sum_{\varepsilon}\int \mathrm{d}^3 r|\vec{r},\varepsilon\rangle\langle\vec{r},\varepsilon|\psi\rangle \tag{3.45}$$

$$\langle\vec{r},\varepsilon|\psi\rangle = \psi_{\varepsilon}(\vec{r}) \tag{3.46}$$

To completely characterize the state of an electron, it is necessary to specify two functions of x, y and z

$$\psi_+(\vec{r}) = \langle \vec{r}, +|\psi\rangle \tag{3.47}$$

$$\psi_-(\vec{r}) = \langle \vec{r}, -|\psi\rangle \tag{3.48}$$

which can be written as **2-component spinor**

$$[\psi](\vec{r}) = \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} \tag{3.49}$$

We can now also define the bra $\langle\psi|$:

$$\langle\psi| = \sum_{\varepsilon} \int \mathrm{d}^3 r \langle\psi|\vec{r}, \varepsilon\rangle\langle\vec{r}, \varepsilon| = \sum_{\varepsilon} \int \mathrm{d}^3 r\, \psi_{\varepsilon}^*(\vec{r})\, \langle\vec{r}, \varepsilon| \tag{3.50}$$

$$[\psi]^{\dagger}(\vec{r}) = \begin{pmatrix} \psi_+^*(\vec{r}) & \psi_-^*(\vec{r}) \end{pmatrix} \tag{3.51}$$

Using the spinor notation we can define the inner product as follows

$$\langle\psi|\varphi\rangle = \sum_{\varepsilon}\int \mathrm{d}^3r\langle\psi|\vec{r},\varepsilon\rangle\langle\vec{r},\varepsilon|\varphi\rangle \tag{3.52}$$

$$= \int \mathrm{d}^3r\left[\psi_+^*(\vec{r})\,\varphi_+(\vec{r}) + \psi_-^*(\vec{r})\,\varphi_-(\vec{r})\right] \tag{3.53}$$

$$= \int \mathrm{d}^3r\,[\psi]^\dagger(\vec{r})\,[\varphi]\,(\vec{r}) \tag{3.54}$$

and we can calculate the norm

$$\langle\psi|\psi\rangle = \int \mathrm{d}^3r\,[\psi]^\dagger(\vec{r})\,[\psi]\,(\vec{r}) = \int \mathrm{d}^3r\left[\left|\psi_+(\vec{r})\right|^2 + \left|\psi_-(\vec{r})\right|^2\right] = 1 \tag{3.55}$$

A general state $|\psi\rangle \in \mathcal{E}$ is the product state $|\psi\rangle = |\varphi\rangle \otimes |\chi\rangle$ where

$$|\varphi\rangle = \int \mathrm{d}^3 r\, \varphi(\vec{r})\, |\vec{r}\rangle \in \mathcal{E}_{\vec{r}} \tag{3.56}$$

$$|\chi\rangle = c_+|+\rangle + c_-|-\rangle \in \mathcal{E}_S \tag{3.57}$$

The spinor has a simple form

$$[\psi](\vec{r}) = \begin{pmatrix} \varphi(\vec{r})\, c_+ \\ \varphi(\vec{r})\, c_- \end{pmatrix} = \varphi(\vec{r}) \begin{pmatrix} c_+ \\ c_- \end{pmatrix} \tag{3.58}$$

where

$$\psi_+(\vec{r}) = \langle \vec{r}, +|\psi\rangle = \langle \vec{r}|\varphi\rangle\langle +|\chi\rangle = \varphi(\vec{r})\, c_+ \tag{3.59}$$

$$\psi_-(\vec{r}) = \langle \vec{r}, -|\psi\rangle = \langle \vec{r}|\varphi\rangle\langle -|\chi\rangle = \varphi(\vec{r})\, c_- \tag{3.60}$$

The normalization factorizes as

$$\langle\psi|\psi\rangle = \langle\varphi|\varphi\rangle\langle\chi|\chi\rangle = \left(|c_+|^2 + |c_-|^2\right) \int \mathrm{d}^3 r\, \left|\varphi(\vec{r})\right|^2 \tag{3.61}$$

β. Operators

$$|\psi'\rangle = A|\psi\rangle \tag{3.62}$$

$$|\psi\rangle \rightarrow [\psi](\vec{r}) \tag{3.63}$$

$$|\psi'\rangle \rightarrow \left[\psi'\right](\vec{r}) \tag{3.64}$$

$$\left[\psi'\right](\vec{r}) = [[A]]\,[\psi](\vec{r}) \tag{3.65}$$

where $[[A]]$ is a 2×2 matrix where the matrix elements remain in general differential operators with respect to the variable $\vec{r}$.

(i) Spin operators:

are defined in $\mathcal{E}_s$ and are acting on ϵ index in $|\vec{r}, \varepsilon\rangle$.

Example – $\hat{S}_+$:

$$\begin{aligned} |\psi'\rangle &= \hat{S}_+|\psi\rangle = \hat{S}_+ \sum_{\epsilon} \int \mathrm{d}^3 r |\vec{r}, \varepsilon\rangle\langle\vec{r}, \varepsilon|\psi\rangle = \hat{S}_+ \int \mathrm{d}^3 r \left(\psi_+(\vec{r})|\vec{r}, +\rangle + \psi_-(\vec{r})|\vec{r}, -\rangle\right) \\ &= \hbar \int \mathrm{d}^3 r \, \psi_-(\vec{r}) \, |\vec{r}, +\rangle \end{aligned} \tag{3.66}$$

where we have used that the spin operator acts only the spin d.o.f.

$$\hat{S}_+|\vec{r}, -\rangle = \hat{S}_+(|\vec{r}\rangle \otimes |-\rangle) = |\vec{r}\rangle \otimes \hat{S}_+|-\rangle = \hbar|\vec{r}, +\rangle \tag{3.67}$$

The result

$$|\psi'\rangle = \hbar \int \mathrm{d}^3 r \, \psi_-(\vec{r}) \, |\vec{r}, +\rangle \tag{3.68}$$

can be summarized as

$$\langle \vec{r}, +|\psi'\rangle = \psi'_+(\vec{r}) = \hbar\psi_-(\vec{r}) \tag{3.69}$$

$$\langle \vec{r}, -|\psi'\rangle = \psi'_-(\vec{r}) = 0 \tag{3.70}$$

which in the spinor notation reads as

$$\left[\psi'\right](\vec{r}) = \hbar \begin{pmatrix} \psi_-(\vec{r}) \\ 0 \end{pmatrix} \tag{3.71}$$

Thus the spin rising operator is in the spinor notation given as

$$\left[\left[\hat{S}_+\right]\right] = \frac{\hbar}{2}\left(\sigma_x + i\sigma_y\right) = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{3.72}$$

(ii) Orbital operators:

leaves always the spin d.o.f. (ϵ) unchanged in $|\vec{r}, \varepsilon\rangle$, and act only on the $\vec{r}$-dependence of spinors.

Examples – $\hat{X}$, $\hat{P}_x$:

$$\psi'_\varepsilon(\vec{r}) = \langle \vec{r}, \varepsilon | \hat{X} | \psi \rangle = x \psi_\varepsilon(\vec{r}) \tag{3.73}$$

$$\psi''_\varepsilon(\vec{r}) = \langle \vec{r}, \varepsilon | \hat{P}_x | \psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \psi_\varepsilon(\vec{r}) \tag{3.74}$$

and the spinors $[\psi'](\vec{r})$ and $[\psi''](\vec{r})$ are obtained from $[\psi](\vec{r})$ by means of 2×2 matrices:

$$\left[\left[\hat{X}\right]\right] = \begin{pmatrix} x & 0 \\ 0 & x \end{pmatrix} \tag{3.75}$$

$$\left[\left[\hat{P}_x\right]\right] = \frac{\hbar}{i} \begin{pmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial x} \end{pmatrix} \tag{3.76}$$

(iii) Mixed operators:

will have the form of 2×2 matrices whose elements are differential operators with respect to $\vec{r}$.

Examples – $\hat{L}_z\hat{S}_z$, $\hat{\vec{S}} \cdot \hat{\vec{P}}$:

$$\left[\left[\hat{L}_z\hat{S}_z\right]\right] = \frac{\hbar}{2}\begin{pmatrix} \frac{\hbar}{i}\frac{\partial}{\partial\phi} & 0 \\ 0 & -\frac{\hbar}{i}\frac{\partial}{\partial\phi} \end{pmatrix} \tag{3.77}$$

$$\left[\left[\hat{\vec{S}} \cdot \hat{\vec{P}}\right]\right] = \frac{\hbar}{2}\left(\sigma_x\hat{P}_x + \sigma_y\hat{P}_y + \sigma_z\hat{P}_z\right) = \frac{\hbar^2}{2i}\begin{pmatrix} \frac{\partial}{\partial z} & \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} & -\frac{\partial}{\partial z} \end{pmatrix} \tag{3.78}$$

COMMENTS:

(i)

$$\langle\psi|\hat{A}|\varphi\rangle = \int \mathrm{d}^3r\,[\psi]^\dagger(\vec{r})\left[\left[\hat{A}\right]\right][\varphi](\vec{r}) \tag{3.79}$$

where $\left[\left[\hat{A}\right]\right]$ is a 2×2 matrix.

(ii) There also exists $|\vec{p},\varepsilon\rangle$ representation given by C.S.C.O. = $\left\{P_x, P_y, P_z, \hat{S}^2, \hat{S}_z\right\}$. The definition of the scalar product yields

$$\langle\vec{r},\varepsilon|\vec{p},\varepsilon'\rangle = \langle\vec{r}|\vec{p}\rangle\langle\varepsilon|\varepsilon'\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{i\vec{p}\cdot\vec{r}/\hbar}\delta_{\varepsilon\varepsilon'} \tag{3.80}$$

In this representation

$$[\bar{\psi}]\,(\vec{p}) \quad = \quad \begin{pmatrix} \bar{\psi}_{+}\,(\vec{p}) \\ \bar{\psi}_{-}\,(\vec{p}) \end{pmatrix} \tag{3.81}$$

where

$$\bar{\psi}_{+}\,(\vec{p}) \quad = \quad \langle \vec{p}, +|\psi\rangle \tag{3.82}$$

$$\bar{\psi}_{-}\,(\vec{p}) \quad = \quad \langle \vec{p}, -|\psi\rangle \tag{3.83}$$

The relation between the momentum representation and the coordinate representation is again given by the Fourier transform

$$\bar{\psi}_{\varepsilon}\,(\vec{p}) = \langle \vec{p}, \varepsilon|\psi\rangle \quad = \quad \sum_{\epsilon'} \int \mathrm{d}^3 r \langle \vec{p}, \varepsilon|\vec{r}, \varepsilon'\rangle\langle \vec{r}, \varepsilon'|\psi\rangle \tag{3.84}$$

$$= \quad \frac{1}{(2\pi\hbar)^{3/2}} \int \mathrm{d}^3 r\, e^{-i\vec{p}\cdot\vec{r}/\hbar} \psi_{\varepsilon}\,(\vec{r}) \tag{3.85}$$

2. Probability calculations for a physical measurement

We can simultaneously measure the position (x, y, z) and spin $(+\frac{\hbar}{2}, -\frac{\hbar}{2})$ of an electron. The probability of finding electron in the infinitesimal volume $\mathrm{d}^3 r$ around the point $\vec{r} = (x, y, z)$ with its spin "up" or "down" are given respectively as

$$\mathrm{d}^3\mathcal{P}(\vec{r}, +) = \left|\langle\vec{r}, +|\psi\rangle\right|^2 \mathrm{d}^3 r = \left|\psi_+(\vec{r})\right|^2 \mathrm{d}^3 r \tag{3.86}$$

$$\mathrm{d}^3\mathcal{P}(\vec{r}, -) = \left|\langle\vec{r}, -|\psi\rangle\right|^2 \mathrm{d}^3 r = \left|\psi_-(\vec{r})\right|^2 \mathrm{d}^3 r \tag{3.87}$$

Consider measurement of the component of the spin along the x-axis

$$|\vec{r}\rangle|\pm\rangle_x = \frac{1}{\sqrt{2}}\left[|\vec{r},+\rangle \pm |\vec{r},-\rangle\right] \tag{3.88}$$

then the probability of finding the electron in d^3r around the point $\vec{r} = (x, y, z)$ with spin "up" along the x-axis is

$$\mathrm{d}^3r \times \left|\frac{1}{\sqrt{2}}\left[\langle\vec{r},+|\psi\rangle + \langle\vec{r},-|\psi\rangle\right]\right|^2 = \frac{1}{2}\left|\psi_+(\vec{r}) + \psi_-(\vec{r})\right|^2 \mathrm{d}^3r \tag{3.89}$$

Measuring momentum of electron:

- we use the components of $|\psi\rangle$ relative to the basis vectors $\{|\vec{p},\varepsilon\rangle\}$. The desired probability of finding electron in d^3p with the spin $\pm\frac{\hbar}{2}$ equals to

$$\mathrm{d}^3\mathcal{P}(\vec{p},\pm) = \left|\langle\vec{p},\pm|\psi\rangle\right|^2 \mathrm{d}^3p = \left|\bar{\psi}_\pm(\vec{p})\right|^2 \mathrm{d}^3p \tag{3.90}$$

Consider now an incomplete measurement. For example we do not measure the spin, then

$$d^3\mathcal{P}(\vec{r}) = \left[\left|\psi_+(\vec{r})\right|^2 + \left|\psi_-(\vec{r})\right|^2\right] d^3r, \tag{3.91}$$

or we are interested in probability that spin along z-axis is $+\frac{\hbar}{2}$, then

$$\mathcal{P}_+ = \int d^3r \left|\psi_+(\vec{r})\right|^2 \tag{3.92}$$