

Spin is a quintessentially quantum property describing the intrinsic magnetic moment (or equivalently, angular momentum) of quantum particles.

1<sup>st</sup> proposed by Uhlenbeck and Goudsmit in 1925 to explain various experimental results such as

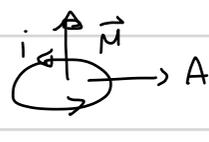
- anomalies in spectroscopic data, including
  - the "fine structure" of Hydrogen (slight shifts of energy levels w/ respect to Bohr/Schrödinger values  $\frac{-13,6}{n^2} \text{eV}$ )
  - the "anomalous Zeeman effect" (shifts in atomic levels under applied magnetic fields)
- the Stern-Gerlach experiment

Pauli soon developed a full theory of spin by extending the postulates of QM. This is the theory we will study here

Later, Dirac showed how the electron's spin arises naturally in a relativistic quantum theory.

To understand the motivations for Pauli's theory, as well as how spin enters in real physical situations, we 1<sup>st</sup> have to recall the connection between angular momentum and magnetic dipole moments

Classical Physics: since magnetic monopoles do not exist, a dipole moment  $\vec{\mu}$  only arises due to a current  $i$  looping around an (oriented) area  $\vec{A}$ , resulting in

$$\vec{\mu} = i\vec{A}$$


In particular, a particle with charge  $q$  and mass  $M$  performing a circular movement with angular momentum  $\vec{L}$  gives rise to the mag. moment

$$\vec{\mu} = \frac{q}{2M} \vec{L} \quad (1)$$

derivation (eg. Griffiths p. 272, or basic physics textbooks)

$$\left. \begin{array}{l} A = \pi r^2, i = \frac{q}{T} \rightarrow \mu = \frac{q\pi r^2}{T} \\ \text{angular mom: } |\vec{L}| = I\omega = M\omega r^2 = \frac{2\pi M r^2}{T} \end{array} \right\} \rightarrow \vec{\mu} = \frac{q}{2M} \vec{L} \quad (\text{since by def point in same direction})$$

In Quantum physics, Eq (1) remains valid, but for the corresponding operator vectors  $\vec{\mu} = (\hat{\mu}_x, \hat{\mu}_y, \hat{\mu}_z)$  and  $\vec{L} = (L_x, L_y, L_z)$ . The rules for quantum (orbital) AM imply that  $\vec{\mu}$  is quantized too:

$$\mu^2 = \left(\frac{q}{2M}\right)^2 l(l+1)\hbar^2; \quad l \in 0, 1, 2, \dots; \quad \mu_z = \frac{q}{2M} \cdot m\hbar \quad (m \in \overbrace{-l, -l+1, \dots, 0, \dots, l-1, l}^{2l+1 \text{ values}})$$

For electrons:  $\mu_z = -m\mu_B$ , where  $\mu_B \equiv \frac{e\hbar}{2m_e}$  is the Bohr magneton  
(basic unit of magnetic moment)

(more generally:  $\vec{\mu} = \frac{\mu_B}{\hbar} \vec{L}$ )

All the experiments mentioned above could be analyzed by considering the hypothetical effect of the electron actually being a 3D body rotating about an axis, thus producing a rotational magnetic moment  $\vec{M}_r$ .

Now, Eq 1 applies to any charge w/ rotational motion - including each portion of a solid charged object rotating about its axis. In this case, summing (integrating) over the entire object we obtain that it will have a rotational magnetic moment

$$\vec{M}_r = \left( \int \frac{\rho_c(\vec{r})}{2\rho_m(\vec{r})} dV \right) \vec{L} \quad \begin{array}{l} \rho_c = \text{charge density} \\ \rho_m = \text{mass density} \end{array}$$

In particular, for each value  $l$  of  $L^2$ ,  $M_z^{\text{rot}}$  can only take one out of  $2l+1$  different possible values (an odd number)

However: the experimental data were only consistent w/a rot. magnetic moment assuming an even number of different values for  $M_z$  - which made no sense!

Uhlenbeck + Goudsmit (Dutch students) made a bold suggestion: the electron has in fact an "intrinsic" mag. moment  $\vec{M}_s$  disconnected from any geometric rotation, but that nevertheless behaves in a similar way as an "ordinary"  $\vec{M}$  - with 2 important differences

- A component of  $\vec{M}$  such as  $M_z$  can only assume two different values - and the same is true for the corresponding "spin" angular momentum,  $S_z$

- The relation between  $\vec{M}_s$  and  $\vec{S}$  is different from Eq 1 by a so-called

"gyromagnetic factor"  $g=2$ .

$$\vec{M}_s = -g \frac{\mu_B}{\hbar} \vec{S}$$

With these two assumptions, nearly all the exper. data (eg. SG experiments) suddenly made sense (except for some details that we will discuss later in this course)

Shortly after, Pauli developed a full theory of "intrinsic" spin, incorporating U+G's concepts, but also extending it in a way that made it adaptable for any particle (not just the electron).

## Pauli theory of spin

Postulates

1) "Spin" is an intrinsic property of particles, corresponding to an internal degree of freedom that is independent of their motion in space. The "spin operator"  $\vec{S}$  is a QM angular momentum vector operator, satisfying the AM commutation relations

$$[S_a, S_b] = i\hbar \epsilon_{abc} S_c$$

→ in particular  $S^2$  can only assume values  $s(s+1)\hbar^2$ , where  $s$  can be integer or half-integer, and components such as  $S_z$  can only have eigenvalues

$$S_z = m_s \hbar, \quad m_s \in -s, -s+1, \dots, s-1, s$$

Note that if  $s$  is half-integer, so is  $m_s$

ii) For each type of particle, the value of  $s$  (or of  $S^2$ ) is fixed.

In particular, for the electron  $s = 1/2$ , so  $S^2 = 3/4 \hbar^2$ .

Same also true for protons and neutrons. However there are particles for which  $s = 1, 3/2, 2$  or even  $1/2!$  (there are also spinless particles,  $s = 0$ )

-> note this is very different both from a classical AM, and also from the normal QM "orbital" AM -> not just because  $s$  is half-integer but also because it cannot be "spun faster" or slower.

iii) The "spin degree of freedom" of a particle is described by a vector in a Hilbert space  $E_s$  that is distinct from the space  $E_r$  of its position state. Furthermore,  $\{S^2, S_z\}$  form a C.S.C.O. for this space. Thus this space has finite dimension  $d = 2s + 1$ , and is spanned by the set  $\{|s, m_s\rangle, -s \leq m_s \leq s\}$  (remember  $s$  is fixed)

For the electron  $d = 2 \times 1/2 + 1 = 2$ , and the basis is  $\{|1/2, 1/2\rangle, |1/2, -1/2\rangle\}$

We usually omit  $s$ , since it is fixed. Other common notations:  $\begin{cases} |m_s = 1/2\rangle = |\uparrow_z\rangle = |+_z\rangle \\ |m_s = -1/2\rangle = |\downarrow_z\rangle = |-_z\rangle \end{cases}$  (sometimes  $1/2$  is omitted)

iv) The full Hilbert space for a particle is the tensor product  $E_r \otimes E_s$ .

ex: a position state of an electron in 3D can be written as a linear combination of a complete basis, such as for example the set  $\{|\Psi_{nlm}\rangle\}_{n=1}^{\infty} \{l=0}^{n-1} \{m=-l}^l$  containing all energy/AM-indexed eigenstates of the standard Hydrogen Hamiltonian.

However, the full state of the electron, including spin, is actually a linear combination of products of the form

$$\{ |\varphi_{n\ell m}\rangle \otimes |+\rangle; |\varphi_{n'\ell'm'}\rangle \otimes |-\rangle \}$$

$$\text{ex: } |\psi\rangle = \sum_{\substack{n\ell m \\ n'\ell'm'}} c_{n\ell m} |\varphi_{n\ell m}\rangle \otimes |+\rangle + c'_{n'\ell'm'} |\varphi_{n'\ell'm'}\rangle \otimes |-\rangle$$

In particular, the H atom has actually twice the number of distinct energy eigenstates for each value of  $E_n$  ( $2n^2$  instead of  $n^2$ ).

### Properties of Spin $\frac{1}{2}$

$$\text{orthonormal basis: } \{|+\rangle, |-\rangle\} \quad |+\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad |-\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\text{general spin state } c_+|+\rangle + c_-|-\rangle, \quad |c_+|^2 + |c_-|^2 = 1$$

$$\text{C.S.C.O: } S^2 |\pm\rangle = \frac{3}{4} \hbar^2 |\pm\rangle \quad S_z |\pm\rangle = \pm \frac{\hbar}{2} |\pm\rangle$$

$$\hookrightarrow S^2 = \frac{3}{4} \hbar^2 \mathbb{I}$$

Recall from general AM theory:

$$\text{Raising/lowering operators: } S_{\pm} |s, m\rangle = \sqrt{s(s\pm 1) \mp m(m\pm 1)} \hbar |s, m\pm 1\rangle \quad [VI-C-40]$$

$$\text{here } s = \frac{1}{2}, m = \pm \frac{1}{2}: \quad S_+ |-\rangle = S_+ |\frac{1}{2}, -\frac{1}{2}\rangle = \sqrt{\frac{3}{4} + \frac{1}{4}} \hbar |\frac{1}{2}, +\frac{1}{2}\rangle = \hbar |+\rangle; \quad S_+ |+\rangle = 0$$

$$S_- |+\rangle = S_- |\frac{1}{2}, +\frac{1}{2}\rangle = \sqrt{\frac{3}{4} - \frac{1}{4}} \hbar |\frac{1}{2}, -\frac{1}{2}\rangle = \hbar |-\rangle; \quad S_- |-\rangle = 0$$

Matrices in  $\{|+\rangle, |-\rangle\}$  basis:

$$S_+ = \hbar \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \quad S_- = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

Spin component operators:  $S_{\pm} = S_x \pm i S_y$

$$\rightarrow S_x = \frac{S_+ + S_-}{2} = \frac{\hbar}{2} \begin{bmatrix} |+\rangle\langle -| + |-\rangle\langle +| \end{bmatrix} \rightarrow S_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$S_y = \frac{S_+ - S_-}{2i} = \frac{\hbar}{2i} \begin{bmatrix} |+\rangle\langle -| - |-\rangle\langle +| \end{bmatrix} \rightarrow S_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

in general  $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$ , where  $\vec{\sigma} = \left( \begin{pmatrix} 0 & 1 \\ i & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right)$  are

known as Pauli matrices

Properties:

- $\sigma_i^2 = 1$ ;  $\sigma_i \sigma_j = \epsilon_{ijk} \sigma_k \Leftrightarrow [\sigma_i, \sigma_j] = 2i \epsilon_{ijk} \sigma_k$
- eigenvalues =  $\pm 1$
- $\text{Tr } \sigma_j = 0$ ;  $\text{Det } \sigma_j = 1$
- $\sigma_j$  Hermitian ( $= \sigma_j^\dagger$ ) and unitary  $\sigma_j^\dagger \sigma_j = \sigma_j^2 = \mathbb{1}$

Spin component operator in direction  $\hat{n} = (\theta, \varphi)$ :

$$S_{\hat{n}} \equiv \vec{S} \cdot \hat{n} = \sin\theta \cos\varphi S_x + \sin\theta \sin\varphi S_y + \cos\theta S_z$$

exercise: check that  $S_{\hat{n}} |\pm\rangle_{\hat{n}} = \pm \frac{\hbar}{2} |\pm\rangle_{\hat{n}}$

$$\text{where } |\pm\rangle_{\hat{n}} = \cos\frac{\theta}{2} |+\rangle_{\hat{z}} + \sin\frac{\theta}{2} e^{i\varphi} |-\rangle_{\hat{z}}$$

→ arbitrary state of spin  $-\frac{1}{2}$  is an eigenstate  $\checkmark$  of  $S_{\hat{n}}$  in some direction  $\hat{n}$

exercise: given a spin  $\frac{1}{2}$  particle in state  $|\psi\rangle = |+\rangle_{\hat{n}}$ , what is

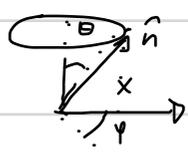
the prob. of measuring  $S_x = +\frac{1}{2}$ ?

$$\text{Projector: } |+\rangle_x \langle +|_x = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \equiv \Pi_{+x}$$

$$\text{prob} = \langle \psi | \Pi_{+x} | \psi \rangle = \langle +_{\hat{n}} | +_x \rangle^2 = \left( \cos\frac{\theta}{2}, \sin\frac{\theta}{2} e^{i\varphi} \right) \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\varphi} \end{bmatrix}$$

$$= \frac{1}{2} \left( \cos\frac{\theta}{2}, \sin\frac{\theta}{2} e^{i\varphi} \right) \cdot \left( \cos\frac{\theta}{2} + \sin\frac{\theta}{2} e^{i\varphi}, \cos\frac{\theta}{2} + \sin\frac{\theta}{2} e^{i\varphi} \right)$$

$$= \frac{1}{2} \left[ \cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} + 2\cos\frac{\theta}{2} \sin\frac{\theta}{2} \left( \frac{e^{i\varphi} + e^{-i\varphi}}{2} \right) \right] = \frac{1}{2} [1 + \sin\theta \cos\varphi]$$



note: show this =  $\cos^2\left(\frac{\alpha}{2}\right)$  where  $\alpha$  angle between  $\hat{n}, \hat{x}$

## Complete description of a particle with spin $\frac{1}{2}$

State space is a tensor product of position and spin parts

Possible basis:  $\{|\vec{r}, +\rangle, |\vec{r}, -\rangle, \forall \vec{r} \in \mathbb{R}^3\}$  (where  $|\vec{r}, +\rangle \equiv |\vec{r}\rangle \otimes |+\rangle$ )

Another possible basis:  $\{|\psi_{nlm}, +\rangle, |\psi_{nlm}, -\rangle\}_{n=1}^{\infty} \begin{matrix} n-1 \\ l=0 \\ m=-l \end{matrix}$

$$\text{Note } \langle \vec{r}, \epsilon | \vec{r}', \epsilon' \rangle = \delta_{\epsilon\epsilon'} \delta(\vec{r} - \vec{r}')$$

$$\langle \psi_{nlm}, \epsilon | \psi_{n'l'm'}, \epsilon' \rangle = \delta_{\epsilon\epsilon'} \delta_{nn'} \delta_{\ell\ell'} \delta_{mm'}$$

Most general state is a combination of all basis elements

$$|\psi\rangle = \left( \sum_{\epsilon=\pm} \int d^3\vec{r} |\vec{r}, \epsilon\rangle \langle \vec{r}, \epsilon | \right) |\psi\rangle = \sum_{\epsilon=\pm} \int d^3\vec{r} \psi_{\epsilon}(\vec{r}) |\vec{r}, \epsilon\rangle$$

$$\text{where } \psi_{\epsilon}(\vec{r}) = \langle \vec{r}, \epsilon | \psi \rangle \in \mathbb{C}$$

One way to see this is to consider that the particle has two position wavefunctions  $\psi_+(\vec{r})$  and  $\psi_-(\vec{r})$  (which can be completely different)

Note that in this most general state position and spin are entangled

## Spinor formalism [optional]

It is often useful to represent the state as a two-component "spinor"

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

Note  $\langle \varphi | \psi \rangle = \int (\varphi_+^*(\vec{r}) \ \varphi_-^*(\vec{r})) \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} d^3r = \int [\varphi]^\dagger(\vec{r}) [\psi](\vec{r}) d\vec{r}$

(similar to regular product of 3D states but containing matrix mult.)

Operators  $A$  also have spinor representation  $A|\psi\rangle \Rightarrow [A][\psi](\vec{r})$

Particularly simple cases:

spin-only operators: act on spinors exactly as the corresponding  $2 \times 2$  matrices

$$\text{ex: } [S_z][\psi](\vec{r}) = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}$$

position-only ops: act diagonally,

$$\begin{aligned} \text{eg } [[P_x]][\psi](\vec{r}) &= \left[ P_x \otimes \mathbb{1} \sum_{\epsilon=\pm} \int d^3\vec{r}' \psi_{\epsilon}(\vec{r}') |\vec{r}', \epsilon\rangle \right] \\ &= \left[ \sum_{\epsilon} \int d^3\vec{r}' (-i\hbar \partial_{x'} \psi_{\epsilon}(\vec{r}') / \partial_{x'} |\vec{r}', \epsilon\rangle \right] = \begin{bmatrix} -i\hbar \frac{\partial}{\partial x} \psi_+(\vec{r}) \\ -i\hbar \frac{\partial}{\partial x} \psi_-(\vec{r}) \end{bmatrix} \end{aligned}$$

$$\therefore \left[ P_x \right] \leftrightarrow -i\hbar \begin{bmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial x} \end{bmatrix}$$

product operator example :  $L_z S_z$

$$L_z \leftrightarrow -i\hbar \frac{\partial}{\partial \varphi} \quad \text{in coordinate basis} \quad S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\rightarrow \left[ L_z S_z \right] \left[ \Psi \right] (\vec{r}) = \left[ \sum_{\epsilon} \int d^3\vec{r} L_z \Psi_{\epsilon}(\vec{r}) |\vec{r}\rangle \otimes S_z |\epsilon\rangle \right]$$

$$= \frac{-i\hbar^2}{2} \sum_{\epsilon} \int d^3\vec{r} \left[ \frac{\partial \Psi_+(\vec{r})}{\partial \varphi} |\vec{r}, +\rangle - \frac{\partial \Psi_-(\vec{r})}{\partial \varphi} |\vec{r}, -\rangle \right] \leftrightarrow \frac{-i\hbar^2}{2} \begin{bmatrix} \frac{\partial \Psi_+(\vec{r})}{\partial \varphi} \\ -\frac{\partial \Psi_-(\vec{r})}{\partial \varphi} \end{bmatrix}$$

$$\therefore \left[ L_z S_z \right] = \frac{-i\hbar^2}{2} \begin{bmatrix} \frac{\partial}{\partial \varphi} & 0 \\ 0 & -\frac{\partial}{\partial \varphi} \end{bmatrix}$$

$$\text{non-product operator. Ex: } \vec{S} \cdot \vec{P} \quad \leftrightarrow \frac{-i\hbar^2}{2} \begin{bmatrix} \frac{\partial}{\partial z} & \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} & -\frac{\partial}{\partial z} \end{bmatrix}$$

Note: the convention adopted in this formalism for ordering the product basis is to first order over  $\vec{r}$  for fixed  $\epsilon = +$ , then order again over  $\vec{r}$  for fixed  $\epsilon = -$ . Thus, in order to be consistent with the general formalism for tensor products developed in II-F, the spin d.o.f. should be the 1<sup>st</sup> element of the tensor product space, i.e., we should write  $|\epsilon, \vec{r}\rangle$  instead of  $|\vec{r}, \epsilon\rangle$ ;  $S_z \leftrightarrow S_z \otimes \mathbb{1}$  etc.

Example of calculation of physical properties

Suppose a H atom is in the spinor state  $\begin{bmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{bmatrix} = [\Psi]$

What is the probability

i) of finding the atom w/ spin  $S_z = +\frac{1}{2}$  (irrespective of position)

$$\begin{aligned} A: P &= \langle \Psi | \left( \mathbb{1}_{\mathbb{R}^3} \otimes |+\rangle\langle+| \right) | \Psi \rangle = \int d^3\vec{r} |\langle \vec{r}, + | \Psi \rangle|^2 = \int d^3\vec{r} |\psi_+(\vec{r})|^2 \\ &= [\Psi]^\dagger \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} [\Psi] \end{aligned}$$

ii) of finding the atom with spin  $S_x = +\frac{1}{2}$ , irrespective of position?

$$|+\rangle\langle+| = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} :$$

$$\begin{aligned} P(S_x = +\frac{1}{2}) &= [\Psi]^\dagger \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} [\Psi] = \frac{1}{2} \int d^3\vec{r} (|\psi_+(\vec{r})|^2 + |\psi_-(\vec{r})|^2 + \psi_+^* \psi_- + \psi_-^* \psi_+(\vec{r})) \\ &= \frac{1}{2} \left( 1 + \int d^3\vec{r} [\psi_+^*(\vec{r}) \psi_-(\vec{r}) + \psi_-^*(\vec{r}) \psi_+(\vec{r})] \right) \end{aligned}$$

porém: spin  $\neq$  rotação orbital... resultado "mais correto" [eq. Dirac].

$$\boxed{\vec{M}_s = -\frac{e}{m} \vec{S}}$$

(ou  $\vec{M}_s = g \left( \frac{-e}{2m} \vec{S} \right)$ , onde  $g=2$  é o "fator giromagnético do elétron")

porém 2: resultado "mais correto ainda" (QED):  $g = 2 + \frac{\alpha}{\pi} + O(\alpha^2) \approx 2.002\dots$

$$-\frac{e}{m} \cdot \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\mu_B = \frac{\hbar e}{2m}$$

The value of  $s$  consistent with experiments is  $s = \frac{1}{2}$  (a half-integer)

Putting it another way

- recheck spinor on b - more examples?
- spinor exercise
- clean up / finish lista 1
- suggest 6 problems