Chapter 14: Spin

Spin has no classical analogue, so the postulates of QM are not helpful in constructing the operators describing spin.

We need to develop some new intuition and mathematical techniques.

The nature of spin

Spin is a form of angular momentum, but not orbital angular momentum. It can be assigned to a point particle, which has no rotating mass elements, and exists even if that particle is at rest (in which case $\vec{r}\times\vec{p}=0$). It is an "intrinsic" property of the particle, similar to charge and mass, although it has a direction which can change in time (charge and mass don't), although its magnitude remains constant in time.

Spin couples to magnetic fields, since a charged spinning particle has a magnetic moment. This is how spin is measured, and indeed the intrinsic magnetic moment of an electron (even when at rest) is the primary observable, and the associated spin angular momentum is a theoretical abstraction.

Experimentally one cannot distinguish between a magnetic moment due to spin and one due to orbital angular momentum of a charge. Both behave like angular momenta, satisfying the same commutator algebra.

Kinematics of spin

Remember our discussion of rotations and the associated eigenvalue problem of the angular momentum operator. We found that for a particle described by a wavefunction with many (n) components, the generator of infinitesimal rotations is not just $\vec{\hat{L}}$. Under rotations <u>two</u> things must happen simultaneously:

$\vec{\hat{L}}$: (1) The values of ψ_i $(i=1,\dots,n)$ are assigned to the rotated point

$\vec{\hat{S}}$: (2) The components of $\vec{\psi}$ get transformed into linear combinations of each other (the "direction" of $\vec{\psi}$ is "rotated")

Step (2) is generated by an $n\times n$ matrix. If $n\neq 3$, the "rotation" of $\vec{\psi}$ is not the same as the rotation of the point $\vec{r}$ at which $\vec{\psi}(\vec{r})$ is located – it is a more general operation. For an infinitesimal rotation ε around $\vec{e}_z$ the wave function in the x-basis transforms like:

$$\Rightarrow \begin{pmatrix}\psi_1'(\vec{r})\\ \psi_2'(\vec{r})\\ \vdots \\ \psi_n'(\vec{r})\end{pmatrix} = \left[\begin{pmatrix}1 & & 0\\ & \ddots & \\ 0 & & 1\end{pmatrix} - \frac{i\varepsilon}{\hbar}\begin{pmatrix}-i\hbar\frac{\partial}{\partial\varphi} & & & 0\\ & -i\hbar\frac{\partial}{\partial\varphi} & & \\ & & \ddots & \\ 0 & & & -i\hbar\frac{\partial}{\partial\varphi}\end{pmatrix} - \frac{i\varepsilon}{\hbar}\begin{pmatrix}S_z^{11} & S_z^{12} & \cdots \\ \vdots & \ddots & \\ \vdots & & S_z^{nn}\end{pmatrix}\right]\begin{pmatrix}\psi_1(\vec{r})\\ \vdots \\ \psi_n(\vec{r})\end{pmatrix}$$

In abstract Hilbert-space language this equation reads

$$|\psi'\rangle = \left(\hat{\mathbb{1}} - \frac{i\varepsilon}{\hbar}\left(\hat{L}_z + \hat{S}_z\right)\right)|\psi\rangle = \left(\hat{\mathbb{1}} - \frac{i\varepsilon}{\hbar}\hat{J}_z\right)|\psi\rangle$$

The wave functions $\vec{\psi}(\vec{r}) = (\psi_1(\vec{r}), \ldots, \psi_n(\vec{r}))$ are the components of the state $|\psi\rangle$ in a basis made up from a direct product of position eigenstates $|\vec{r}\rangle$ and $\hat{S}_z$-eigenstates $|s_z\rangle$,

$S_z|s_z\rangle = s_z|s_z\rangle$ $(s_z = m_1\hbar, \ldots, m_n\hbar)$ where $s_z = m_1\hbar, \ldots, m_n\hbar$ are the n eigenvalues of $\hat{S}_z$ and we have used the representation $|s_z = m_i\hbar\rangle \equiv \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \leftarrow i^{th}$ row.

Generalizing to rotations around any axis gives

$$\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$$

We now need to figure out how many components (n) we need to describe electrons, and what are the corresponding matrix representations of $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$.

As generators of rotations, $\hat{J}_i$ must satisfy the commutation relations

$$[\hat{J}_i, \hat{J}_j] = i\hbar\, \varepsilon_{ijk} \underbrace{\hat{J}_k}$$

Since $\hat{\vec{L}}$ and $\hat{\vec{S}}$ act on different factors of the

Hilbert space states $|\vec{r}\rangle \otimes |s_z\rangle$ (or in different subspaces of the corresponding direct product space), they commute:

$$[\hat{L}_i, \hat{S}_j] = 0 \quad \forall\, i,j = 1,2,3$$

$$\Rightarrow [\hat{J}_i, \hat{J}_j] = \underbrace{[\hat{L}_i, \hat{L}_j]}_{= i\hbar\varepsilon_{ijk}\hat{L}_k} + [\hat{S}_i, \hat{S}_j]$$

$$\qquad\qquad + \; i\hbar\,\varepsilon_{ijk}\hat{S}_k$$

$$\Rightarrow \boxed{[\hat{S}_i, \hat{S}_j] = i\,\varepsilon_{ijk}\hat{S}_k}$$

So spin, orbital and total angular momentum all satisfy the same commutation relations.

Now let's address the question how many components we need. The answer is that electrons have spin $\frac{\hbar}{2}$, so $\hat{\vec{S}}^2$ has eigenvalue $s(s+1)\hbar^2 = \frac{3}{4}\hbar^2$, and $\hat{S}_z$ has correspondingly eigenvalues $s_z = m\hbar$ with $m = s, s-1, \ldots, -s$ $= \frac{1}{2}, -\frac{1}{2}$.

$\Rightarrow$ only two eigenvalues of s_z $\Rightarrow$ 2 component wave function:

$$(\langle\vec{r}|\otimes\langle s_z|)|\psi\rangle = \langle\vec{r}, s_z|\psi\rangle = \psi(\vec{r}, s_z) = C_+\psi_+(\vec{r})\cdot\begin{pmatrix}1\\0\end{pmatrix} + C_-\psi_-(\vec{r})\begin{pmatrix}0\\1\end{pmatrix}$$

probability amplitude for electron with $s_z = \frac{1}{2}\hbar$ at $\vec{r}$

prob. amplitude for electron with $s_z = -\frac{1}{2}\hbar$ at $\vec{r}$

Hence

$$|\psi\rangle \xrightarrow[\hat{\vec{R}},\,\hat{S}_z \text{ basis}]{} \begin{pmatrix}\tilde{\psi}_+(\vec{r})\\ \tilde{\psi}_-(\vec{r})\end{pmatrix} \qquad (\tilde{\psi}_\pm = C_\pm\psi_\pm)$$

The corresponding matrices that represent $\hat{S}_x, \hat{S}_y, \hat{S}_z$ in this 2-dimensional space are the 2×2 blocks corresponding the colums and rows labelled $(\frac{1}{2},\frac{1}{2})$ and $(\frac{1}{2},-\frac{1}{2})$ in the block-diagonal matrices for J_x, J_y, J_z on p. 328:

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

$$= \frac{\hbar}{2}\sigma_x \qquad\qquad = \frac{\hbar}{2}\sigma_y \qquad\qquad = \frac{\hbar}{2}\sigma_z$$

($\sigma_x, \sigma_y, \sigma_z$ = Pauli matrices)

Let us now consider an ensemble of electrons prepared in a state of zero momentum, $\vec{p}=0$:

$$\hat{\vec{P}}|\psi\rangle = 0$$

In our basis representation, $\hat{\vec{P}}$ acts only on the spatial part of the wave function, so we need its representation in the x-basis:

$$\begin{pmatrix} -i\hbar\vec{\nabla}\psi_+(\vec{r}) \\ -i\hbar\vec{\nabla}\psi_-(\vec{r}) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

$\Rightarrow$ ψ_+ and ψ_- are both independent of x, y, z.

$$\Rightarrow \hat{\vec{L}}|\psi\rangle = (\hat{\vec{R}}\times\vec{P})|\psi\rangle = 0$$

$\Rightarrow$ The state has zero orbital momentum.

But it's spin is nonzero: $S_z\begin{pmatrix}\psi_+ \\ \psi_-\end{pmatrix} = \begin{pmatrix}\psi_+ \\ -\psi_-\end{pmatrix}$

ψ_+ is the amplitude for measuring $s_z = +\frac{\hbar}{2}$,

ψ_- is the amplitude for measuring $s_z = -\frac{\hbar}{2}$

The total spin operator $\hat{\vec{S}}^2$ is represented by

$$\vec{S}^2 = S_x^2 + S_y^2 + S_z^2 = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdot 3 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hbar^2 \begin{pmatrix} \frac{1}{2}(\frac{1}{2}+1) & 0 \\ 0 & \frac{1}{2}(\frac{1}{2}+1) \end{pmatrix}$$

$$= s(s+1)\hbar^2 \hat{\mathbb{1}}$$

It yields the value $\frac{3}{4}\hbar^2$ on any state $|\psi\rangle$ – the spins of an electron is always ½ and never changes.

Normalization of the "spinor states"

$$|\psi\rangle \longrightarrow \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}$$

$$1 = \langle\psi|\psi\rangle = \sum_{s_z} \langle\psi|\vec{r}, s_z\rangle\langle\vec{r}, s_z|\psi\rangle\, d^3r$$

$$= \int d^3r \left(|\psi_+(\vec{r})|^2 + |\psi_-(\vec{r})|^2\right)$$

$$\hat{\mathbb{1}} = \sum_{s_z} \int d^3r\ |\vec{r}, s_z\rangle\langle\vec{r}, s_z|$$

If the Hamiltonian is separable into an orbital and spin part,

$$\hat{H} = \hat{H}_o + \hat{H}_s$$

with no so-called spin-orbit coupling (such couplings arise, however, in relativistic electron theory), then the states $|\psi(t)\rangle$ factorize into

$$|\psi(t)\rangle = |\psi_o(t)\rangle \otimes |\psi_s(t)\rangle$$

where $|\psi_o(t)\rangle$ evolves with $\hat{H}_o$ and $|\psi_s(t)\rangle$ evolves independently with $\hat{H}_s$.

Let us study the structure and evolution of $|\psi_s(t)\rangle$ in greater depth.

- Basis: $|s, s_z\rangle \equiv |s, m\hbar\rangle \equiv |s, m\rangle \quad (s = \frac{1}{2}, m = \pm\frac{1}{2})$

$$|\tfrac{1}{2}\,\tfrac{1}{2}\rangle \leftrightarrow \begin{pmatrix}1\\0\end{pmatrix}$$
$$|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle \underset{S_z\text{ basis}}{\longleftrightarrow} \begin{pmatrix}0\\1\end{pmatrix}$$

- General spin state:

$$|\psi_s\rangle = |\chi\rangle = \alpha|\tfrac{1}{2}\,\tfrac{1}{2}\rangle + \beta|\tfrac{1}{2},-\tfrac{1}{2}\rangle \longleftrightarrow \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

- Normalization:

$$1 = \langle\chi|\chi\rangle \underset{S_z\text{basis}}{\longleftrightarrow} (\alpha^* \beta^*)\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = |\alpha|^2 + |\beta|^2$$

- spin expectation value:

$$\langle\tfrac{1}{2}, \pm\tfrac{1}{2}|\,\hat{\vec{S}}\,|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle = \pm\frac{\hbar}{2}\vec{e}_z. \qquad (\Rightarrow \langle\tfrac{1}{2},\pm\tfrac{1}{2}|\hat{S}_{x,y}|\tfrac{1}{2},-\tfrac{1}{2}\rangle = 0)$$

- eigenstates for other spin components:

Consider $S_n \equiv \vec{n}\cdot\hat{\vec{S}}$ with $\vec{n}$ some unit vector

$$\Rightarrow \langle\vec{n},\pm|\,\hat{\vec{S}}\,|\vec{n},\pm\rangle = \pm\frac{\hbar}{2}\vec{n}$$

where $|\vec{n},\pm\rangle$ is an eigenstate of $\vec{n}\cdot\hat{\vec{S}}$ with eigenvalue $\pm\hbar/2$. (spin "up" or "down" in the direction of $\vec{n}$)

In more detail:

$$\vec{n} = (\sin\vartheta\cos\varphi,\ \sin\vartheta\sin\varphi,\ \cos\vartheta) = (n_x, n_y, n_z)$$

$|\vec{n},\pm\rangle$ are eigenvectors of

$$\vec{n}\cdot\hat{\vec{S}} = n_x\hat{S}_x + n_y\hat{S}_y + n_z\hat{S}_z \longleftrightarrow \frac{\hbar}{2}\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z\end{pmatrix}$$
$$= \frac{\hbar}{2}\begin{pmatrix}\cos\vartheta & \sin\vartheta\, e^{-i\varphi} \\ \sin\vartheta\, e^{i\varphi} & -\cos\vartheta\end{pmatrix}$$

$$|\vec{n},+\rangle \longleftrightarrow \begin{pmatrix} \cos\left(\frac{\vartheta}{2}\right) e^{-i\varphi/2} \\ \sin(\vartheta/2)\, e^{i\varphi/2} \end{pmatrix}$$

$$|\vec{n},-\rangle \longleftrightarrow \begin{pmatrix} -\sin(\vartheta/2)\, e^{-i\varphi/2} \\ \cos(\vartheta/2)\, e^{i\varphi/2} \end{pmatrix}$$

Proof: $\vec{n}\cdot\hat{\vec{S}}\,|\vec{n},+\rangle \Longleftrightarrow \frac{\hbar}{2}\begin{pmatrix} \cos\vartheta \cos\vartheta/2\, e^{-i\varphi/2} + \sin\vartheta \sin\vartheta/2\, e^{-i\varphi/2} \\ \sin\vartheta \cos\vartheta/2\, e^{i\varphi/2} - \cos\vartheta \sin\vartheta/2\, e^{+i\varphi/2} \end{pmatrix}$

$$= \frac{\hbar}{2}\begin{pmatrix} \cos\vartheta/2\, e^{-i\varphi/2} \\ \sin\vartheta/2\, e^{i\varphi/2} \end{pmatrix} \longleftrightarrow +\frac{\hbar}{2}\,|\hat{\vec{n}},\vec{S}\rangle$$

and similarly for $|\vec{n},-\rangle$.

- Can verify that

$$\langle\vec{n},\pm|\hat{\vec{S}}|\vec{n},\pm\rangle = \pm\frac{\hbar}{2}\left(\sin\vartheta\cos\varphi\,\vec{e}_x + \sin\vartheta\sin\varphi\,\vec{e}_y + \cos\vartheta\,\vec{e}_z\right)$$

$$= \pm\frac{\hbar}{2}\vec{n}$$

- Interesting: not only can we compute $\langle\hat{\vec{S}}\rangle$ given a state vector, but we can also reconstruct the state vector when given $\langle\hat{\vec{S}}\rangle$! This is because the general state $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ has only 3 [(2 complex = 4 real) minus 1 normalization constraint] real degrees of freedom.

Pauli matrices

$$\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}} \longleftrightarrow \sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix} \quad \sigma_y = \begin{pmatrix}0&-i\\i&0\end{pmatrix} \quad \sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

$$[\hat{\sigma}_i,\hat{\sigma}_j]_+ = 2\,\delta_{ij}\,\hat{\mathbb{1}}_{2\times 2} \quad \left(\text{anticommute if } i\neq j;\ \sigma_i^2 = \mathbb{1}\ (i=1,2,3)\right)$$

$$(\vec{n}\cdot\hat{\vec{\sigma}})^2 = \hat{\mathbb{1}}: \quad (n_i\hat{\sigma}_i)(n_j\hat{\sigma}_j) = n_i n_j\,\hat{\sigma}_i\hat{\sigma}_j = \frac{1}{2}n_i n_j [\hat{\sigma}_i,\hat{\sigma}_j]_+$$

$$= \frac{1}{2}n_i n_j\, 2\delta_{ij}\hat{\mathbb{1}} = \vec{n}^2\,\hat{\mathbb{1}} = \hat{\mathbb{1}}.$$

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\,\varepsilon_{ijk}\,\hat{\sigma}_k \qquad \text{(angular momentum algebra)}$$

$$\Rightarrow (\vec{A}\cdot\hat{\vec{\sigma}})(\vec{B}\cdot\vec{\sigma}) = A_i B_j\, \hat{\sigma}_i \hat{\sigma}_j = A_i B_j \left(\tfrac{1}{2}[\hat{\sigma}_i,\hat{\sigma}_j]_+ + \tfrac{1}{2}[\hat{\sigma}_i,\hat{\sigma}_j]_-\right)$$

$$= A_i B_j \left(\tfrac{1}{2}\cdot 2\delta_{ij}\,\hat{\mathbb{1}} + \tfrac{1}{2}\, 2i\,\varepsilon_{ijk}\,\hat{\vec{\sigma}}_k\right)$$

$$= \vec{A}\cdot\vec{B}\,\hat{\mathbb{1}} + i\,(\vec{A}\times\vec{B})\cdot\hat{\vec{\sigma}}$$

$$\mathrm{Tr}(\sigma_i\sigma_j) = \mathrm{Tr}\left(\tfrac{1}{2}[\sigma_i,\sigma_j]_+ + \tfrac{1}{2}[\hat{\sigma}_i,\hat{\sigma}_j]_-\right)$$

$$= \mathrm{Tr}(\delta_{ij}\,\mathbb{1}_{2\times 2}) + i\,\varepsilon_{ijk}\,\underbrace{\mathrm{Tr}(\sigma_k)}_{0}$$

$$= 2\delta_{ij}$$

- Let us view the identity $\mathbb{1}_{2\times2}$ as a fourth Pauli matrix, $\sigma_0 = \mathbb{1}_{2\times 2}$

$$\Rightarrow \mathrm{Tr}(\sigma_\alpha \sigma_\beta) = 2\,\delta_{\alpha\beta}$$

$\Rightarrow$ the matrices σ_α are linearly independent:

let $\sum_\alpha c_\alpha \sigma_\alpha = 0 \Rightarrow \sigma_\beta \sum_\alpha c_\alpha \sigma_\alpha = 0$

$$\Rightarrow \sum_\alpha c_\alpha \mathrm{Tr}(\sigma_\alpha\sigma_\beta) = \sum_\alpha c_\alpha 2\delta_{\alpha\beta} = 0 \Rightarrow c_\beta = 0\ \forall\beta.$$

- Since any 2×2 matrix M has only 4 complex degrees of freedom, it can be written as

$$M = \sum_\alpha m_\alpha \sigma_\alpha \qquad m_\alpha \in \mathbb{C}$$

with $m_\alpha = \frac{1}{2}\mathrm{Tr}(M\sigma_\alpha)$

Rotation operators

$$\underbrace{\mathcal{U}[\hat{R}(\vec{\vartheta})]}_{} = e^{-i\vec{\theta}\cdot\hat{\vec{S}}/\hbar} = e^{-i\vec{\theta}\cdot\hat{\vec{\sigma}}/2}$$

$$= e^{-i\frac{\vartheta}{2}\hat{\theta}\cdot\hat{\vec{\sigma}}} = \sum_{n=0}^{\infty}\left(-\frac{i\vartheta}{2}\right)^n \frac{1}{n!}\left(\hat{\theta}\cdot\hat{\vec{\sigma}}\right)^n$$

$$= \sum_{n\,\text{even}}\left(-\frac{i\vartheta}{2}\right)^n \frac{1}{n!}\hat{\mathbb{1}} + \sum_{n\,\text{odd}}\left(-\frac{i\vartheta}{2}\right)^n \frac{1}{n!}\hat{\theta}\cdot\hat{\vec{\sigma}}$$

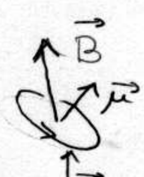
$$= \hat{\mathbb{1}}\cdot\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k)!}\left(\frac{\vartheta}{2}\right)^{2k} - i\,\hat{\theta}\cdot\hat{\vec{\sigma}}\sum_{k=1}\frac{(-1)^k}{(2k+1)!}\left(\frac{\vartheta}{2}\right)^{2k+1}$$

$$= \hat{\mathbb{1}}\cos\frac{\vartheta}{2} - i\,\hat{\theta}\cdot\hat{\sigma}\sin\left(\frac{\vartheta}{2}\right)$$

Time evolution – Spin dynamics

1. Classically:

Interaction of a magnetic moment $\vec{\mu}$ with a magnetic field $\vec{B}$:



$$\mathcal{H}_{int} = -\vec{\mu}\cdot\vec{B}$$

torque on the current loop:

$$\vec{T} = \vec{\mu}\times\vec{B}$$

lowest energy state: $\vec{\mu} \parallel \vec{B}$

Example: current $\vec{I}$ caused by single charge q of mass m going around a circle of radius r (area $a = \pi r^2$):

$$I = \frac{\Delta Q}{\Delta t} = \frac{q v}{2\pi r}$$

$$\mu = I\frac{a}{c} = \frac{qv}{2\pi r}\frac{\pi r^2}{c} = \frac{q}{2mc} mvr = \frac{q}{2mc}\cdot l$$

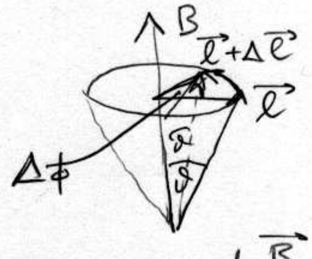
where l = orbital angular momentum

$$\Rightarrow \boxed{\vec{\mu} = \gamma \vec{l} = \frac{q}{2mc}\vec{l}} \qquad \left(\gamma = \frac{q}{2mc} = \text{"gyromagnetic ratio"}\right)$$

Equation of motion:

$$\frac{d\vec{l}}{dt} = \vec{T} = \vec{\mu}\times\vec{B} = \gamma\left(\vec{l}\times\vec{B}\right)$$

In small Δt:



$$\Delta\vec{l} = \gamma\left(\vec{l}\times\vec{B}\right)\Delta t$$

$$\Delta l = \gamma l B \sin\vartheta \, \Delta t$$

$(\Delta\vec{l} \perp \vec{l}, \vec{B}) \Rightarrow \vec{l}$ precesses around $\vec{B}$

$$\Delta\phi = \left(\frac{-\Delta l}{l\sin\vartheta}\right) = -\gamma B \, \Delta t$$

$$\Rightarrow \boxed{\vec{\omega}_0 = -\gamma\vec{B}}$$ precession frequency (clockwise for positive charge)

2. Quantum mechanically:

$$\hat{H} = \frac{\left(\hat{\vec{P}} - \frac{q}{c}\hat{\vec{A}}\right)^2}{2m} = \frac{\hat{\vec{P}}^2}{2m} - \frac{q}{2mc}\left(\hat{\vec{P}}\cdot\hat{\vec{A}} + \hat{\vec{A}}\cdot\hat{\vec{P}}\right) + \frac{q^2|\hat{\vec{A}}|^2}{2mc^2}$$

Assume $\vec{B} = B\vec{e}_z$, $\vec{A} = \frac{B}{2}\left(-y\vec{e}_x + x\vec{e}_y\right)$ $(\Rightarrow \vec{\nabla}\cdot\vec{A} = 0$ Coulomb gauge)

and small B so that $\frac{q^2}{c^2}|A|^2 \ll \frac{q}{c}\vec{P}\cdot\vec{A}$:

Compute

$$\hat{\vec{P}}\cdot\hat{\vec{A}}|\psi\rangle \longrightarrow -i\hbar\vec{\nabla}\cdot\left(\vec{A}\psi(\vec{r})\right) = -i\hbar\vec{A}\cdot\vec{\nabla}\psi(\vec{r}) \rightarrow \hat{\vec{A}}\cdot\hat{\vec{P}}|\psi\rangle$$

So in this gauge the interaction between the moving particle and the magnetic field is approximately

$$\hat{H}_{int} = -\frac{q}{2mc}2\hat{\vec{A}}\cdot\hat{\vec{P}} = -\frac{q}{mc}\frac{B}{2}\left(-\hat{Y}\hat{P}_x + \hat{X}\hat{P}_y\right) = -\frac{q}{2mc}\hat{\vec{L}}\cdot\hat{\vec{B}} = -\hat{\vec{\mu}}\cdot\hat{\vec{B}}$$

with $\hat{\vec{\mu}} \equiv \frac{q}{2mc}\hat{\vec{L}}$, just like in the classical case.

The z-component of $\hat{\vec{\mu}}$ has eigenvalues

$$\mu_z = \frac{q}{2mc} L_z = \frac{q\hbar}{2mc}(0, \pm 1, \pm 2, \dots)$$

For the electron

$$\mu_e \equiv \frac{e\hbar}{2mc} \approx 0.6 \times 10^{-8} \frac{\text{eV}}{\text{G}} \qquad \text{electron Bohr magneton}$$

For a nucleon

$$\mu_N = \frac{e\hbar}{2Mc} \approx 0.3 \times 10^{-11} \frac{\text{eV}}{\text{G}} \qquad \text{nucleon Bohr magneton} \approx \frac{1}{2000}\mu_e$$

Ehrenfest's thm: $\langle \hat{\vec{L}} \rangle$ precesses around $\vec{B}$ just as the classical $\vec{\ell}$ does.

Spin magnetic moment

Analogous to $\hat{\vec{\mu}} = \gamma \hat{\vec{L}}$ for a circling charge,

introduce $\boxed{\hat{\vec{\mu}} = \gamma \hat{\vec{S}}}$ for a charged particle with spin.

We write $\boxed{\gamma = g\left(-\frac{e}{2mc}\right)}$ where g is a constant multiplying the Bohr magneton that arises in the orbital case.

$$\Rightarrow \hat{H}_{int} = -\hat{\vec{\mu}} \cdot \hat{\vec{B}} = \frac{ge}{2mc} \hat{\vec{S}} \cdot \vec{B} = \frac{ge\hbar}{4mc} \hat{\vec{\sigma}} \cdot \vec{B}$$

The intrinsic magnetic moment due to spin is $\frac{g}{2}$ magnetons.

Experimentally, $g \approx 2$ (deviations due to QED effects)

$\Rightarrow$ The gyromagnetic ratio for spin is twice as large as for orbital angular momentum!

($g=2$ is predicted by the Dirac equation; quantum field theoretical corrections from QED arise from coupling between $\vec{S}$ and vacuum fluctuations in $\vec{B}$ $\Rightarrow$ $g_{QED} = 2\left[1+\frac{\alpha}{2\pi}+O(\alpha^2)\right]$

$$= 2\cdot[1.00115965214\bullet(\pm 28)] \text{ to order } \alpha^3$$

$$g_{exp} = 2\cdot[1.0011596521884(\pm 43)] \quad ! \;)$$

Spin dynamics in a magnetic field:

$$\hat{H}_s = -\hat{\vec{\mu}}\cdot\vec{B} = -\gamma\,\hat{\vec{S}}\cdot\vec{B} \qquad \left(\gamma = -\frac{e}{mc}\right)$$

$$|\psi_s(t)\rangle = \hat{U}_s(t)\,|\psi_s(0)\rangle \qquad \text{(spin factor of the particle state only)}$$

$$\hat{U}_s(t) = e^{i\gamma t(\vec{S}\cdot\vec{B})/\hbar}$$

This is a rotation operator by the angle

$$\boxed{\vec{\theta}(t) = -\gamma\vec{B}t} \quad !$$

$\Rightarrow \langle\hat{\vec{S}}\rangle$ precesses around $\vec{B}$ at frequency

$\boxed{\vec{\omega}_0 = -\gamma\vec{B}}$, just as in classical physics!

$$\boxed{\hat{U}_s(t) = \hat{\mathbb{1}}\cos(\omega_0 t) + i(\hat{B}\cdot\hat{\vec{\sigma}})\sin(\omega_0 t)} \underset{\hat{B}=\vec{e}_z}{\longleftrightarrow} \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & -e^{-i\omega_0 t/2} \end{pmatrix}$$

Putting back the orbital degrees of freedom:

$$\hat{H} = \hat{H}_0 + \hat{H}_s \qquad |\psi\rangle = |\psi_0\rangle \otimes |\chi_s\rangle$$

Example: hydrogen atom, $\hat{H} = \hat{H}_0$ independent of spin

$\Rightarrow$ spin is constant in time. S_z eigenstates:

$$|nlm\rangle \longmapsto |n\,l\,m; m_s = +\tfrac{1}{2}\rangle \rightarrow \psi_{nlm}(r,\vartheta,\varphi)\chi_+ \equiv \begin{pmatrix}\psi_{nlm}(r,\vartheta,\varphi)\\ 0\end{pmatrix}$$

spinless electron

$$\text{or} \quad |nlm; m_s = -\tfrac{1}{2}\rangle \rightarrow \psi_{nlm}(r,\vartheta,\varphi)\chi_- \equiv \begin{pmatrix}0\\ \psi_{nlm}(r,\vartheta,\varphi)\end{pmatrix}$$

Since $\hat{H}$ is spin-independent, these states have the same energy eigenvalues as for the spinless electron

Example: hydrogen atom in a weak magnetic field $\vec{B} = B\vec{e}_z$:

due to the smallness of $\frac{m}{M}$, we can ignore the coupling of the proton's spin and orbital magnetic moments to $\vec{B}$ when compared with the analogous coupling to the electron magnetic moment:

$$\hat{H} = \hat{H}_{\text{Coulomb}} - \underbrace{\left(\frac{-e}{2mc}\right)\hat{L}_z}_{\mu^e_{z,\text{orbital}}} B - \underbrace{\left(\frac{-e}{mc}\right)\hat{S}_z}_{\mu^e_{z,\text{intrinsic}}} B$$

Since $\hat{H}_{\text{Coulomb}}$ commutes with $\hat{L}^2, \hat{L}_z, \hat{S}_z$, and $\hat{L}_z, \hat{S}_z$ commute with $\hat{L}^2$, $\hat{H}$ has the same eigenstates as $\hat{H}_0$, but with different energy eigenvalues:

$$\hat{H}|nlmm_s\rangle = \left(-\frac{R_y}{n^2} + \frac{eB\hbar}{2m_ec}(m + 2m_s)\right)|nlmm_s\rangle$$

The magnetic field splits the degeneracy between the $2l+1$ magnetic substates m and between the spin up and down states, $m_s = \pm 1$. Some degeneracies remain, though:

The ground state splits into 2 levels:

$$E_{n=1} = -R_y \pm \frac{e\hbar B}{2mc} \qquad (m_s = \pm 1/2)$$

The first excited state $n=2$, which was $4\times 2 = 8$-fold degenerate, splits into 5 levels:

$$E_{n=2} = -\frac{R_y}{4} + \frac{e\hbar B}{2mc} \times \begin{cases} 2 & (l m m_s) = (1 1 \tfrac{1}{2}) \\ 1 & (l m m_s) = (1 0 \tfrac{1}{2}) \text{ or } (0 0 \tfrac{1}{2}) \\ 0 & (l m m_s) = (1, 1, -\tfrac{1}{2}) \text{ or } (1, -1, \tfrac{1}{2}) \\ -1 & (l m m_s) = (1 0 -\tfrac{1}{2}) \text{ or } (0 0 -\tfrac{1}{2}) \\ -2 & (l m m_s) = (1, -1, -\tfrac{1}{2}) \end{cases}$$

and so on. $\Rightarrow$ more spectral lines!

$\Rightarrow$ "Zeeman effect".

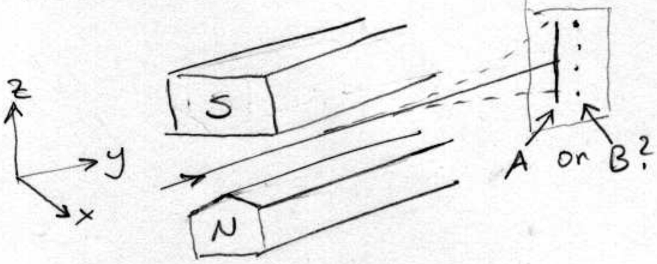
Example: $\hat{H} = \hat{H}_{Coulomb} + a\,\hat{\vec{L}}\cdot\hat{\vec{S}}$

(the relativistic origin of the $\hat{\vec{L}}\cdot\hat{\vec{S}}$ term will be explained later)

Since this depends on all 3 components of $\hat{\vec{L}}$ and $\hat{\vec{S}}$ and these don't commute with each other, the states $|nlmm_s\rangle$ are not eigenstate of $\hat{H}$, and no separation of orbital and spin degrees of freedom is possible. So the eigenstates will not have the form $|\psi_0\rangle \otimes |\chi_s\rangle$, but be linear superpositions of such states that diagonalize $\hat{\vec{L}}\cdot\hat{\vec{S}}$

Details to follow...

Stern - Gerlach experiment



<u>inhomogeneous</u> magnetic field,

$$\vec{B} = B_z(z)\vec{e}_z, \quad \frac{\partial B_z}{\partial z} < 0$$

beam of electrons in y direction, parallel to the edge of the N magnet, through region where

$\frac{\partial B_z}{\partial z} < 0.$

The inhomogenous $\vec{B}$-field exerts a force on the electrons due to their $\vec{\mu}_s \cdot \vec{B}$ coupling:

$$\vec{F} = -\vec{\nabla}\mathcal{H} = +\vec{\nabla}(\vec{\mu}\cdot\vec{B}) = \mu_z \frac{\partial B_z}{\partial z}\vec{e}_z$$

(If there is also a $\frac{\partial B_z}{\partial x}$ and $\frac{\partial B}{\partial y}$ term, or $B_x \neq 0$, the associated force vanishes on average, since the spin precesses in the x-y plane.)

Classically, s_z can take any value, so the force has a continuous distribution, depending on the direction of $\vec{\mu}$ $\rightarrow$ deflected beam traces a continuous vertical line on a screen behind the magnet.

Quantum mechanically, s_z is quantized

$\Rightarrow$ discrete dots ($2s+1$ of them) on the screen

spin up $\rightarrow \mu_z$ is down

$\frac{\partial B_z}{\partial z} < 0 \rightarrow$ force is up

If

$$\psi_{initial} = \underset{\substack{\uparrow \\ \text{c.m. motion} \\ \text{of atom}}}{e^{ik_{CM}y_{CM}}}\psi_{100}(\vec{r})\begin{bmatrix}1\\0\end{bmatrix}$$

$$\Rightarrow \psi_{out} = e^{i(k_y y_{CM} + k_z z_{CM})} \psi_{100}(\vec{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

If

$$\psi_{initial} = e^{i k_{CM} y_{CM}} \psi_{100} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

then

$$\psi_{out} = e^{i(k_y y_{CM} + k_z z_{CM})} \psi_{100} \begin{pmatrix} \alpha \\ 0 \end{pmatrix} + e^{i(k_y y_{CM} - k_z z_{CM})} \psi_{100} \begin{pmatrix} 0 \\ \beta \end{pmatrix}$$

kick from downward force

$\Rightarrow$ beam split into two beams.