Spin and Angular Momentum

The electron, as well as other particles, have an intrinsic angular momentum or spin. Historically, the spin of the electron was first discovered (or introduced) as a way to explain details of the atomic spectra. However, its physical origin lies in relativistic quantum theory, in the Dirac equation. In fact, we already saw that photons have spin.

Since the notion of spin is inherently related to angular momentum, let us review the properties of the latter.

In QM, the (orbital) angular momentum operator is

$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$ where $\hat{\vec{r}}$ and $\hat{\vec{p}}$ are ops.

Clearly $\hat{L}_i^\dagger = \hat{L}_i$ $(i = 1,2,3)$ (or x, y, z)

it's hermitean.

From this definition it follows (see my Physics 480 Notes) that the L_i's obey the following algebra

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

and

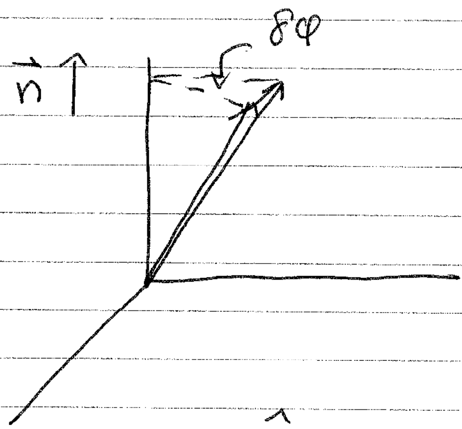
$$[\hat{L}_i, \hat{r}_j] = i\hbar\, \varepsilon_{ijk} \hat{r}_k$$

In particular, ~~for~~ given an arbitrary vector $\vec{n}$, Here I will summarize the results we derived in Physics 480 (see my lecture notes pages 268 - 288)

Let $|\psi\rangle$ be some state of the Hilbert space and $U(R)$ be the unitary operator representing the action of rotations on this state vector

$$|\psi_R\rangle = U[R]\,|\psi\rangle$$

In Phys 480 we examined first the action of an infinitesimal rotation



$$\vec{\delta\varphi} = \pm|\delta\varphi|\,\vec{n}$$

$$\delta\vec{r} = \vec{\delta\varphi}\wedge\vec{r}$$ is the rotation

$\Rightarrow \langle\psi_R|\hat{\vec{X}}|\psi_R\rangle$ is the rotated expectation value of the position vector operator

$$\langle\psi_R|\hat{\vec{X}}|\psi_R\rangle = \langle\psi|U[R]^\dagger\,\hat{\vec{X}}\,U[R]|\psi\rangle$$

$$= \mathbb{R}\,\langle\psi|\hat{\vec{X}}|\psi\rangle$$

rotation matrix

$$\Rightarrow \langle \psi_R | \hat{\vec{X}} | \psi_R \rangle - \langle \psi | \hat{\vec{X}} | \psi \rangle =$$

$$= \delta\vec{\varphi} \wedge \langle \psi | \hat{\vec{X}} | \psi \rangle + \cdots$$

$$\Rightarrow \mathcal{U}[R] = \hat{I} - \frac{i}{\hbar} \underbrace{\delta\vec{\varphi} \cdot \vec{L}}_{\delta\varphi\, \vec{n} \cdot \vec{L}} + \cdots \Rightarrow \frac{d}{d\varphi} \langle \psi | \hat{\vec{X}} | \psi \rangle = $$

$$= \vec{n} \wedge \langle \psi | \hat{\vec{X}} | \psi \rangle$$

Finite rotations

$$\mathcal{U}[R] = e^{-\frac{i}{\hbar} \vec{\varphi} \cdot \vec{L}}$$

i.e. $\vec{n} \cdot \vec{L}$ generates infinitesimal transformation (rotations) $\parallel$ to $\vec{n}$.

$$\Rightarrow |\psi_R\rangle = e^{-\frac{i}{\hbar} \vec{\varphi} \cdot \vec{L}} |\psi\rangle$$

and $|\vec{x}'\rangle = e^{-\frac{i}{\hbar} \vec{\varphi} \cdot \vec{L}} |\vec{x}\rangle$

if $\vec{x}' = \mathbb{R}\, \vec{x}$

The Angular Momentum Algebra

$$\vec{L} \equiv \hat{\vec{X}} \wedge \hat{\vec{P}}$$

$\hat{X}_1 = \hat{x}$ $\quad \hat{L}_x = \hat{L}_1$

$\hat{X}_2 = \hat{y}$ $\quad \hat{L}_y = \hat{L}_2$

$\hat{X}_3 = \hat{z}$ $\quad \hat{L}_z = \hat{L}_3$

$$\Rightarrow \left[\hat{L}_i, \hat{X}_j\right] = i\hbar\, \varepsilon_{ijk}\, \hat{X}_k$$

$$\left[\vec{n}\cdot\hat{\vec{L}}, \hat{\vec{X}}\right] = i\hbar\left(\hat{\vec{X}} \wedge \vec{n}\right)$$

cross product

$$\left[\vec{n}\cdot\hat{\vec{L}}, \hat{\vec{P}}\right] = i\hbar\left(\hat{\vec{P}} \wedge \vec{n}\right)$$

$$\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\, \varepsilon_{ijk}\, \hat{L}_k \qquad \left(\hat{\vec{L}} \times \hat{\vec{L}} = i\hbar \hat{\vec{L}}\right)$$

$$\left[\hat{L}_i, \hat{\vec{L}}^2\right] = 0$$

L15 <u>The eigenvalue problem:</u>

We will now review the eigenstates and eigenvectors of $\hat{L}_z$ and $\hat{\vec{L}}^2$ which follow from this algebra.

We begin by defining $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y \equiv \hat{L}_1 \pm i\hat{L}_2$
(raising and lowering ops.

Since $[\hat{L}_z, \hat{\vec{L}}^2] = 0$ they can be diagonalized simultaneously.

also we denote the states by

$$\hat{\vec{L}}^2 |\alpha, \beta\rangle = \alpha |\alpha, \beta\rangle$$

$$\hat{L}_z |\alpha, \beta\rangle = \beta |\alpha, \beta\rangle$$

Now

$$[\hat{L}_z, \hat{L}_\pm] = \pm \hbar \hat{L}_\pm \quad \text{(it is an "eigenoperator")}$$

$$[\hat{\vec{L}}^2, \hat{L}_\pm] = 0$$

$$[\hat{L}_+, \hat{L}_-] = 2\hbar \hat{L}_z$$

Consider the state $\hat{L}_+ |\alpha, \beta\rangle$. Let us show that it is an eigenstate of $\hat{L}_z$ and $\hat{\vec{L}}^2$:

$$\Rightarrow \quad \hat{L}_z \hat{L}_+ |\alpha, \beta\rangle = \left([\hat{L}_z, \hat{L}_+] + \hat{L}_+ \hat{L}_z \right) |\alpha, \beta\rangle$$

$$= \hbar \hat{L}_+ |\alpha, \beta\rangle + \hat{L}_+ \hat{L}_z |\alpha, \beta\rangle$$

$$= \hbar \hat{L}_+ |\alpha, \beta\rangle + \beta \hat{L}_+ |\alpha, \beta\rangle$$

$$= (\hbar + \beta) \hat{L}_+ |\alpha, \beta\rangle$$

$\Rightarrow$ $\hat{L}_+ |\alpha, \beta\rangle$ is an eigenvector of $\hat{L}_z$ with eigenvalue $\hbar + \beta$

$$\hat{\vec{L}}^2 \hat{L}_{+} |\alpha,\beta\rangle = \Big(\underbrace{[\hat{\vec{L}}^2, \hat{L}_+]}_{0} + \hat{L}_+ \hat{\vec{L}}^2 \Big) |\alpha,\beta\rangle$$

$$= \alpha \, \hat{L}_+ |\alpha,\beta\rangle$$

$\Rightarrow$ $\hat{L}_+ |\alpha,\beta\rangle$ is an eigenvector of $\hat{\vec{L}}^2$ with eigenvalue α

$$\Rightarrow \boxed{\hat{L}_+ |\alpha,\beta\rangle = C_+(\alpha,\beta) \; |\alpha, \hbar+\beta\rangle}$$

Since $\langle\alpha,\beta| \hat{L}_i^2 |\alpha,\beta\rangle = \| \hat{L}_i |\alpha,\beta\rangle \|^2 \geq 0$

(since $\hat{L}_i = \hat{L}_i^\dagger$)

$$\Rightarrow \langle\alpha,\beta| (\hat{\vec{L}}^2 - \hat{L}_z^2) |\alpha,\beta\rangle = \underbrace{\langle\alpha,\beta| (\hat{L}_x^2 + \hat{L}_y^2) |\alpha,\beta\rangle}_{\geq 0}$$

but $\langle\alpha\beta| (\hat{\vec{L}}^2 - \hat{L}_z^2) |\alpha,\beta\rangle = (\alpha - \beta^2) \| |\alpha,\beta\rangle \|^2 \geq 0$

$$\Rightarrow \alpha \geq \beta^2$$

$\Rightarrow \exists$ β_{max} and β_{min} s.t

$$-\sqrt{\alpha} \leq \beta_{min} \leq \beta \leq \beta_{max} < \sqrt{\alpha}$$

β_{max} / $\hat{L}_+ |\alpha, \beta_{max}\rangle = 0$ since otherwise the bound is violated.

Also $\hat{L}_- \hat{L}_+ = \hat{\vec{L}}^2 - \hat{L}_z^2 - \hbar \hat{L}_z$ (check!)

$$\Rightarrow \left(\hat{\vec{L}}^2 - \hat{L}_z^2 - \hbar \hat{L}_z\right) |\alpha, \beta_{max}\rangle = 0$$

$$\alpha - \beta_{max}^2 - \hbar \beta_{max} = 0$$

$$\Rightarrow \alpha = \beta_{max}(\hbar + \beta_{max})$$

Consider now the state

$\hat{L}_-^k |\alpha, \beta_{max}\rangle$ $\qquad (k \in \mathbb{Z}^+)$

$$\Rightarrow \hat{L}_-^k |\alpha, \beta_{max}\rangle \propto |\alpha, \beta_{max} - \hbar k\rangle$$

$\Rightarrow$ for some k

$(\beta_{max} - \hbar k)^2 > \alpha$ and the bound is violated again

Let $\beta_{min} = \beta_{max} - \hbar k$ $\Rightarrow$ $\beta_{max} - \beta_{min} = \hbar k$ where $k \in \mathbb{Z}^+$

$\Rightarrow$ $\hat{L}_- |\alpha, \beta_{min}\rangle = 0$ must be true or the lower bound is violated

$\Rightarrow \hat{L}_+ \hat{L}_- |\alpha, \beta_{min}\rangle = 0$

Using $\hat{L}_+ \hat{L}_- = \hat{\vec{L}}^2 - \hat{L}_z^2 + \hbar \hat{L}_z$

$$\Rightarrow \left(\hat{\vec{L}}^2 - \hat{L}_z^2 + \hbar \hat{L}_z \right) |\alpha, \beta_{min}\rangle = 0$$

$$\Rightarrow \alpha - \beta_{min}^2 + \hbar \beta_{min} = 0$$

$$\alpha = \beta_{min} (\hbar + \beta_{min}) \quad \text{same eqn!}$$

$$\Rightarrow \beta_{min} = -\beta_{max}$$

But $\beta_{max} - \beta_{min} = \hbar k$ where $k \in \mathbb{Z}^+$

$$\Rightarrow 2\beta_{max} = \hbar k$$

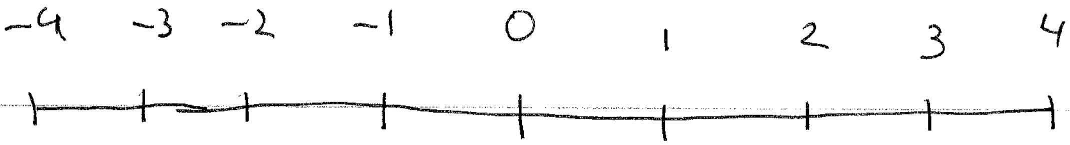
$$\Rightarrow \beta_{max} = -\beta_{min} = \frac{\hbar k}{2}$$

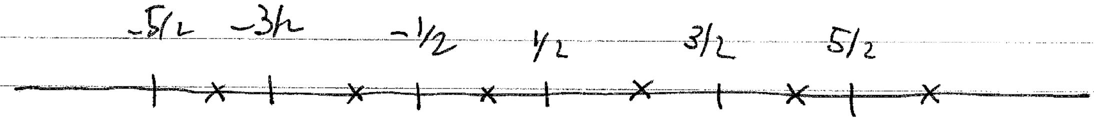
$\Rightarrow$ the eigenvalues of $\hat{L}_z$ are half integers $\times \hbar$

$\hat{\vec{L}}^2$ are $\hbar^2 l(l+1)$

$$l = \frac{k}{2}$$

The cases $l \in \mathbb{Z}$ (i.e. k even) are the usual angular momentum states

k even:


k odd


Let us denote by $j = \frac{k}{2}$ $\qquad$ $\alpha = \hbar^2 j(j+1)$, $\beta = \hbar m$

and m $\qquad -j \le m \le j$ in integer steps.

$$\hat{\vec{L}}^2 |j,m\rangle = \hbar^2 j(j+1)|j,m\rangle \qquad j \in \tfrac{1}{2}\mathbb{Z}^+$$

$$\hat{L}_z |j,m\rangle = \hbar m |j,m\rangle$$

For orbital motion the spectrum of $\hat{\vec{L}}^2$ and $\hat{L}_z$ is restricted to $l \in \mathbb{Z}$ $\qquad l = 0, 1, 2, \dots$

What are the other states?

The 1/2-integral states represent spin states.

$$\hat{L}_- |j,m\rangle = \hbar\sqrt{j(j+1)-m(m-1)}\,|j,m-1\rangle$$

$$\hat{L}_+ |j,m\rangle = \hbar\sqrt{j(j+1)-m(m+1)}\,|j,m+1\rangle$$

[the normalization follows from $\hat{L}_-|jm\rangle = C_-(jm)|j,m-1\rangle$, with
$\hat{L}_+\hat{L}_- = \hbar^2\hat{\vec{L}}^2 - \hat{L}_z^2 - \hbar\hat{L}_z$]

$\Rightarrow$ We discover that the angular momentum eigenstates $|lm\rangle$ are arranged in <u>multiplets</u>, i.e. vector spaces of dimension $2j+1$ = # of degenerate (= same l) eigenvectors.

The group whose generators satisfy the algebra

$[L_i, L_j] = i\hbar\, \varepsilon_{ijk}\, L_k$

is the (Lie group) $SU(2)$

and what we have done is to construct the representations of $SU(2)$. The representation with $j \equiv l \in \mathbb{Z}^+$ form the representations of the group of rotations $SO(3)$. In each one of these vector spaces (or reps.) the angular momentum ops or generators become $(2l+1)\times(2l+1)$ matrices.

<u>Examples</u>

(a) $l=1$, $m = 0, \pm 1$ and the vector space is three-dimensional. Clearly, the states are

$|1,1\rangle, |1 0\rangle$ and $|1,-1\rangle$

$$\Rightarrow \quad \hat{L}_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

[Note: photons have intrinsic ang. momentum $\pm\hbar$ $\Rightarrow$ the spin is $\underline{\underline{1}}$ but the state with $S_z = 0$ is missing because photons are massless.]

$$\hat{L}_+ = \hbar \begin{bmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix} \qquad \hat{L}_- = \hbar \begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix}$$

$$\hat{L}_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad \hat{L}_y = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}$$

which satisfy the algebra. It is easy to check that this has the required form for a generator of infinitesimal rotations in $d=3$.

(b) $j = \frac{1}{2}$, the dimension of the space is $\underline{\underline{2}}$ and the eigenvectors are $|\frac{1}{2},\frac{1}{2}\rangle$, $|\frac{1}{2},-\frac{1}{2}\rangle$

$|\frac{1}{2},\frac{1}{2}\rangle \equiv |\uparrow\rangle$; $|\frac{1}{2},-\frac{1}{2}\rangle \equiv |\downarrow\rangle$

$\Rightarrow$ we get 2×2 matrices.

$$\hat{L}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{L}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{L}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

It is customary to use the notation $\hat{L} \equiv \vec{S}$ for 1/2 integer reps. and $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

are the Pauli matrices $\sigma_z, \sigma_x, \sigma_y$.

$\Rightarrow \vec{S} = \frac{\hbar}{2}\vec{\sigma}$

These matrices have special properties:

① clearly $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

and $\sigma_x^\dagger = \sigma_x$, $\sigma_y^\dagger = \sigma_y$, $\sigma_z^\dagger = \sigma_z$

[this also known as a Clifford algebra)

and ② $[\sigma_i, \sigma_j] = 2i\, \varepsilon_{ijk}\, \sigma_k$

$$\{\sigma_i, \sigma_j\} \equiv \sigma_i \sigma_j + \sigma_j \sigma_i = 2\, \delta_{ij}\, I$$

$$\Rightarrow \sigma_i \sigma_j = \delta_{ij} + i\, \varepsilon_{ijk}\, \sigma_k$$

$$\Rightarrow \hat{S}_i \hat{S}_j = \frac{\hbar^2}{4} \delta_{ij} + i\, \varepsilon_{ijk} \frac{\hbar}{2} \hat{S}_k$$

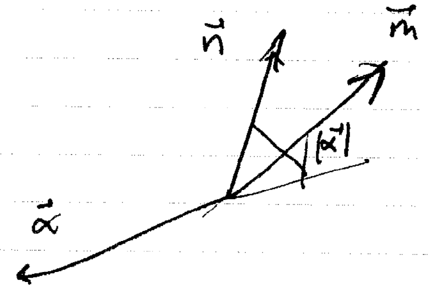
similarly

③ $\vec{S}^2 = \frac{\hbar^2}{4} \times 3 = \hbar^2\, \frac{1}{2}(\frac{1}{2}+1)$

④ $(\vec{a}.\vec{\sigma})(\vec{b}.\vec{\sigma}) = a_i b_j\, \sigma_i \sigma_j = \vec{a}.\vec{b} + i\, \vec{a}\times\vec{b}.\,\vec{\sigma}$

Rotations in Spin Space

Let $\vec{n}$ and $\vec{m}$ be two vectors related by a rotation $\vec{\alpha}$ $\Rightarrow$ $\vec{S}.\vec{n} = e^{-\frac{i}{\hbar}\vec{S}.\vec{\alpha}}\, \vec{S}.\vec{m}\, e^{\frac{i}{\hbar}\vec{S}.\vec{\alpha}}$



$\Rightarrow$ If $\vec{S}.\vec{m}\,|\vec{m}\uparrow\rangle = +\frac{\hbar}{2}|\vec{m}\uparrow\rangle$

$$\Rightarrow \vec{S}.\vec{n}\; e^{-\frac{i}{\hbar}\vec{S}.\vec{\alpha}}\,|\vec{m}\uparrow\rangle = e^{-\frac{i}{\hbar}\vec{S}.\vec{\alpha}}\;\vec{S}.\vec{m}\,|\vec{m}\uparrow\rangle$$
$$= \frac{\hbar}{2} e^{-\frac{i}{\hbar}\vec{S}.\vec{\alpha}}\,|\vec{m}\uparrow\rangle$$

$$\Rightarrow e^{-\frac{i}{\hbar}\vec{S}.\vec{\alpha}}\,|\vec{m}\uparrow\rangle = |\vec{n}\uparrow\rangle$$
$$e^{-\frac{i}{\hbar}\vec{S}.\vec{\alpha}}\,|\vec{m}\downarrow\rangle = |\vec{n}\downarrow\rangle$$

$\Rightarrow e^{-\frac{i}{\hbar}\vec{S}.\vec{\alpha}}$ rotates the eigenstates of $\vec{S}.\vec{m}$ <u>into</u> the eigenstates of $\vec{S}.\vec{n}$.

Also notice that $\hat{d}(\vec{\alpha}) = e^{-\frac{i}{\hbar}\vec{\alpha}.\vec{S}} \equiv e^{-\frac{i}{2}\vec{\alpha}.\vec{\sigma}}$

$$\Rightarrow \hat{d}(\vec{\alpha}) = e^{-\frac{i}{2}\vec{\alpha}.\vec{\sigma}} = \sum_{n=0}^{\infty} \frac{\left(-\frac{i}{2}\right)^n}{n!}(\vec{\alpha}.\vec{\sigma})^n$$

$$(\vec{\alpha}.\vec{\sigma})^2 = (\vec{\alpha}.\vec{\sigma})(\vec{\alpha}.\vec{\sigma}) = (\vec{\alpha}.\vec{\alpha})\,I + i\,\underbrace{\vec{\alpha}\times\vec{\alpha}}_{=0}.\vec{\sigma}$$

$$\Rightarrow (\vec{\alpha}.\vec{\sigma})^2 = |\alpha|^2\, I$$
$$\Rightarrow (\vec{\alpha}.\vec{\sigma})^3 = |\alpha|^2\,\vec{\alpha}.\vec{\sigma}$$
$$\Rightarrow (\vec{\alpha}.\vec{\sigma})^{2k} = |\alpha|^{2k}\, I$$
$$(\vec{\alpha}.\vec{\sigma})^{2k+1} = |\alpha|^{2k}\,\vec{\alpha}.\vec{\sigma}$$

$$\Rightarrow \hat{d}(\vec{\alpha}) = \sum_{n=0}^{\infty}\left[\frac{\left(-\frac{i}{2}\right)^{2n}}{(2n)!}(\vec{\alpha}.\vec{\sigma})^{2n} + \frac{\left(-\frac{i}{2}\right)^{2n+1}}{(2n+1)!}(\vec{\alpha}.\vec{\sigma})^{2n+1}\right]$$
$$= \left[\sum_{n=0}^{\infty}\left(-\frac{i}{2}\right)^{2n}\frac{|\alpha|^{2n}}{(2n)!}\right]\hat{I} + (-i)\left(\sum_{n=0}^{\infty}\frac{\left(-\frac{i}{2}\right)^{2n+1}|\alpha|^{2n+1}}{(2n+1)!}\right)\frac{\vec{\alpha}.\vec{\sigma}}{|\alpha|}$$

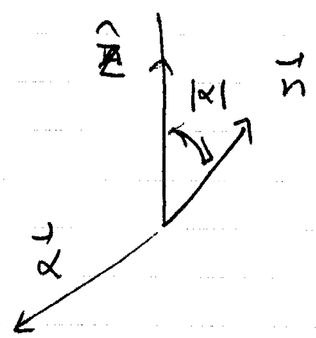
$$\Rightarrow \quad \hat{d}(\vec{\alpha}) = e^{-\frac{i}{2}\vec{\alpha}\cdot\vec{\sigma}} = \hat{I}\cos\frac{|\alpha|}{2} - i\,\frac{\vec{\alpha}\cdot\vec{\sigma}}{|\alpha|}\,\sin\left(\frac{|\alpha|}{2}\right)$$

$$\Rightarrow |\uparrow\rangle = |\tfrac{1}{2},\tfrac{1}{2}\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$

$$|\downarrow\rangle = |\tfrac{1}{2},-\tfrac{1}{2}\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

$$\Rightarrow \quad e^{-\frac{i}{2}\vec{\alpha}\cdot\vec{\sigma}}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}\cos\frac{|\alpha|}{2} - i\sin\frac{|\alpha|}{2}\,\frac{\alpha_z}{|\alpha|} \\[2ex] \frac{(-i\alpha_x + i\alpha_y)}{|\alpha|}\sin\frac{|\alpha|}{2}\end{pmatrix}$$

where $\vec{\alpha}$ is the rotation that takes $\hat{z} \to \vec{n}$



Notice the following

$$\hat{d}(2\pi\hat{\alpha}) = e^{-\frac{i}{2}2\pi\hat{\alpha}\cdot\vec{\sigma}} = \hat{I}\overset{-1}{\cos\pi} - i\,\vec{\sigma}\cdot\hat{\alpha}\,\overset{0}{\sin\pi}$$

unit vector

$$\Rightarrow \hat{d}(2\pi\hat{\alpha}) = -\hat{I}$$ (a 2π rotation is represented by $-I$)

while $\hat{d}(0) = \hat{I}$

$\Rightarrow$ the spin rep. of SU(2) is <u>double valued</u>.

$\Rightarrow$ $\hat{d}(\vec{\alpha})$ and $\hat{d}(\vec{\alpha} + 2\pi\hat{\alpha}) = -\hat{d}(\vec{\alpha})$ are the same rotation.

In summary, we have constructed the Hilbert spaces for states with a well defined total spin S and z-projection S_z, $|S, m_s\rangle$

$$\vec{S}^2 \, |S, m_s\rangle = \hbar^2 s(s+1) \, |S, m_s\rangle$$

$$S_z \, |S, m_s\rangle = \hbar \, m_s \, |S, m_s\rangle$$

where $S = 0, \frac{1}{2}, 1, \ldots$ and $|m_s| \leq S$

The <u>dimensions</u> of these spaces (or <u>representations</u>) are $2S+1$. In these spaces the states are constructed from the highest projection state $|S, S\rangle$ by applying the lowering ops. $S^{\pm} = S_x \pm i S_y$

$$S^{\pm} |S, m_s\rangle = \hbar \sqrt{S(S+1) - m_s(m_s \pm 1)} \, |S, m_s \pm 1\rangle$$

These relations define the matrix elements of the three generators S_x, S_y and S_z in ~~the~~ each space. Notice that the commutation relations are always the same

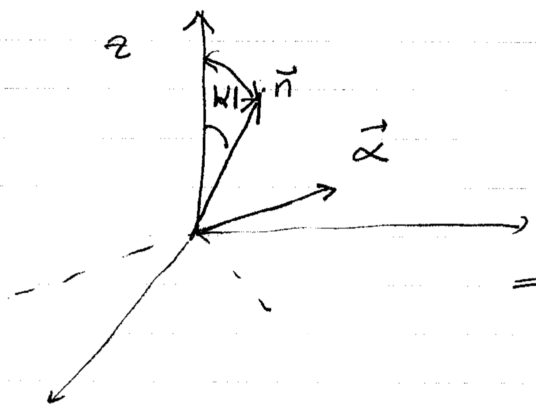
$$[S_i, S_j] = i\hbar \, \varepsilon_{ijk} S_k$$

Rotations in each space are ~~spec~~ represented by unitary matrices, of rank $2S+1$,

$$e^{-i \frac{\vec{\alpha} \cdot \vec{S}}{\hbar}}$$

Thus, if $|S, m_s\rangle$ is a state polarized along the z-axis with projection (S_z) $\frac{\hbar}{2} m_s$, the state

$$e^{-i\vec{\alpha}\cdot\vec{S}} |s, m_s\rangle$$ is polarized along the $\vec{n}$ axis rotated by $|\alpha|$ from the z axis around the axis $\frac{\vec{\alpha}}{|\alpha|}$.



$$\Rightarrow \quad \vec{S}\cdot\vec{n}\; e^{-i\vec{\alpha}\cdot\vec{S}} |s, m_s\rangle = \hbar m_s\, e^{-i\vec{\alpha}\cdot\vec{S}} |s, m_s\rangle$$

(L16) Including the spacial degrees of freedom

Thus, in a non-relativistic system, spin is an additional label (or quantum number) and the wave functions become vectors with 2s+1 components,

$$\psi(\vec{r}) = \begin{bmatrix} \psi_s(\vec{r}) \\ \psi_{s-1}(\vec{r}) \\ \vdots \\ \psi_{-s}(\vec{r}) \end{bmatrix}$$

For $s = \frac{1}{2}$ we have spinors, two component vectors

$$\psi(\vec{r}) = \begin{bmatrix} \psi_\uparrow(\vec{r}) \\ \psi_\downarrow(\vec{r}) \end{bmatrix} \quad \text{or "spinors"}$$

$$\Rightarrow \quad \psi_{m_s}(\vec{r}) = \langle \vec{r}; s, m_s | \psi \rangle$$

$\Rightarrow \quad \psi_\uparrow(\vec{r}) = \langle \vec{r}, \uparrow | \psi \rangle \quad , \quad \psi_\downarrow(\vec{r}) = \langle \vec{r}, \downarrow | \psi \rangle$

Probab. density to find a particle at $\vec{r}$:

$$|\psi_\uparrow(\vec{r})|^2 + |\psi_\downarrow(\vec{r})|^2$$

Total Probab to find a particle with $|\uparrow\rangle$

$$\int d^3r \; |\psi_\uparrow(\vec{r})|^2$$

Normalization:

$$\langle \psi | \psi \rangle = \int d^3r \left(|\psi_\uparrow(\vec{r})|^2 + |\psi_\downarrow(\vec{r})|^2 \right) = 1$$

$$\langle \phi | \psi \rangle \equiv \int d^3r \sum_{m_s} \phi^*_{m_s}(\vec{r}) \, \psi_{m_s}(\vec{r})$$

L30

Total Angular Momentum:

$$\underset{\substack{\uparrow \\ \text{orbital}}}{\vec{J} = \vec{L}} + \underset{\substack{\uparrow \\ \text{spin}}}{\vec{S}} \qquad [L_i, S_j] = 0$$

(since they act on $\neq$ Hilbert spaces)

$\Rightarrow \vec{J}$ generates rotations in real and spin space.

What is the action of $\vec{J}$ on states $|\vec{r}_0; s, m_s\rangle$?

$$e^{-i\vec{\alpha}\cdot\vec{J}} |\vec{r}_0; s, m_s\rangle = e^{-i\vec{\alpha}\cdot(\vec{L}+\vec{S})} |\vec{r}_0; s, m_s\rangle$$

$$= e^{-i\vec{\alpha}\cdot\vec{L}} e^{-i\vec{\alpha}\cdot\vec{S}} |\vec{r}_0; s, m_s\rangle =$$

(because $[S_i, L_j] = 0$)

$$= e^{-i\vec{\alpha}\cdot\vec{L}} |\vec{r}_0\rangle \times e^{-i\vec{\alpha}\cdot\vec{S}} |s, m_s\rangle$$

$$= \underset{\substack{\uparrow \\ \text{rotated } \vec{r}_0}}{|\vec{r}_0'\rangle} \times \underset{\substack{\uparrow \\ \text{rotated spin polarization.}}}{|s, \vec{n}\cdot\vec{S} = m_s\rangle}$$

$\Rightarrow$ the state $|\psi'\rangle = e^{+i\vec{\alpha}\cdot\vec{J}}|\psi\rangle$

$$\Rightarrow \langle \vec{r}_0; s\, m_s | \psi' \rangle = \langle \vec{r}_0; s\, m_s | e^{i\vec{\alpha}\cdot\vec{J}} | \psi \rangle$$

$$= \langle \underbrace{\vec{r}_0{}'}_{\text{rotated point}}; s, \underbrace{\vec{\alpha}\cdot\vec{n} = \hbar m_s}_{\text{rotated spin projection.}} | \psi \rangle$$

<u>Spin magnetic moment.</u>

How does the spin manifest itself? One of the main consequences of the $\exists$ of spin is the $\exists$ of a magnetic moment. By <u>analogy</u> with the <u>orbital</u> magnetic moment of a state with angular momentum $\vec{L}$ (mass m and charge e (with its sign))

$$\vec{M}_{orb} = \frac{e}{2mc}\vec{L}$$

there is a spin magnetic moment, whose origin is purely relativistic,

$$\vec{M}_{spin} = g\frac{e}{2mc}\vec{S}$$

where g is the <u>Landé g factor</u> (gyromagnetic). For a free particle of spin $\frac{1}{2}$ (in the Dirac theory), $g = 2$.

(However, radiative e.m. corrections change this #).

$$\Rightarrow \quad \vec{M}_{tot} = \vec{M}_{orb} + \vec{M}_{spin} = \frac{e}{2mc}(\vec{L} + g\vec{S})$$

$$\cong \frac{e}{2mc}(\vec{L} + 2\vec{S})$$

which is $\neq$ from $\frac{e}{2mc}\vec{J}$

$\Rightarrow$ $\vec{M}_{tot}$ <u>is</u> <u>not</u> ~~parallel~~ parallel to $\vec{J}$

[proton: $g \simeq 5.59$ and for electrons $g - 2 \approx \frac{e^2}{2\pi\hbar c} + O\left(\left(\frac{e^2}{\hbar c}\right)^2\right)$]

[neutron: $g = -3.83$ in spite of the fact that it is a neutral particle.]

<u>Energy of a magnetic moment:</u> $-\vec{M}\cdot\vec{B}$

$$\Rightarrow \quad H_{spin} = -\vec{M}_{spin}\cdot\vec{B} \qquad \text{(Zeeman term)}$$

If we include the orbital motion

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \vec{M}_{spin}\cdot\vec{B} - \frac{e^2}{|\vec{r}|}$$

<u>Pauli Equation</u>

Coulomb interaction in a central potential.

If $\vec{B}$ is uniform we can write

$$\vec{A} = -\frac{1}{2}\vec{r}\times\vec{B} \qquad (\text{in the transverse gauge } \vec{\nabla}\cdot\vec{A} = 0)$$

To <u>first order in $\vec{B}$</u>, we find $(g=2)$

$$H = H_0 - \frac{e}{2mc}(\vec{A}\cdot\vec{p} + \vec{p}\cdot\vec{A}) - \frac{e}{mc}\vec{S}\cdot\vec{B}$$

$$= H_0 - \frac{e}{2mc}\vec{B}\cdot(\vec{L} + 2\vec{S}) = H_0 - \vec{M}_{tot}\cdot\vec{B}$$

Let $\vec{B} = B\,\hat{z}$

$$\Rightarrow H_{int} = -\frac{eB}{2mc}\left(L_z + 2S_z\right)$$

<u>without spin</u> the levels are $|n, l, m_l\rangle$

$\Rightarrow$ level splitting

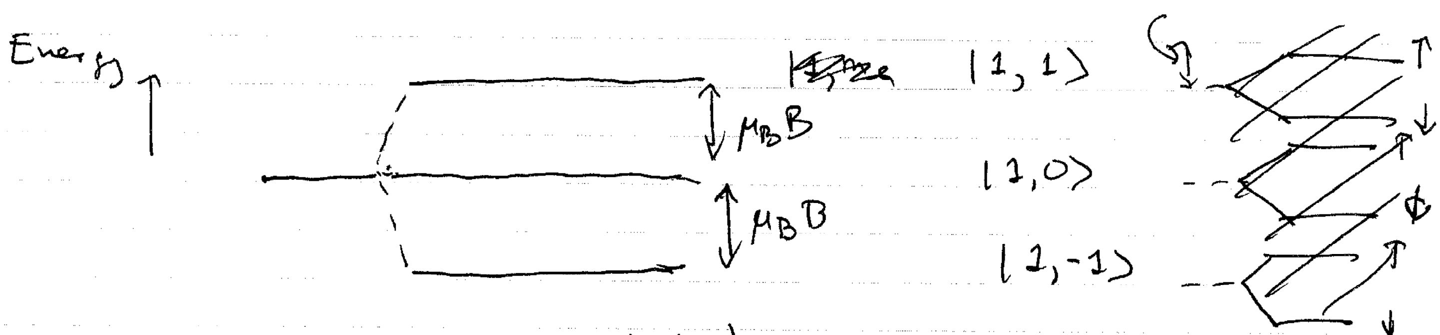
$$(\Delta E)_{no\ spin} = \langle n\,l\,m_l | H_{int} | n\,l\,m_l\rangle$$

$$= -\frac{e\hbar}{2mc} B\, m_l$$

$$\equiv \mu_B B\, m_l$$

$$\mu_B = \left|\frac{e\hbar}{2mc}\right| = 0.927 \times 10^{-20}\ \frac{\text{ergs}}{\text{gauss}} \quad \text{(Bohr magneton)}$$

$\Rightarrow$ without spin the state $l = 1$ has a three-fold degeneracy which is lifted

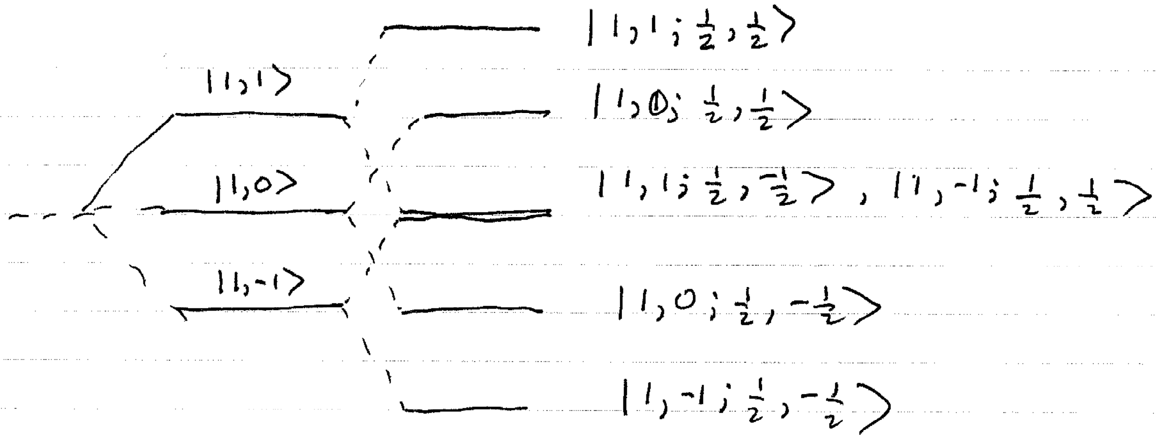


<u>with spin:</u> (no spin-orbit)

$|n; l, m_l; s, m_s\rangle$

$$\Delta E = \langle n; l, m_l; s, m_s | H_{int} | n; l, m_l; s, m_s\rangle$$

$$= \mu_B B\,(m_l + 2m_s)$$



Spin-Orbit Interaction:

The relativistic motion of particles in external potentials generate new effects that we haven't discussed so far. The most important ones are: Spin-Orbit and the related Thomas Precession.

According to relativity a moving particle of charge e and velocity $\vec{v}$ in an electric field $\vec{E}$, sees a magnetic field $-\frac{\vec{v}}{c}\times\vec{E}$ (to lowest order in $|\vec{v}|/c$) $\Rightarrow$ this extra magnetic field couples to the spin leading to the extra term

$$-\frac{|e|}{mc}\,\vec{S}\cdot\left(\frac{\vec{v}}{c}\times\vec{E}\right)$$

There is an additional relativistic effect (Thomas Precession)

$$+\frac{|e|}{2mc}\,\vec{S}\cdot\left(\frac{\vec{v}}{c}\times\vec{E}\right)$$

$$\Rightarrow\quad H_{S.O.} = -\frac{|e|}{2mc^2}\,\vec{S}\cdot\vec{v}\times\vec{E}$$

Central Potential $: |e|\vec{E} = \vec{\nabla} V(\vec{r}) = \vec{r}\,\frac{1}{r}\,\frac{dV}{dr}$

$$\Rightarrow \quad H_{s.o.} = +\,\frac{1}{2mc^2}\,\frac{1}{r}\left(\frac{dV}{dr}\right)\vec{S}\cdot\vec{r}\times\vec{v}$$

$$\Rightarrow \quad \boxed{H_{s.o.} = \frac{1}{2m^2c^2}\,\frac{1}{r}\left(\frac{dV}{dr}\right)\vec{L}\cdot\vec{S}}$$

<u>Pauli Equation</u>: Schrödinger equation with spin

$$\psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \qquad \text{(easy to generalize)} \qquad \left(\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right)$$

$$i\hbar\,\frac{\partial}{\partial t}\begin{pmatrix} \psi_\uparrow(\vec{r},t) \\ \psi_\downarrow(\vec{r},t) \end{pmatrix} =$$

$$= \left[\frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}(\vec{r},t)\right)^2 \cdot \hat{I} - \frac{g}{2}\,\frac{e\hbar}{2mc}\,\vec{\sigma}\cdot\vec{B}(\vec{r},t)\right.$$

$$\left. + \; V(\vec{r})\cdot\hat{I}\right]\begin{pmatrix} \psi_\uparrow(\vec{r},t) \\ \psi_\downarrow(\vec{r},t \end{pmatrix}$$

$$\vec{\sigma}\cdot\vec{B} = \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}$$

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Spin Precession

Neglect for now the orbital motion.

$$H_{spin} = -\frac{g}{2}\frac{e}{mc}\vec{S}\cdot\vec{B}(t) = -\frac{g}{4}\frac{e\hbar}{mc}\vec{\sigma}\cdot\vec{B}(t)$$

Heisenberg operator: $\hat{S}_i(t)$

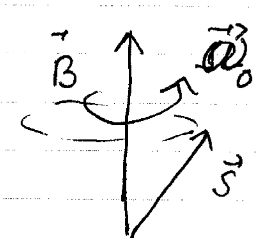
$$\Rightarrow i\hbar\frac{dS_i(t)}{dt} = \left[S_i(t), H_{spin}(t)\right]$$

$$= -\frac{g}{2}\frac{e}{mc}\left[S_i(t), S_j(t)\right]B_j(t)$$

$$= -\frac{g}{2}\frac{e}{mc}\,i\hbar\,\varepsilon_{ijk}S_k(t)\,B_j(t)$$

$$\Rightarrow \underbrace{\frac{d\vec{S}}{dt}}_{\text{rate of change of angular momentum}} = +g\frac{e}{2mc}\vec{S}\times\vec{B} = \underbrace{\vec{M}_{spin}\times\vec{B}}_{\text{torque}}$$

$$\frac{d\vec{S}}{dt} = -g\frac{e}{2mc}\vec{B}\times\vec{S}$$



$$\Rightarrow \vec{\omega}_0 = -g\frac{e}{2mc}\vec{B}$$ (Larmor frequency)

$$= +\frac{g|e|}{2mc}\vec{B}$$ $\Rightarrow$ if the polarization of the initial state is not parallel to $\vec{B}$, the polarization precesses around $\vec{B}$.

For electrons $\quad \omega_0 = g\frac{eB}{2mc}$ and $\frac{|\omega_0|}{2\pi B} \simeq 2.8 \frac{\text{MHz}}{\text{gauss}}$

$\Rightarrow$ if at $t=0$ the spin is polarized $\parallel \vec{x}$

$$\Rightarrow \langle S_x(0)\rangle = \langle \hat{x}\uparrow | S_x(0) | \hat{x}\uparrow\rangle = \frac{\hbar}{2}$$

$$\langle S_y(0)\rangle = \langle S_z(0)\rangle = 0$$

$$\Rightarrow \langle S_x(t)\rangle = \frac{\hbar}{2}\cos\omega_0 t$$

$$\langle S_y(t)\rangle = -\frac{\hbar}{2}\sin\omega_0 t$$

$$\langle S_z(t)\rangle = 0$$

In the Schrödinger rep.:

$$|\psi(t)\rangle = e^{-iH\cdot t/\hbar}|\psi(0)\rangle$$

$$= e^{i\omega_0 t\, S_z/\hbar}|\psi(0)\rangle$$

$$\left[\text{since } |\vec{n}\uparrow\rangle = e^{-i\vec{\alpha}\cdot\vec{S}/\hbar}|\uparrow\rangle\right]$$

$\Rightarrow$ the spin rotates around $-\vec{z}$ with velocity ω_0 $\quad (e>0)$

<u>Spin Resonance</u>:

Since the spin precesses <u>negatively</u> (positively) about $\hat{z}$ for $e>0$ ($e<0$), with angular velocity ω_0, if we observe the spin in a coordinate frame rotating negatively (positively) about $\hat{z}$ with ang. vel. ω_0, the spin will appear not to precess at all. In other words, it is as if in the rotating frame there was an extra magnetic field that cancelled $\vec{B}$.

If a coord-frame rotates by $-\omega$ about $\hat{z}$ $\Rightarrow$ the effective field is

$$B_{eff} = B_0 - \frac{2mc\omega}{ge}$$

$\Rightarrow$ If we could apply a weak field that remains stationary along the x axis of the rotating frame with ang. vel. $-\omega_0$ about $\hat{z}$, then in this rot. frame the spin will feel only this field and would precess about it.

If the field begin $|\uparrow\rangle$ $\Rightarrow$ after a $180°$ precession $\rightarrow |\downarrow\rangle$ (no matter how weak the field is).

In the lab. frame this expt. means an radio freq. magnetic field

$$B_x = \frac{B_1}{2}\cos\omega t \qquad B_y = -\frac{B_1}{2}\sin\omega t \qquad B_z = 0$$

$\omega = \omega_0$

& in practice one uses $B_x = B_1 \cos\omega t$

$B_y = 0$ $\qquad \omega \simeq \omega_0$

$B_z = 0$

$$\vec{B} = \frac{B_1}{2}\begin{pmatrix}\cos\omega t\\ -\sin\omega t\\ 0\end{pmatrix} + \frac{B_1}{2}\begin{pmatrix}\cos\omega t\\ \sin\omega t\\ 0\end{pmatrix}$$

rotates with $+\omega$ and counter to the precessing spin $\Rightarrow$ high freq wiggles that average out to 0.

$(B_1 \ll B_0)$

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Schrödinger Rep:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = -\frac{e\hbar}{2mc}\frac{g}{2}\left(B_0\sigma_z + B_1\cos\omega t\,\sigma_x\right)|\psi(t)\rangle$$

rotated state

$$|\psi(t)\rangle = e^{\frac{i}{2}\omega t\,\sigma_z}|\psi'(t)\rangle$$

$$\Rightarrow i\frac{d}{dt}|\psi'(t)\rangle = \left[\left(\frac{\omega-\omega_0}{2}\right)\sigma_z - \omega_1\cos\omega t\left(e^{-\frac{i\omega t\sigma_z}{2}}\sigma_x e^{\frac{i\omega t\sigma_z}{2}}\right)\right]|\psi'(t)\rangle$$

$$\omega_1 = \frac{geB_1}{4mc} \qquad \omega_0 = \frac{geB_0}{\cancel{4}2mc}$$

$$e^{-i\frac{\omega t}{2}\sigma_z}\sigma_x e^{+i\frac{\omega t}{2}\sigma_z} =$$

$$= \left(\cos\left(\frac{\omega t}{2}\right)I - i\sin\left(\frac{\omega t}{2}\right)\sigma_z\right)\sigma_x\left(\cos\frac{\omega t}{2}I - i\sin\frac{\omega t}{2}\sigma_z\right)$$

$$= e^{-i\omega t\sigma_z}\sigma_x = \cos\omega t\,\sigma_x + \sin(\omega t)\,\sigma_y$$

$$\Rightarrow \cos\omega t\; e^{-\frac{i\omega t}{2}\sigma_z}\sigma_x e^{\frac{i\omega t}{2}\sigma_z} =$$

$$= \cos^2\omega t\,\sigma_x + \frac{1}{2}\sin 2\omega t\,\sigma_y$$

$$= \frac{1}{2}\sigma_x + \underbrace{\frac{1}{2}\left(\sigma_x\cos 2\omega t + \sigma_y\sin 2\omega t\right)}_{\text{high freq. terms}}$$

$$i \frac{d}{dt}|\psi'(t)\rangle = \left[\left(\frac{\omega-\omega_0}{2}\right)\sigma_z - \frac{\omega_1}{2}\sigma_x\right]|\psi'(t)\rangle + \text{high freq. terms}$$

$$|\psi'(t)\rangle = e^{-i\frac{\Omega t}{2}\hat{\sigma}}|\psi'(0)\rangle$$

$$\Omega = \sqrt{(\omega-\omega_0)^2 + \omega_1^2}$$

$$\hat{\sigma} = \frac{\omega-\omega_0}{\Omega}\sigma_z - \frac{\omega_1}{\Omega}\sigma_x$$

$$[\hat{\sigma}^2 = I]$$

$$\Rightarrow |\psi(t)\rangle = e^{i\frac{\omega t}{2}\sigma_z} e^{-i\frac{\Omega t}{2}\hat{\sigma}}|\psi(0)\rangle$$

Suppose that, at $t=0$, the state is

$$|\psi(0)\rangle = |\hat{z}\uparrow\rangle \equiv |\uparrow\rangle$$

$\Rightarrow$ the amplitude to be in the state $|\downarrow\rangle$ at time t is

$$\langle\downarrow|\psi(t)\rangle = \langle\downarrow| e^{i\frac{\omega t}{2}\sigma_z} e^{-i\frac{\Omega t}{2}\hat{\sigma}}|\uparrow\rangle$$

$$= e^{-i\frac{\omega t}{2}}\langle\downarrow| e^{-i\frac{\Omega t}{2}\hat{\sigma}}|\uparrow\rangle$$

$$= e^{-i\frac{\omega t}{2}}\langle\downarrow|\left(\cos\frac{\Omega t}{2} - i\hat{\sigma}\sin\frac{\Omega t}{2}\right)|\uparrow\rangle$$

$$= e^{-i\frac{\omega t}{2}}(-i)\sin\frac{\Omega t}{2}\langle\downarrow|\hat{\sigma}|\uparrow\rangle$$

(since $\langle\downarrow|\uparrow\rangle = 0$)

and $\langle\downarrow|\hat{\sigma}|\uparrow\rangle = \langle\downarrow|\left[\left(\frac{\omega-\omega_0}{\Omega}\right)\sigma_z - \frac{\omega_1}{2}\sigma_x\right]|\uparrow\rangle$

$$= \left(\frac{\omega-\omega_0}{\Omega}\right)\underbrace{\langle\downarrow|\sigma_z|\uparrow\rangle}_{=0} - \frac{\omega_1}{\Omega}\langle\downarrow|\sigma_x|\uparrow\rangle$$

$$= \left(\frac{\omega-\omega_0}{\Omega}\right)\cdot 0 - \frac{\omega_1}{\Omega}\cdot 1$$

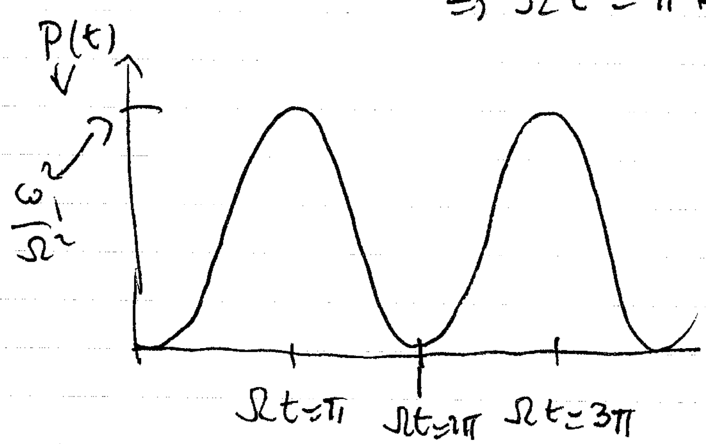
$$\Rightarrow \quad \langle\downarrow|\psi(t)\rangle = +i\frac{\omega_1}{\Omega}e^{-i\frac{\omega t}{2}}\sin\left(\frac{\Omega t}{2}\right)$$

$$\Rightarrow \quad P_\downarrow(t) = |\langle\downarrow|\psi(t)\rangle|^2 = \frac{\omega_1^2}{2\Omega^2}(1-\cos\Omega t) = \frac{\omega_1^2}{\Omega^2}\sin^2\left(\frac{\Omega t}{2}\right)$$

Maximum value of $P_\downarrow(t) = \frac{\omega_1^2}{\cancel{2}\Omega^2}\times\cancel{2} = \frac{\omega_1^2}{(\omega-\omega_0)^2+\omega_1^2}$

and it occurs for $\cos\Omega t = -1$

$$\Rightarrow \Omega t = \pi + 2n\pi \quad / \quad t = \frac{\pi}{\Omega}, \ldots$$



If $\omega-\omega_0 \gg \omega_1 \Rightarrow P_\downarrow(t) \ll 1$

but $\omega \to \omega_0 \Rightarrow P_\downarrow(t) \to 1$

(Resonance)

$\Rightarrow$ the spin absorbed an energy $\hbar\omega_0$ from the rf field.

This phenomenon is the basis of spin resonance techniques
(NMR, ESR, ...)