Spins

Drehimpuls $$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} = \vec{r} \times (-i\hbar\vec{\nabla}) = \begin{pmatrix} \hat{L}_x \\ \hat{L}_y \\ \hat{L}_z \end{pmatrix} = \begin{pmatrix} yp_z - zp_y \\ zp_x - xp_z \\ xp_y - yp_x \end{pmatrix}$$

Bsp.: H-Atom

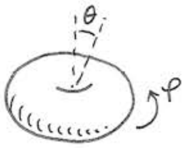
s:
$(\ell=0)$

$\psi \sim e^{-r/r_0}$

$\hat{\vec{L}}\psi = 0$

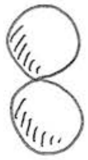
$|\psi|^2 = const$

p:
$(\ell=1)$



$\psi_\pm \sim f(r)\, e^{\pm i\varphi} \sin\theta \qquad m = \pm 1$

$\hat{L}_z \psi_\pm = \pm\hbar\psi_\pm = \hbar m \psi_\pm$



$\psi_0 \sim g(r) \cos\theta \qquad m = 0$

$\hat{L}_z \psi_0 = 0$

usw.: Quantenzahlen (ℓ, m) $\quad -\ell \leq m \leq \ell$, $m \in \mathbb{Z}$

ℓ → Drehimpuls

m → Projektion (in z)

Drehimpuls-Eigenschaften

$$[\hat{L}_x, \hat{L}_y] = \underbrace{[y p_z, z p_x]}_{y p_x \underbrace{[p_z, z]}_{-i\hbar}} + \underbrace{[z p_y, x p_z]}_{p_y x \underbrace{[z, p_z]}_{i\hbar}}$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$ "Drehimpuls-Algebra"

"& zyklisch"

$$.. y .. z = ... x$$
$$.. z .. x = ... y$$

$$[\hat{L}_x, \hat{\vec{L}}^2] = [\hat{L}_x, \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2]$$
$$= ... = 0$$

analog $\hat{L}_y, \hat{L}_z$

⇒ Wähle Basis von Eigenzuständen (simultan) zu $\hat{\vec{L}}^2$ & $\hat{L}_z$ (oder $\hat{\vec{L}}^2$ & $\hat{L}_x$ etc.)
Erlaubte Werte von $\hat{\vec{L}}^2$ & $\hat{L}_z$?
Matrixelemente von $\hat{L}_x, \hat{L}_y$?

Sei $\hat{L}_\pm \equiv \hat{L}_x \pm i \hat{L}_y$

$$\Rightarrow \quad [\hat{L}_z, \hat{L}_+] = ... = \hbar \hat{L}_+$$

⇒ falls $\hat{L}_z |\psi\rangle = \hbar m |\psi\rangle$:

$$\hat{L}_z \hat{L}_+ |\psi\rangle = \Big(\hat{L}_+ \hat{L}_z + \underbrace{[\hat{L}_z, \hat{L}_+]}_{\hbar \hat{L}_+}\Big) |\psi\rangle$$
$$= \hbar (m+1) \hat{L}_+ |\psi\rangle$$

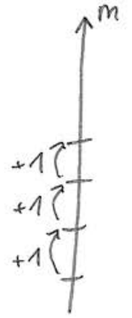
⇒ $\overset{|\tilde{\psi}\rangle = \hat{L}_+|\psi\rangle}{\text{ist}}$ EZ zum EW $\hbar(m+1)$

Aber: $|\tilde{\Psi}\rangle$ nicht normiert!

$$\langle\tilde{\Psi}|\tilde{\Psi}\rangle = \langle\Psi|\underbrace{\hat{L}_+^+}_{\hat{L}_-}\hat{L}_+|\Psi\rangle = \dots$$

$$= \langle\Psi|\hat{\vec{L}}^2 - \hat{L}_z^2 - \hbar\hat{L}_z|\Psi\rangle$$

$$= \langle\Psi|\hat{\vec{L}}^2|\Psi\rangle - \hbar^2 m(m+1)$$



Serie endet, falls $\hat{\vec{L}}^2|\Psi\rangle = \hbar^2 l(l+1)|\Psi\rangle$

& dann $m=+l \Rightarrow |\tilde{\Psi}\rangle = 0$

(& Serie muß enden, weil sonst $\langle\tilde{\Psi}|\tilde{\Psi}\rangle < 0$ ↯)

Analog: $\hat{L}_- \quad \Rightarrow \quad m \geq -l$

$m = -l, -l+1, \dots, l-1, l \quad \}$ 2l+1 Zustände

$\Rightarrow \quad l-(-l) = 2l$ muß $\in \mathbb{Z}$ sein

$\Rightarrow \quad l$ ganzzahlig $(l=0,1,2,\dots)$

oder

halbzahlig $(l=\frac{1}{2},\frac{3}{2},\dots)$

Normierung $\Rightarrow \quad |l,m+1\rangle = \dfrac{|\tilde{\Psi}\rangle}{\sqrt{\langle\tilde{\Psi}|\tilde{\Psi}\rangle}}$

$$\Rightarrow |\tilde{\Psi}\rangle = \hat{L}_+|l,m\rangle = \hbar\sqrt{l(l+1)-m(m+1)}\;|l,m+1\rangle$$

analog

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

z.B. $l=2$:

$$\hat{L}_+ = \hbar\begin{array}{c|l} \left[\begin{matrix} 0 & \sqrt{4} & & & \\ & 0 & \sqrt{6} & & \\ & & 0 & \sqrt{6} & \\ & & & 0 & \sqrt{4} \\ & & & & 0 \end{matrix}\right] & \begin{matrix} \leftarrow m=+2 \\ \leftarrow m=+1 \\ \leftarrow 0 \\ \leftarrow -1 \\ \leftarrow -2 \end{matrix} \end{array} \quad \& \; \hat{L}_- = \hat{L}_+^+$$

$$\Rightarrow \hat{L}_x = \frac{1}{2}(\hat{L}_+ + \hat{L}_-) = \dots$$

Spin $\frac{1}{2}$: $(l=\frac{1}{2})$

→ schreibe: $\hat{\vec{S}}$ (statt $\hat{\vec{L}}$)

S (statt l)

$$\hat{\vec{S}}^2 = \hbar^2 \cdot \frac{1}{2}\left(\frac{1}{2}+1\right) = \hbar^2 \cdot \frac{3}{4}$$

$$\hat{S}_z = \frac{\hbar}{2} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\hat{\sigma}_z}$$

Pauli-Matrizen

$$\hat{S}_x = \frac{\hbar}{2} \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\hat{\sigma}_x}$$

$$\hat{S}_y = \frac{\hbar}{2} \underbrace{\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}_{\hat{\sigma}_y}$$

$[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z$

& zykl.

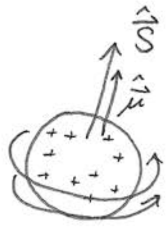
$\hat{\sigma}_x^2 = 1 = \hat{\sigma}_y^2 = \hat{\sigma}_z^2$

$\{\hat{\sigma}_x, \hat{\sigma}_y\} = 0$ usw.

$|S=\frac{1}{2}, m=+\frac{1}{2}\rangle \equiv |\uparrow\rangle$ "spin up"

$|S=\frac{1}{2}, m=-\frac{1}{2}\rangle \equiv |\downarrow\rangle$ "spin down"

Zeeman-Energie



$$\hat{H} = -\hat{\vec{\mu}} \cdot \vec{B}$$

magnetisches Moment : $\hat{\vec{\mu}} = \frac{1}{2}\int d^3\vec{r}\ \hat{\vec{r}} \times \hat{\vec{j}}$ [in SI]

$$\hat{\vec{\mu}} = g\frac{\mu_B}{\hbar}\hat{\vec{S}} \qquad (\text{oder: } \hat{\vec{L}})$$

"Bohr-Magneton"

g-Faktor

$\mu_B = \frac{|q_e|\hbar}{2m_e}$ [SI] $= \frac{|q_e|\hbar}{2m_e c}$ [CGS]

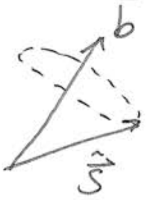
[z.B. $g=-2$ für $\overset{e^-}{\text{Spin}}$
$g=-1$ für orbitale Bewgg]

$$\Rightarrow \quad \hat{H} = \hat{\vec{S}}\cdot\vec{b} \qquad \Big(\vec{b} = -\frac{1}{\hbar}g\mu_B\vec{B}\Big)$$

(Frequenz)

Für $\vec{b} \parallel \hat{z}$: $|S, m\rangle$ mit $E = \hbar b m$

Bewgglg.: $\frac{d}{dt}\hat{\vec{S}}(t) = \frac{1}{i\hbar}[\hat{\vec{S}}(t), \hat{H}(t)]$
$= \dots = \underline{\underline{\vec{b}\times\hat{\vec{S}}}}$



$\Rightarrow$ Präzession mit Freq. $|\vec{b}|$ um $\vec{b}$
Winkel $\varphi = |\vec{b}|\cdot t$

Lsg.: $\hat{\vec{S}}(t) = e^{\frac{i}{\hbar}\hat{H}t}\,\hat{\vec{S}}(0)\,e^{-\frac{i}{\hbar}\hat{H}t}$

$$= \underbrace{e^{\frac{i}{\hbar}(\hat{\vec{S}}\vec{b})t}\ \hat{\vec{S}}(0)\,e^{-\frac{i}{\hbar}(\hat{\vec{S}}\vec{b})t}}_{\text{Drehung eines Spins (oder: des Koord.sys.)}}$$

z.B. Spin $\frac{1}{2}$, $\vec{b} = b\cdot\hat{e}_z$, $\varphi = bt$ $\Rightarrow$

$$\hat{\vec{\sigma}}(t) = e^{\frac{i}{2}\hat{\sigma}_z\varphi}\,\hat{\vec{\sigma}}(0)\,e^{-\frac{i}{2}\hat{\sigma}_z\varphi}$$

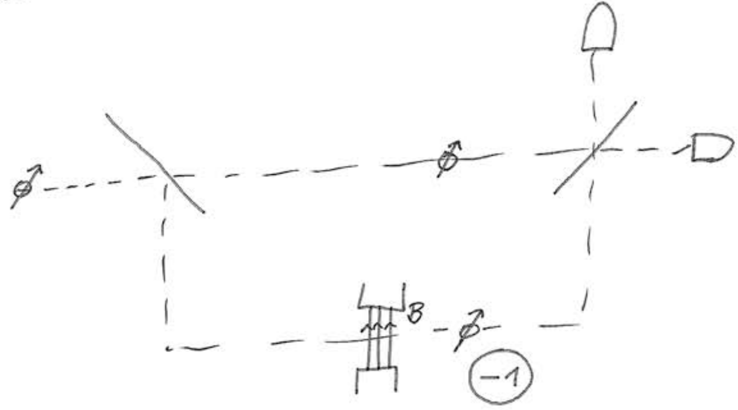
Drehung der Wellenfkt.: $e^{-\frac{i}{2}\hat{\sigma}_z\varphi}|\psi(0)\rangle$

⇒ für $\varphi = 2\pi$:

$$|\Psi'\rangle = e^{-\frac{i}{2}\hat{\sigma}_z \varphi}|\Psi(0)\rangle = -|\Psi(0)\rangle$$

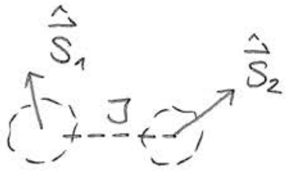
(!)

beobachtet in Interferenzexperimenten:



Spin-Kopplung

z.B. $\hat{H} = J \underbrace{\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2}$ "Heisenberg-Kopplung"



Jeder Spin spürt den anderen als Magnetfeld

$$= \hat{S}_{x1}\hat{S}_{x2} + \hat{S}_{y1}\hat{S}_{y2} + \hat{S}_{z1}\hat{S}_{z2}$$

$$= \frac{1}{2}\left(\hat{S}_{+1}\hat{S}_{-2} + \hat{S}_{-1}\hat{S}_{+2}\right) + \hat{S}_{z1}\hat{S}_{z2}$$

Gesamtspin: $\hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2$

wir haben:

$$[\hat{\vec{S}}, \hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2] = 0$$ ⇒ Gesamtspin erhalten unter Dynamik!

$$\hat{\vec{S}}_1 \hat{\vec{S}}_2 = \frac{1}{2}\left[\hat{\vec{S}}^2 - \hat{\vec{S}}_1^2 - \hat{\vec{S}}_2^2\right]$$

Bsp.: $S_1 = S_2 = \frac{1}{2}$ (Zwei gekoppelte Spin $\frac{1}{2}$)

⇒ alte Basis $|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$

Eigenbasis zu $\hat{H}$?
d.h. zu $\hat{\vec{S}}^2, \hat{S}_z, (\hat{\vec{S}}_1^2, \hat{\vec{S}}_2^2)$:

$|\Phi_{+1}\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 = |\uparrow\uparrow\rangle$

$\hat{S}_z |\uparrow\uparrow\rangle = (\hat{S}_{z1} + \hat{S}_{z2})|\uparrow\uparrow\rangle = \hbar |\uparrow\uparrow\rangle$

$|\Phi_{-1}\rangle = |\downarrow\downarrow\rangle$

⇒ $\hat{S}_z |\downarrow\downarrow\rangle = -\hbar |\downarrow\downarrow\rangle$

$|\Phi_0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$

⇒ $\hat{S}_z |\Phi_0\rangle = 0$

$\hat{\vec{S}}^2 |\Phi_j\rangle = \ldots = \hbar^2 1 (1+1) |\Phi_j\rangle$ ~~"Triplett"~~

⇒ $S = 1$

$$\hat{H} |\Phi_j\rangle = \frac{J}{2}\left[\hat{\vec{S}}^2 - \hat{\vec{S}}_1^2 - \hat{\vec{S}}_2^2\right] |\Phi_j\rangle = J \frac{\hbar^2}{4} |\Phi_j\rangle$$

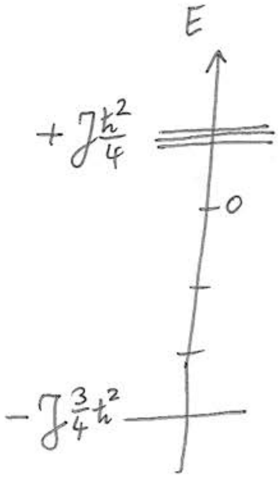
$|\Phi_{0,\pm 1}\rangle$: "Triplett"

$$|\Psi_0> = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow> - |\downarrow\uparrow>\right)$$

$$\hat{S}_z|\Psi_0> = 0$$

$$\hat{\vec{S}}^2|\Psi_0> = 0 \quad \Rightarrow S = 0 \qquad , \qquad \hat{H}|\Psi_0> = \dots = -J\frac{3}{4}\hbar^2|\Psi_0>$$

"Singlett"



Allgemeine Spin-Kopplung

S_1, S_2 bel.

$\Rightarrow$ $(2S_1+1)\cdot(2S_2+1)$-dim. Produkt-Hilbertraum!

Konstruiere darin Eigenbasis zu $\hat{\vec{S}}^2, \hat{S}_z$!

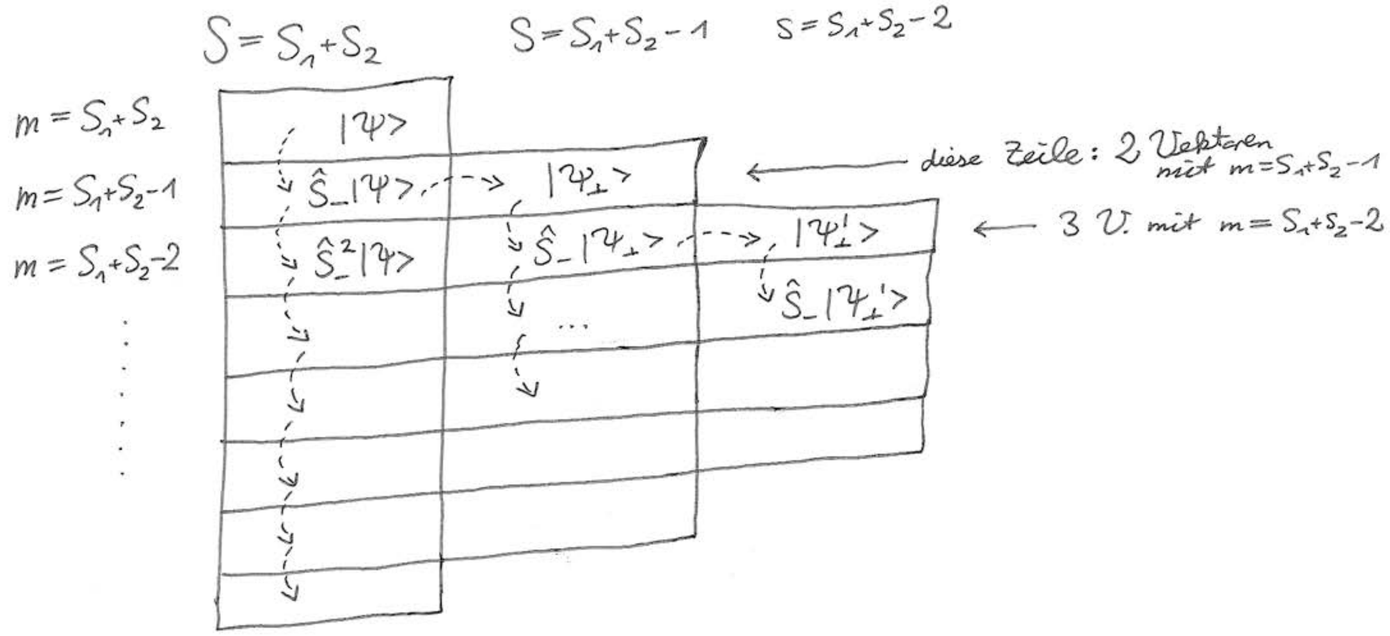
Starte von
$$|\psi\rangle = |S_1, m_1 = S_1, S_2, m_2 = S_2\rangle \quad (\text{analog zu } |\uparrow\uparrow\rangle)$$

$$\hat{S}_z|\psi\rangle = \underbrace{\hbar(\overset{S}{\cancel{m}}_1 + \overset{S}{\cancel{m}}_2)}_{\text{max. mögl. } S_z\text{-EW}}|\psi\rangle$$

$\Rightarrow$ $S = S_1 + S_2$ ist max. Wert von S !

Check: $\hat{\vec{S}}^2|\psi\rangle = \ldots = \hbar^2 S(S+1)|\psi\rangle$
mit $S = S_1 + S_2$ ✓

Schema:



Jede Zeile: alle Vektoren zu m, also
~~$|m_1, m_2 = m - m_1\rangle, |m_1 + m_2$~~
$|m_1, m_2\rangle$ mit $m_1 + m_2 = m$
$-S_1 \leq m_1 \leq S_1$
$-S_2 \leq m_2 \leq S_2$

Raum zu $m = S_1 + S_2 - 1$ ist 2-dim.

$$\left(|S_1, S_2-1\rangle \ \& \ |S_1-1, S_2\rangle \right)$$

$\Rightarrow$ $|\Psi_+\rangle$ ist der Vektor, der in diesem Raum orthagonal zu $|\tilde{\Psi}\rangle = \hat{S}_-|\Psi\rangle$ ist

$$\Rightarrow \quad |\Psi_+\rangle = |S_1, S_2-1\rangle - \frac{|\tilde{\Psi}\rangle\langle\tilde{\Psi}|S_1, S_2-1\rangle}{\langle\tilde{\Psi}|\tilde{\Psi}\rangle}$$

analog alle weiteren!

Es ergibt sich: $S_{min} = |S_1 - S_2|$

$$\Rightarrow \sum_{S=S_{min}}^{S_{max}=S_1+S_2} (2S+1) = (2S_1+1)\cdot(2S_2+1)$$

gesamte Basis ✓

Darstellung der neuen Basis in der (S_{z1}, S_{z2})-Produktbasis:

„Clebsch-Gordan-Koeffizienten“

$$|\underset{\downarrow \atop \text{zu } \hat{S}^2}{S}, \underset{\downarrow \atop \text{zu } \hat{S}_z}{m}\rangle = \sum_{m_1=-S_1}^{+S_1} \sum_{m_2=-S_2}^{+S_2} |S_1, m_1, S_2, m_2\rangle \langle S_1, m_1, S_2, m_2 | S, m\rangle$$