Review: H atom with electron spin $\hat{\vec{S}} = \frac{\hbar}{2}\vec{\sigma}$ $S = \frac{1}{2}$

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} - \frac{Z\alpha\hbar c}{r} + \hat{V}_{LS}$$

↳ due to relativistic effects

$$\hat{V}_{LS} = \frac{\hbar^2}{2m^2c^2}\left(\frac{1}{r}\frac{d}{dr}V(r)\right)\hat{\vec{L}}\cdot\hat{\vec{S}}$$

dim. less.

$l\cdot(l+1)$ $S\cdot(S+1)$

m m_s

$$\Rightarrow \hat{H} = \text{radial part} + \dots \hat{\vec{L}}^2 + \dots \hat{\vec{L}}\cdot\hat{\vec{S}}$$

Problem: $[\hat{H}, \hat{L}_j] \neq 0$ and $[\hat{H}, \hat{S}_j] \neq 0$

if $=0$ rotational inv. in coord. space

if $=0$ rotational inv. in spin space

But: $\left[\hat{H}, \underbrace{\hat{\vec{L}} + \hat{\vec{S}}}_{\hat{\vec{J}}}\right] = 0$!

→ $\hat{H}$ is only invariant under rotations in coordinate + spin space

Because $[\hat{L}_j, \hat{S}_k] = 0$ (different spaces!)

→ $[\hat{J}_j, \hat{J}_k] = i\varepsilon_{jkl}\hat{J}_l$ obey angular mom. algebra

→ $|J\, J_z\rangle$ simultaneous eigenstates

$$\hat{\vec{J}}^2 |J\, J_z\rangle = J(J+1)\,|J\, J_z\rangle$$

$$\hat{J}_z |J\, J_z\rangle = J_z\,|J\, J_z\rangle$$

Use $\quad \hat{\vec{L}} \cdot \hat{\vec{S}} = \frac{1}{2}\left(\hat{\vec{J}}^2 - \hat{\vec{S}}^2 - \hat{\vec{L}}^2\right)$

$$\Rightarrow \quad \hat{H} = \text{radial part} + \cdots \hat{\vec{L}}^2 + \cdots \frac{1}{2}\left(\vec{J}^2 - \vec{S}^2 - \vec{L}^2\right)$$

$$\Rightarrow \quad [\hat{H}, \hat{\vec{J}}_k] = 0 = [\hat{H}, \underbrace{\hat{\vec{L}}^2}_{\ell(\ell+1)}] = [\hat{H}, \hat{\vec{S}}^2] = [\hat{H}, \hat{\vec{J}}^2]$$

$\hat{H}$ hat gute Eigenzustände $|E\, \ell\, s\, J\, J_z\rangle$

nicht $|n\, \ell\, m\rangle\, |s\, m_s\rangle$

Simultane Eigenzustände von $\hat{\vec{L}}^2$, $\hat{\vec{S}}^2$, $\hat{\vec{J}}^2 = (\hat{\vec{L}} + \hat{\vec{S}})^2$, $\hat{J}_z$

$$|\underbrace{(\ell\, s)\, J}\, J_z\rangle$$

ℓ und S sind gekoppelt addiert zu J

$$\hat{\vec{J}}^2\, |(\ell s) J J_z\rangle = J(J+1)\, |(\ell s) J J_z\rangle$$

$$\hat{J}_z\, |(\ell s) J J_z\rangle = J_z\, |(\ell s) J J_z\rangle$$

$$\hat{\vec{L}}^2\, |(\ell s) J J_z\rangle = \ell(\ell+1)\, |(\ell s) J J_z\rangle$$

$$\hat{\vec{S}}^2\, |(\ell s) J J_z\rangle = s(s+1)\, |(\ell s) J J_z\rangle$$

Wie konstruieren wir $\underbrace{|(\ell s) J J_z\rangle}$ aus $\underbrace{|\ell m\rangle\, |s\, m_s\rangle}$ da?

muss für $\ell = 2$, $s = \frac{1}{2}$ auch 10 Zustände geben!

geg. ℓ, s, Dimension: $(2\ell+1)\cdot(2s+1)$

Bsp. $\ell = 2$, $s = \frac{1}{2}$ 10 Zustände

$m = -2, -1, 0, 1, 2 \qquad m_s = -\frac{1}{2}, \frac{1}{2}$

Im allg. $\underbrace{|(ls)\,j\,j_z\rangle}_{\text{gekoppelt}} = \sum\limits_{\underbrace{m,m_s}_{m+m_s=j_z}} C^{l\,s\,j\,j_z}_{m\,m_s}\, \underbrace{|l m\rangle |s m_s\rangle}_{\text{ungekoppelt}}$

① $\hat{J}_z\, |l m\rangle |s m_s\rangle = (\hat{L}_z + \hat{S}_z)\, |l m\rangle |s m_s\rangle$

$= (m + m_s)\, |l m\rangle |s m_s\rangle$

$\Rightarrow$ $j_z = m + m_s$ $\qquad j_z = -j, -j+1, \dots, j-1, j$

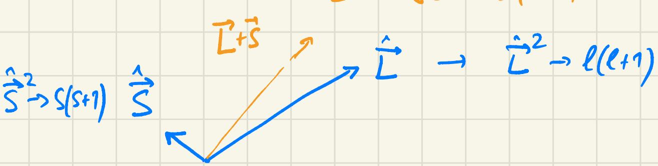
② $\Rightarrow$ $|l - s| \leq \underset{\text{positiv!}}{j} \leq l + s$ $\qquad j = |l-s|, |l-s|+1, \dots, l+s-1, l+s$

Bsp. $\frac{3}{2} \leq j \leq \frac{5}{2}$

Dimensionscheck: $j = \frac{5}{2}$ $\quad j_z = -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$ $\quad (2j+1) = 6$

$j = \frac{3}{2}$ $\quad j_z = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$ $\quad (2j+1) = 4$

$\overline{10}$!



③ Ein Zustand mit max. $j_z = l + s$: $|(ls)\, l+s\;\, l+s\rangle = |l l\rangle |s s\rangle$

min $j_z = -(l+s)$: $|(ls)\, l+s\;\, -(l+s)\rangle = |l, -l\rangle |s, -s\rangle$ ✓

④ $\hat{\vec{J}}^2 \overset{\text{Kap. 8}}{=} \hat{J}_\mp \hat{J}_\pm + \hat{J}_z (\hat{J}_z \pm 1)$

$\Rightarrow$ $\underset{\hat{J}_- \hat{J}_+ + \hat{J}_z(\hat{J}_z+1)}{\hat{\vec{J}}^2}\, |l l\rangle |s s\rangle = \underbrace{(l+s)}_{j}\, \underbrace{(l+s+1)}_{j+1}\, |l l\rangle |s s\rangle$

$\hat{J}_- \hat{J}_+ \to = 0$

$$\Rightarrow \hat{\vec{J}}^2 \, |l,-l\rangle |s,-s\rangle \overset{?}{=} J(J+1)\, |l,-l\rangle |s,-s\rangle$$

$$\underset{\shortparallel}{} \hat{J}_+ \underbrace{\hat{J}_-}_{0} + \hat{J}_z(\hat{J}_z - 1) = \underbrace{-(l+s)(-l-s-1)}_{(l+s)(l+s+1)} \, |l,-l\rangle |s,-s\rangle \quad ✓$$

(5) Zustände mit $J_z - 1, J_z - 2, \ldots, -J_z$ durch Anwenden von

$$\hat{J}_- = \hat{L}_- + \hat{S}_-$$

auf $|(ls)\, l+s \;\; l+s\rangle$

$$\begin{matrix} l+s & l+s-1 \\ & -2 \\ & -3 \\ & \vdots \end{matrix}$$

<u>Beispiel:</u> Addition von zwei $s = \frac{1}{2}$ spins.

$s_1 = \frac{1}{2}$, $\hat{\vec{S}}_1$; $s_2 = \frac{1}{2}$, $\hat{\vec{S}}_2$, $\hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2$

ungekoppelt: Dim. 4 Gesamtspin

Starte bei max. S, max S_z

$|(s_1 = \frac{1}{2})(s_2 = \frac{1}{2})\, S = 1, m_S = 1\rangle$

Gesamt $\hat{S}_-$ ↓

$S = 1$, $S_z = 1$ $\quad \underset{(\frac{1}{2}\frac{1}{2})}{|} S = 1, S_z = 1\rangle = \underset{C^{11}_{\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}}}{1} |s_1 = \frac{1}{2}, m_{s_1} = \frac{1}{2}\rangle |s_2 = \frac{1}{2}, m_{s_2} = \frac{1}{2}\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2$

$S = 1$, $S_z = 0$ $\quad \underset{(\frac{1}{2}\frac{1}{2})}{|} S = 1, S_z = 0\rangle = \underbrace{\frac{1}{\sqrt{S(S+1) - \cdots}}}_{\frac{1}{\sqrt{2}}} \hat{S}_- \underset{(\frac{1}{2}\frac{1}{2})}{|} S = 1, S_z = 1\rangle$

$$= \frac{1}{\sqrt{2}} (\hat{S}_{1-} + \hat{S}_{2-}) |\uparrow\rangle_1 |\uparrow\rangle_2 .$$

$$= \frac{1}{\sqrt{2}} \left(|\downarrow\rangle_1 |\uparrow\rangle_2 + |\uparrow\rangle_1 |\downarrow\rangle_2 \right) \qquad C^{10}_{\frac{1}{2}\frac{1}{2}\frac{1}{2}-\frac{1}{2}} = \frac{1}{\sqrt{2}}$$

$\hat{S}_-$ ↓

$S = 1$, $S_z = -1$ $\quad \underset{(\frac{1}{2}\frac{1}{2})}{|} S = 1, S_z = -1\rangle = \frac{1}{\sqrt{2}} (\hat{S}_{1-} + \hat{S}_{2-}) \frac{1}{\sqrt{2}} \left(|\downarrow\rangle|\uparrow\rangle + |\uparrow\rangle|\downarrow\rangle \right)$

$=0$ $\quad =0$

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

$$|S=1, S_z=-1\rangle = 1\,|s_1=\tfrac{1}{2}, m_{s_1}=-\tfrac{1}{2}\rangle\,|s_2=\tfrac{1}{2}, m_{s_2}=-\tfrac{1}{2}\rangle$$

Spin Triplett, Symmetrische Spin-zustände $\quad C^{1\,-1}_{\frac{1}{2}\,-\frac{1}{2}\,\frac{1}{2}\,-\frac{1}{2}}$

fehlt noch $S=0$ Zustand $S_z=0$

benutze $|S=0, S_z=0\rangle$ orthogonal zu $|S=1, S_z\rangle$

$$\Rightarrow \quad \underset{(\frac{1}{2}\frac{1}{2})}{|S=0, S_z=0\rangle} = \frac{1}{\sqrt{2}}\Big(|s_1=\tfrac{1}{2}, m_{s_1}=\tfrac{1}{2}\rangle\,|s_2=\tfrac{1}{2}\rangle\,|m_{s_2}=-\tfrac{1}{2}\rangle - |s_1=\tfrac{1}{2}, m_{s_1}=-\tfrac{1}{2}\rangle\,|s_2=\tfrac{1}{2}, m_{s_2}=+\tfrac{1}{2}\rangle \Big)$$

$$= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2 \right)$$

Spin Singlett, antisymmetrischer Spinzustand

allg. $\quad |S=0, S_z=0\rangle = c_1\,|\uparrow\rangle_1|\downarrow\rangle_2 + c_2\,|\downarrow\rangle_1|\uparrow\rangle_2$

bestimme c_1, c_2 aus Orthonormalität

Allgemein $\quad |(l\,s)\,J\,J_z\rangle = \sum\limits_{\substack{m, m_s \\ m+m_s=J}} \underbrace{C^{J J_z}_{l m s m_s}}_{\text{Clebsch-Gordan Koeffizient}} |l\,m\rangle\,|s\,m_s\rangle$

Benutze $\hat{\mathbb{1}} = \sum_{\substack{l\,m \\ s\,m_s}} |l m\rangle\, |s\, m_s\rangle \langle l m|\, \langle s\, m_s|$

$$= \sum_{\substack{l s \\ J J_z}} |(l s)\, J J_z\rangle \langle (l s)\, J J_z|$$

$$\Longrightarrow \quad |(l s)\, J J_z\rangle = \sum_{m, m_s} |l m\rangle\, |s\, m_s\rangle\, \underbrace{\langle l\, m; s\, m_s | (l s)\, J J_z\rangle}_{= C^{J J_z}_{l m s m_s}}$$

$C^{J J_z}_{l m s m_s} \neq 0$ für $J_z = m + m_s$ und $|l - s| \leq J \leq l + s$

$C^{J J_z}_{l m s m_s} = \text{reell}$