Inhaltsverzeichnis

1 Spinfunktionen für $n_{el} = 4$

1.1 Quantenzahlen und Abkürzung als Ket

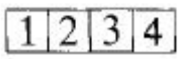
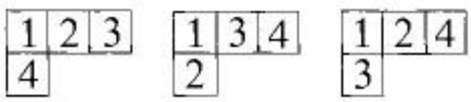
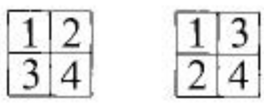
$n_{el} = 4$ d.h. $S = \{0, 1, 2\}$ und

- $M_S = \{0\}$ für $S = 0$ bzw. $2S + 1 = 1$
- $M_S = \{-1, 0, 1\}$ für $S = 1$ bzw. $2S + 1 = 3$
- $M_S = \{-2, -1, 0, 1, 2\}$ für $S = 2$ bzw. $2S + 1 = 5$

d.h. mögliche Fälle für $|S\ M_S\rangle$ lauten:

- $|0 \quad 0\rangle$
- $|1 \quad 1\rangle$
- $|1 \quad 0\rangle$
- $|1 \quad -1\rangle$
- $|2 \quad 2\rangle$
- $|2 \quad 1\rangle$
- $|2 \quad 0\rangle$
- $|2 \quad -1\rangle$
- $|2 \quad -2\rangle$

Der Fall $\uparrow\uparrow\uparrow\uparrow$ muss symmetrisch sein und kann nur im Fall $S = 2$ vorkommen. D.h. $S = 2$ gehört zum Tableau [4], das nur Kästchen nur symmetrisch (= in 1 Reihe) kombiniert. Analog weitergegangen folgt: [31] gehört zu $S = 1$ und $[2^2]$ gehört zu $S = 0$.

[4]	[3 1]	$[2^2]$
		
$\|2 \quad 2\rangle$ $\|2 \quad 1\rangle$ $\|2 \quad 0\rangle$ $\|2 \quad -1\rangle$ $\|2 \quad -2\rangle$	$\|1 \quad 1\rangle$ $\|1 \quad 0\rangle$ $\|1 \quad -1\rangle$	$\|0 \quad 0\rangle$

1.2 Funktionen

Funktionen konstruieren anhand der M_S-Werte und daraus folgender mögl. m_s Kombinationen. Vorzeichen anhand des Young-Tableau:

- [4] :

- $\begin{array}{|c|c|c|c|}\hline 1&2&3&4\\\hline\end{array}$:
  * $|2 \quad 2\rangle = (\alpha\alpha\alpha\alpha)$
  * $|2 \quad 1\rangle = \frac{1}{\sqrt{4}}\left[(\alpha\alpha\alpha\beta) + (\alpha\alpha\beta\alpha) + (\alpha\beta\alpha\alpha) + (\beta\alpha\alpha\alpha)\right]$
  * $|2 \quad 0\rangle = \frac{1}{\sqrt{6}}\left[(\alpha\alpha\beta\beta) + (\beta\alpha\beta\alpha) + (\alpha\beta\alpha\beta) + (\beta\beta\alpha\alpha) + (\alpha\beta\beta\alpha) + (\beta\alpha\alpha\beta)\right]$
  * $|2 \quad -1\rangle = \frac{1}{\sqrt{4}}\left[(\alpha\beta\beta\beta) + (\beta\alpha\beta\beta) + (\beta\beta\alpha\beta) + (\beta\beta\beta\alpha)\right]$
  * $|2 \quad -2\rangle = (\beta\beta\beta\beta)$

• $[3 \quad 1]$:

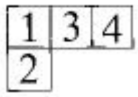
- $\begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4\\\cline{1-1}\end{array}$:
  * $|1 \quad 1\rangle = \frac{1}{\sqrt{2}}\left[(\alpha\alpha\alpha\beta) - (\beta\alpha\alpha\alpha)\right]$
  * $|1 \quad 0\rangle = \frac{1}{\sqrt{4}}\left[(\alpha\alpha\beta\beta) - (\beta\alpha\beta\alpha) + (\alpha\beta\alpha\beta) - (\beta\beta\alpha\alpha)\right]$
  * $|1 \quad -1\rangle = \frac{1}{\sqrt{2}}\left[(\alpha\beta\beta\beta) - (\beta\beta\beta\alpha)\right]$
- $\begin{array}{|c|c|c|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array}$:
  * $|1 \quad 1\rangle = \frac{1}{\sqrt{2}}\left[(\alpha\beta\alpha\alpha) - (\beta\alpha\alpha\alpha)\right]$
  * $|1 \quad 0\rangle = \frac{1}{\sqrt{4}}\left[(\alpha\beta\alpha\beta) - (\beta\alpha\beta\alpha) + (\alpha\beta\beta\alpha) - (\beta\alpha\alpha\beta)\right]$
  * $|1 \quad -1\rangle = \frac{1}{\sqrt{2}}\left[(\alpha\beta\beta\beta) - (\beta\alpha\beta\beta)\right]$
- $\begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array}$:
  * $|1 \quad 1\rangle = \frac{1}{\sqrt{2}}\left[(\alpha\alpha\beta\alpha) - (\beta\alpha\alpha\alpha)\right]$
  * $|1 \quad 0\rangle = \frac{1}{\sqrt{4}}\left[(\alpha\alpha\beta\beta) - (\beta\alpha\alpha\beta) - (\beta\beta\alpha\alpha) + (\alpha\beta\beta\alpha)\right]$
  * $|1 \quad -1\rangle = \frac{1}{\sqrt{2}}\left[(\alpha\beta\beta\beta) - (\beta\beta\alpha\beta)\right]$

• $[2^2]$:

- $\begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline\end{array}$
  * $|0 \quad 0\rangle = \frac{1}{\sqrt{4}}\left[(\alpha\alpha\beta\beta) + (\beta\beta\alpha\alpha) - (\alpha\beta\beta\alpha) - (\beta\alpha\alpha\beta)\right]$
- $\begin{array}{|c|c|}\hline 1&3\\\hline 2&4\\\hline\end{array}$
  * $|0 \quad 0\rangle = \frac{1}{\sqrt{4}}\left[(\alpha\beta\alpha\beta) + (\beta\alpha\beta\alpha) - (\alpha\beta\beta\alpha) - (\beta\alpha\alpha\beta)\right]$

1.3 Herleitung Spinfunktionen

Vorfaktoren entsprechen nicht dem Normierungsfaktor, werden nur z.T. zur Nachvollziehbarkeit hier mitgeschrieben; grün hinterlegt = $\hat{A}\hat{S}$ und $\hat{S}\hat{A}$. identisch, bold = Unterschiedssummanden zw. $\hat{A}\hat{S}$ und $\hat{S}\hat{A}$.

		
	$\hat{A}\hat{S}$	$\hat{S}\hat{A}$
$M_S = 0 \leftrightarrow 1 = 3 = 4 = \alpha,\ 2 = \beta$	$\hat{A}\,(\alpha\alpha\alpha)\,\beta$ $= \alpha\beta\alpha\alpha - \beta\alpha\alpha\alpha$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\alpha\alpha$ $= 6\ \alpha\beta\alpha\alpha - 6\ \beta\alpha\alpha\alpha$
$M_S = 1 \leftrightarrow 1 = 3 = \alpha,\ 2 = 4 = \beta$	$\hat{A}\,(\alpha\alpha\beta + \beta\alpha\alpha + \alpha\beta\alpha)\,\beta$ $= \alpha\beta\alpha\beta - \beta\alpha\alpha\beta\ \boldsymbol{+\beta\beta\alpha\alpha}\ - \beta\alpha\beta\alpha + \alpha\beta\beta\alpha \boldsymbol{-\alpha\alpha\beta\beta}$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\alpha\beta$ $= \alpha\beta\alpha\beta + \alpha\beta\alpha\beta + \alpha\beta\beta\alpha + \beta\beta\alpha\alpha + \alpha\beta\beta\alpha + \beta\beta\alpha\alpha$ $-\beta\alpha\alpha\beta - \beta\alpha\alpha\beta - \beta\alpha\beta\alpha - \beta\beta\alpha\alpha - \beta\alpha\beta\alpha - \beta\beta\alpha\alpha$ $= 2\ \alpha\beta\alpha\beta + 2\ \alpha\beta\beta\alpha$ $-2\ \beta\alpha\alpha\beta - 2\ \beta\alpha\beta\alpha$
$M_S = -1 \leftrightarrow 1 = \alpha,\ 2 = 3 = 4 = \beta$	$\hat{A}\,(\alpha\beta\beta + \beta\alpha\beta + \beta\beta\alpha)\,\beta$ $= \alpha\beta\beta\beta - \beta\alpha\beta\beta + \beta\beta\alpha\beta - \beta\alpha\beta\beta + \beta\beta\beta\alpha - \beta\alpha\beta\beta$ $= \alpha\beta\beta\beta - 3\beta\alpha\beta\beta + \beta\beta\alpha\beta + \beta\beta\beta\alpha$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\beta\beta$ $= \alpha\beta\beta\beta + \beta\beta\alpha\beta + \alpha\beta\beta\beta + \beta\beta\beta\alpha + \beta\beta\beta\alpha + \beta\beta\alpha\beta$ $-\beta\alpha\beta\beta - \beta\beta\alpha\beta - \beta\alpha\beta\beta - \beta\beta\beta\alpha - \beta\beta\beta\alpha - \beta\beta\alpha\beta$ $= 2\ \alpha\beta\beta\beta - 2\ \beta\alpha\beta\beta$

	$\begin{array}{\|c\|c\|c\|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array}$	
	$\hat{A}\hat{S}$	$\hat{S}\hat{A}$
$M_S = 0 \leftrightarrow 1 = 2 = 4 = \alpha,\ 3 = \beta$	$\hat{A}\,(\alpha\alpha\alpha)\,\beta$ $= \alpha\alpha\beta\alpha - \beta\alpha\alpha\alpha$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\alpha\alpha$ $= 6\ \alpha\alpha\beta\alpha - 6\ \beta\alpha\alpha\alpha$
$M_S = 1 \leftrightarrow 1 = 2 = \alpha,\ 3 = 4 = \beta$	$\hat{A}\,(\alpha\alpha\beta + \beta\alpha\alpha + \alpha\beta\alpha)\,\beta$ $= \alpha\alpha\beta\beta - \beta\alpha\alpha\beta \boldsymbol{+\beta\alpha\beta\alpha} - \beta\beta\alpha\alpha + \alpha\beta\beta\alpha \boldsymbol{-\alpha\beta\alpha\beta}$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\alpha\beta$ $= \alpha\alpha\beta\beta + \alpha\alpha\beta\beta + \alpha\beta\beta\alpha + \beta\alpha\beta\alpha + \alpha\beta\beta\alpha + \beta\alpha\beta\alpha$ $-\beta\alpha\alpha\beta - \beta\alpha\alpha\beta - \beta\beta\alpha\alpha - \beta\alpha\beta\alpha - \beta\alpha\beta\alpha - \beta\beta\alpha\alpha$ $= 2\ \alpha\alpha\beta\beta + 2\ \alpha\beta\beta\alpha - 2\ \beta\alpha\alpha\beta - 2\ \beta\beta\alpha\alpha$
$M_S = -1 \leftrightarrow 1 = \alpha,\ 2 = 3 = 4 = \beta$	$\hat{A}\,(\alpha\beta\beta + \beta\alpha\beta + \beta\beta\alpha)\,\beta$ $= \alpha\beta\beta\beta - \beta\beta\alpha\beta + \beta\alpha\beta\beta - \beta\beta\alpha\beta + \beta\beta\beta\alpha - \beta\beta\alpha\beta$ $= \alpha\beta\beta\beta - 3\beta\beta\alpha\beta \boldsymbol{+\beta\alpha\beta\beta + \beta\beta\beta\alpha}$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\beta\beta$ $= \alpha\beta\beta\beta + \beta\alpha\beta\beta + \alpha\beta\beta\beta + \beta\beta\beta\alpha + \beta\beta\beta\alpha + \beta\alpha\beta\beta$ $-\beta\beta\alpha\beta - \beta\alpha\beta\beta - \beta\beta\alpha\beta - \beta\beta\beta\alpha - \beta\alpha\beta\beta - \beta\beta\beta\alpha$ $= 2\ \alpha\beta\beta\beta - 2\ \beta\beta\alpha\beta$

	$\begin{array}{\|c\|c\|c\|}\hline 1 & 2 & 3 \\ \hline 4 \\ \cline{1-1}\end{array}$	
	$\hat{A}\hat{S}$	$\hat{S}\hat{A}$
$M_S = 0 \leftrightarrow 1 = 2 = 3 = \alpha,\ 4 = \beta$	$\hat{A}\,(\alpha\alpha\alpha)\,\beta$ $= \alpha\alpha\alpha\beta - \beta\alpha\alpha\alpha$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\alpha\alpha$ $= 6\ \alpha\alpha\alpha\beta\ {-6}\ \beta\alpha\alpha\alpha$
$M_S = 1 \leftrightarrow 1 = 2 = \alpha,\ 3 = 4 = \beta$	$\hat{A}\,(\alpha\alpha\beta + \alpha\beta\alpha + \beta\alpha\alpha)\,\beta$ $= \alpha\alpha\beta\beta - \beta\alpha\beta\alpha + \alpha\beta\alpha\beta - \beta\beta\alpha\alpha$ $\cancel{+\beta\alpha\alpha\beta - \beta\alpha\alpha\beta}$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\alpha\alpha$ $= \alpha\alpha\beta\beta + \alpha\alpha\beta\beta + \alpha\beta\alpha\beta + \beta\alpha\alpha\beta + \alpha\beta\alpha\beta + \beta\alpha\alpha\beta$ $-\beta\alpha\beta\alpha - \alpha\beta\beta\alpha - \beta\beta\alpha\alpha - \beta\alpha\beta\alpha - \alpha\beta\beta\alpha - \beta\beta\alpha\alpha$ $= 2\ \alpha\alpha\beta\beta - 2\ \alpha\beta\alpha\beta - 2\ \beta\alpha\beta\alpha - 2\ \alpha\beta\beta\alpha$ $\boldsymbol{+2\ \beta\alpha\alpha\beta - 2\ \beta\beta\alpha\alpha}$
$M_S = -1 \leftrightarrow 1 = \alpha,\ 2 = 3 = 4 = \beta$	$\hat{A}\,(\alpha\beta\beta)\,\beta$ $= \alpha\beta\beta\beta - \beta\beta\beta\alpha$	$\hat{S}\,(\alpha\beta - \beta\alpha)\,\beta\beta$ $= \alpha\beta\beta\beta + \beta\alpha\beta\beta + \beta\beta\alpha\beta + \alpha\beta\beta\beta + \beta\beta\alpha\beta + \beta\alpha\beta\beta$ $-\beta\beta\beta\alpha - \beta\alpha\beta\beta - \beta\beta\beta\alpha - \beta\beta\alpha\beta - \beta\alpha\beta\beta - \beta\beta\alpha\beta$ $= 2\ \alpha\beta\beta\beta - 2\ \beta\beta\beta\alpha$ (2. Teil: Festhalten des Index 4, der nun an 1. Stelle steht!)

	$\begin{array}{\|c\|c\|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array}$	
	$\hat{A}\hat{S}$	$\hat{S}\hat{A}$
$M_S = 0 \leftrightarrow 1 = 2 = \alpha,\ 3 = 4 = \beta$	$\hat{A}\,(\alpha\alpha)\,(\beta\beta)$ $\alpha\alpha\beta\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha + \beta\beta\alpha\alpha$ $+\alpha\alpha\beta\beta - \alpha\beta\alpha\beta - \beta\alpha\beta\alpha + \beta\beta\alpha\alpha$ $= 2\ \alpha\alpha\beta\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha\ \boldsymbol{-\alpha\beta\alpha\beta - \beta\alpha\beta\alpha}\ {+2}\ \beta\beta\alpha\alpha$ (wenn Wegfall von Termen nach S nicht beachtet wird, und nur 1234 ersetzt werden, ergibt sich eine Wiederholung aller Summanden = Dopplung)	$\hat{S}\,(\alpha\beta - \beta\alpha)\,(\alpha\beta - \beta\alpha)$ $= \hat{S}\,(\alpha\beta - \beta\alpha)\,\alpha\beta - \hat{S}\,(\alpha\beta - \beta\alpha)\,\beta\alpha$ $= \alpha\alpha\beta\beta - \beta\alpha\alpha\beta - \alpha\beta\beta\alpha + \beta\beta\alpha\alpha + \alpha\alpha\beta\beta - \alpha\beta\alpha\beta - \beta\alpha\beta\alpha + \beta\beta\alpha\alpha + \alpha\alpha\beta\beta$ $-\beta\alpha\beta\alpha - \alpha\beta\alpha\beta + \beta\beta\alpha\alpha + \alpha\alpha\beta\beta - \alpha\beta\beta\alpha - \beta\alpha\alpha\beta + \beta\beta\alpha\alpha$ $= 4\ \alpha\alpha\beta\beta - 4\ \beta\alpha\alpha\beta - 4\ \alpha\beta\beta\alpha - 4\ \beta\beta\alpha\alpha$

	$\begin{array}{\|c\|c\|}\hline 1&3\\\hline 2&4\\\hline\end{array}$	
	$\hat{A}\hat{S}$	$\hat{S}\hat{A}$
$M_S = 0 \leftrightarrow$ $1 = 2 = \alpha$, $3 = 4 = \beta$	$\hat{A}\,(\alpha\beta + \beta\alpha)\,(\alpha\beta + \beta\alpha)$ $= \hat{A}\,(\alpha\beta + \beta\alpha)\,\alpha\beta - \hat{A}\,(\alpha\beta + \beta\alpha)\,\beta\alpha$ $= \alpha\alpha\beta\beta - \alpha\alpha\beta\beta - \alpha\alpha\beta\beta + \alpha\alpha\beta\beta$ $+\beta\alpha\alpha\beta - \beta\alpha\alpha\beta - \beta\alpha\alpha\beta + \beta\alpha\alpha\beta$ $-\alpha\beta\beta\alpha + \alpha\beta\beta\alpha + \alpha\beta\beta\alpha - \alpha\beta\beta\alpha$ $-\beta\beta\alpha\alpha + \beta\beta\alpha\alpha + \beta\beta\alpha\alpha - \beta\beta\alpha\alpha$ $= 0$	$\hat{S}\,(\alpha\alpha - \alpha\alpha)\,(\beta\beta - \beta\beta)$ $= \hat{S}\,(\alpha\alpha - \alpha\alpha)\,\beta\beta - \hat{S}\,(\alpha\alpha - \alpha\alpha)\,\beta\beta$ $= \alpha\alpha\beta\beta + \beta\alpha\alpha\beta + \alpha\beta\beta\alpha + \beta\beta\alpha\alpha$ $-\alpha\alpha\beta\beta - \alpha\beta\alpha\beta - \beta\alpha\beta\alpha - \beta\beta\alpha\alpha$ $= \beta\alpha\alpha\beta + \alpha\beta\beta\alpha - \alpha\beta\alpha\beta - \beta\alpha\beta\alpha$

1.4 Überlappungsintegrale

1. Überlappungsintegrale zw. versch. Tableaus sind orthogonal
2. Überlappungsintegrale $= 0$ zwischen den versch. Kets eines Tableaus (da M_S und damit die Anzahl der Spins ja verschieden, kann nie gleiche Folge vorkommen)
3. Überlappungsintegrale zw. versch. Tableaus eines Diagramms ($=$ Form des Tableaus) können 0 oder $1/2$ sein: 0 wenn M_S versch., sonst $1/2$

			[4]					[3 1]									$[2^2]$	
			$\begin{smallmatrix}1&2&3&4\end{smallmatrix}$					$\begin{smallmatrix}1&2&3\\4\end{smallmatrix}$			$\begin{smallmatrix}1&2&4\\3\end{smallmatrix}$			$\begin{smallmatrix}1&3&4\\2\end{smallmatrix}$			$\begin{smallmatrix}1&2\\3&4\end{smallmatrix}$	$\begin{smallmatrix}1&3\\2&4\end{smallmatrix}$
			$\|2\,2\rangle$	$\|2\,1\rangle$	$\|2\,0\rangle$	$\|2\,-1\rangle$	$\|2\,-2\rangle$	$\|1\,1\rangle$	$\|1\,0\rangle$	$\|1\,-1\rangle$	$\|1\,1\rangle$	$\|1\,0\rangle$	$\|1\,-1\rangle$	$\|1\,1\rangle$	$\|1\,0\rangle$	$\|1\,-1\rangle$	$\|0\,0\rangle$	$\|0\,0\rangle$
[4]	$\begin{smallmatrix}1&2&3&4\end{smallmatrix}$	$\|2\,2\rangle$	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
		$\|2\,1\rangle$	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
		$\|2\,0\rangle$	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
		$\|2\,-1\rangle$	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
		$\|2\,-2\rangle$	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
[3 1]	$\begin{smallmatrix}1&2&3\\4\end{smallmatrix}$	$\|1\,1\rangle$	0	0	0	0	0	1	0	0	1/2	0	0	1/2	0	0	0	0
		$\|1\,0\rangle$	0	0	0	0	0	0	1	0	0	1/2	0	0	1/2	0	0	0
		$\|1\,-1\rangle$	0	0	0	0	0	0	0	1	0	0	1/2	0	0	1/2	0	0
	$\begin{smallmatrix}1&2&4\\3\end{smallmatrix}$	$\|1\,1\rangle$	0	0	0	0	0	1/2	0	0	1	0	0	1/2	0	0	0	0
		$\|1\,0\rangle$	0	0	0	0	0	0	1/2	0	0	1	0	0	1/2	0	0	0
		$\|1\,-1\rangle$	0	0	0	0	0	0	0	1/2	0	0	1	0	0	1/2	0	0
	$\begin{smallmatrix}1&3&4\\2\end{smallmatrix}$	$\|1\,1\rangle$	0	0	0	0	0	1/2	0	0	1/2	0	0	1	0	0	0	0
		$\|1\,0\rangle$	0	0	0	0	0	0	1/2	0	0	1/2	0	0	1	0	0	0
		$\|1\,-1\rangle$	0	0	0	0	0	0	0	1/2	0	0	1/2	0	0	1	0	0
$[2^2]$	$\begin{smallmatrix}1&2\\3&4\end{smallmatrix}$	$\|0\,0\rangle$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1/2
	$\begin{smallmatrix}1&3\\2&4\end{smallmatrix}$	$\|0\,0\rangle$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1/2	1

2 Raumfunktionen

2.1 Quantenzahlen und Abkürzung als Ket

4 Elektronen, von denen jeweils 2 im e_{1g} und im e_{2g} Orbital sind:

$$l_1 = 1, \quad l_2 = -1, \quad l_3 = 2, \quad l_4 = -2$$

D.h. $L = 0, 2, 4$ und

- $M_L = \{\}$ für $L = 0$
- $M_L = \{-2, -1, 0, 1, 2\}$ für $L = 2$
- $M_L = \{-4, -3, -2, -1, 0, 1, 2, 3, 4\}$ für $L = 4$

d.h. mögliche Fälle für $|L\ M_L\rangle$ lauten:

- $|0\ 0\rangle$
- $|2 \quad 2\rangle$, $|2 \quad 1\rangle$, $|2 \quad 0\rangle$, $|2 \quad -1\rangle$, $|2 \quad -2\rangle$
- $|4 \quad 4\rangle$, $|4 \quad 3\rangle$, $|4 \quad 2\rangle$, $|4 \quad 1\rangle$, $|4 \quad 0\rangle$, $|4 \quad -1\rangle$, $|4 \quad -2\rangle$, $|4 \quad -3\rangle$, $|4 \quad -4\rangle$

adjungierte Young-Tableaus zu denen der Spinfunktionen:

$[1^4]$	$[13]$	$[2^2]$
$\begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array}$	$\begin{array}{cc} 1 & 2 \\ 3 & \\ 4 & \end{array} \quad \begin{array}{cc} 1 & 3 \\ 2 & \\ 4 & \end{array} \quad \begin{array}{cc} 1 & 4 \\ 2 & \\ 3 & \end{array}$	$\begin{array}{cc} 1 & 2 \\ 3 & 4 \end{array} \quad \begin{array}{cc} 1 & 3 \\ 2 & 4 \end{array}$
$\|4 \quad 4\rangle$ $\|4 \quad 3\rangle$ $\|4 \quad 2\rangle$ $\|4 \quad 1\rangle$ $\|4 \quad 0\rangle$ $\|4 \quad -1\rangle$ $\|4 \quad -2\rangle$ $\|4 \quad -3\rangle$ $\|4 \quad -4\rangle$	$\|2 \quad 2\rangle$ $\|2 \quad 1\rangle$ $\|2 \quad 0\rangle$ $\|2 \quad -1\rangle$ $\|2 \quad -2\rangle$	$\|0 \quad 0\rangle$

2.2 Funktionen

2.2.1 1. Antisymmetrisieren, 2. Symmetrisieren

- $[1^4]$
  - $\begin{array}{|c|}\hline 1\\ \hline 2\\ \hline 3\\ \hline 4\\ \hline \end{array}$:
    * $+1234-1243-1324+1342+1423-1432$
      $-2134+2143+2314-2341-2413+2431$
      $+3124-3142-3214+3241+3412-3421$
      $-4123+4132+4213-4231-4312+4321$
      $= \begin{vmatrix} 1 & 1 & 1 & 1\\ 2 & 2 & 2 & 2\\ 3 & 3 & 3 & 3\\ 4 & 4 & 4 & 4 \end{vmatrix}$
    * Integrale:
      $+D + 1/6 \cdot (cd|dc) + 1/6 \cdot (bc|cb) - 1/6 \cdot (bd|db) - 1/6 \cdot (ab|ba) - 1/6 \cdot (ac|ca) - 1/6 \cdot (ad|da)$

- $[21^2]$
  - $\begin{array}{|c|c|}\hline 1 & 4\\ \hline 2 \\ \cline{1-1} 3 \\ \cline{1-1} \end{array}$
    * $\hat{S}\,(123+312+231-213-132-321)\,4$
      $= 1234 + 4231 + 3124 + 3421 + 2314 + 2341$
      $-2134 - 2431 - 1324 - 4321 - 3214 - 3241$
      $= \left|123\right|4$
      bzw. $abcd + dbca + bcad + dcab + cabd + dabc$
      $-bacd - dacb - acbd - dcba - cbad - dbac = \left|abc\right| d$
    * Integrale mit Vorfaktoren $\frac{1}{\sqrt{12}}$ werden zu:
      $+D + \frac{1}{3} \cdot (ad|da) - 1 \cdot (ab|ba) - 1 \cdot (bc|cb) - 1 \cdot (ac|ca) + \frac{1}{3} \cdot (bd|db) + \frac{1}{3} \cdot (cd|dc)$
  - $\begin{array}{|c|c|}\hline 1 & 3\\ \hline 2 \\ \cline{1-1} 4 \\ \cline{1-1} \end{array}$
    * $\hat{S}\,(124+412+241-214-142-421)\,3$
      $= 1234 + 3214 + 4132 + 4312 + 2431 + 2413$
      $-2134 - 2314 - 1432 - 3412 - 4231 - 4213$
      bzw. $abcd + cbad + bdca + cdba + dacb + cadb$
      $-bacd - cabd - adcb - cdab - dbca - cbda$
    * Integrale mit Vorfaktoren $\frac{1}{\sqrt{12}}$ werden zu:
      $+D + \frac{1}{3} \cdot (ac|ca) - 1 \cdot (ab|ba) - 1 \cdot (bd|db) - 1 \cdot (ad|da) + \frac{1}{3} \cdot (bc|cb) + \frac{1}{3} \cdot (cd|dc)$

- $\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1} 4 \\ \cline{1-1}\end{array}$

  * $\hat{S}\,(134+413+341-143-431-314)\,2$
    $= 1234 + 2134 + 4213 + 4123 + 3241 + 3142$
    $-1243 - 2143 - 4231 - 4132 - 3214 - 3124$
    bzw. $abcd + bacd + cbda + bcda + dbac + bdac$
    $-abdc - badc - dbca - bdca - cbad - bcad$
  * Integrale: $+D + \frac{1}{3}\cdot(ab|ba) - 1\cdot(cd|dc) - 1\cdot(ad|da) - 1\cdot(ac|ca) + \frac{1}{3}\cdot(bc|cb) + \frac{1}{3}\cdot(bd|db)$

- $[2^2]$

  - $\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 & 4 \\ \hline\end{array}$

    * $\hat{S}(12-21)(34-43) = \left[\hat{S}(12-21)34\right] - \left[\hat{S}(12-21)43\right]$
      $= 1234 + 3214 + 1432 + 3412 - 2134 - 2314 - 4132 - 4312$
      $-1243 - 3241 - 1423 - 3421 + 2143 + 2341 + 4123 + 4321$
      bzw. $abcd + cbad + adcb + cdab - bacd - cabd - bdca - cdba$
      $-abdc - dbac - acdb - dcab + badc + dabc + bcda + dcba$
    * Integrale
      $+D + \frac{1}{2}\cdot(ac|ca) + \frac{1}{2}\cdot(bd|db) - 1\cdot(ab|ba) - 1\cdot(cd|dc) + \frac{1}{2}\cdot(bc|cb) + \frac{1}{2}\cdot(ad|da)$

  - $\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array}$

    * $\hat{S}(13-31)(24-42) = \left[\hat{S}(13-31)24\right] - \left[\hat{S}(13-31)42\right]$
      $= 1234 + 2134 + 1243 + 2143 - 3214 - 3124 - 4213 - 4123$
      $-1432 - 2431 - 1342 - 2341 + 3412 + 3421 + 4312 + 4321$
      bzw. $abcd + bacd + adcb + dbca + dacb + bdca$
      $-cbad - bcad - cdab - dbac - bdac - dcab$
    * Integrale
      $+D + \frac{1}{2}\cdot(ab|ba) + 1\cdot(bd|db) + \frac{1}{2}\cdot(ad|da) - 1\cdot(ac|ca) + \frac{1}{2}\cdot(bc|cb) + \frac{1}{2}\cdot(cd|dc)$

- $[3\quad 1]$:

  - $\begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline 4 \\ \cline{1-1}\end{array}$:

    * $\hat{S}\,(14-41)\,23$
      $= 1234 + 2134 + 1324 + 3214 + 2314 + 3124$
      $-4231 - 4132 - 4321 - 4213 - 4123 - 4312$

  - $\begin{array}{|c|c|c|}\hline 1 & 3 & 4 \\ \hline 2 \\ \cline{1-1}\end{array}$:

    * $\hat{S}\,(12-21)\,34$
      $= 1234 + 3214 + 1243 + 4231 + 3241 + 4213$
      $-2134 - 2314 - 2143 - 2431 - 2341 - 2413$

  - $\begin{array}{|c|c|c|}\hline 1 & 2 & 4 \\ \hline 3 \\ \cline{1-1}\end{array}$:

    * $\hat{S}\,(13 - 31)\,24$
      $= 1234 + 2134 + 1432 + 4231 + 2431 + 4132$
      $-3214 - 3124 - 3412 - 3241 - 3142 - 3421$

- $[4]$:

  - $\begin{array}{|c|c|c|c|}\hline 1 & 2 & 3 & 4 \\ \hline\end{array}$:

    * $1234 + 1243 + 1324 + 1342 + 1423 + 1432$
      $+2134 + 2143 + 2314 + 2341 + 2413 + 2431$
      $+3124 + 3142 + 3214 + 3241 + 3412 + 3421$
      $+4123 + 4132 + 4213 + 4231 + 4312 + 4321$

2.2.2 1. Symmetrisieren, 2. Antisymmetrisieren

- $[1^4]$
  - $\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline 4\\\hline\end{array}$:
    * $+1234 - 1243 - 1324 + 1342 + 1423 + 1432$
      $-2134 - 2143 - 2314 - 2341 - 2413 + 2431$
      $+3124 - 3142 + 3214 + 3241 - 3412 - 3421$
      $-4123 + 4132 - 4213 - 4231 - 4312 - 4321$
      $= \begin{vmatrix} 1 & 1 & 1 & 1\\ 2 & 2 & 2 & 2\\ 3 & 3 & 3 & 3\\ 4 & 4 & 4 & 4\end{vmatrix}$
      bzw. $\begin{vmatrix} a & b & c & d\\ a & b & c & d\\ a & b & c & d\\ a & b & c & d\end{vmatrix} =$
      $+abcd - abdc - acbd + adbc + acdb + adcb$
      $-bacd - badc - cabd - dabc - cadb + dacb$
      $+bcad - bdac + cbad + dbac - cdab - dcab$
      $-bcda + bdca - cbda - dbca - cdba - dcba$
    * Integrale:
      $+D + 1/6 \cdot (cd|dc) + 1/6 \cdot (bc|cb) - 1/6 \cdot (bd|db) - 1/6 \cdot (ab|ba) - 1/6 \cdot (ac|ca) - 1/6 \cdot (ad|da)$

- $[21^2]$
  - $\begin{array}{|c|c|}\hline 1 & 4\\\hline 2 & \multicolumn{1}{c}{}\\\cline{1-1} 3 & \multicolumn{1}{c}{}\\\cline{1-1}\end{array}$
    * $\hat{A}\,(14 + 41)\,23$
      $= 1234 - 2134 - 1324 - 3214 + 2314 + 3124$
      $+4231 - 4132 - 4321 - 4213 + 4123 + 4312$
      bzw. $abcd - bacd - acbd - cbad + cabd + bcad$
      $+dbca - bdca - dcba - cbda + bcda + cdba$
    * Integrale
      $+D - \frac{1}{2} \cdot (ab|ba) - 1 \cdot (bc|cb) - \frac{1}{2} \cdot (ac|ca) + 1 \cdot (ad|da) - \frac{1}{2} \cdot (bd|db) - \frac{1}{2} \cdot (cd|dc)$
  - $\begin{array}{|c|c|}\hline 1 & 3\\\hline 2 & \multicolumn{1}{c}{}\\\cline{1-1} 4 & \multicolumn{1}{c}{}\\\cline{1-1}\end{array}$
    * $\hat{A}\,(13 + 31)\,24$
      $= 1234 - 2134 - 1432 - 4231 + 2431 + 4132$
      $+3214 - 3124 - 3412 - 3241 + 3142 + 3421$
      bzw. $abcd - bacd - adcb - dbca + dacb + bdca$
      $+cbad - bcad - cdab - dbac + bdac + dcab$

    * Integrale
      $+D - 1/2 \cdot (ab|ba) - 1 \cdot (bd|db) - \frac{1}{2} \cdot (ad|da) + 1 \cdot (ac|ca) - \frac{1}{2} \cdot (bc|cb) - \frac{1}{2} \cdot (cd|dc)$

  - $\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & \\ \cline{1-1} 4 & \\ \cline{1-1}\end{array}$
    * $\hat{A}\,(12 + 21)\,34$
      $= 1234 - 3214 - 1243 - 4231 + 3241 + 4213$
      $+2134 - 2314 - 2143 - 2431 + 2341 + 2413$
      bzw. $abcd - cbad - abdc - dbca + dbac + cbda$
      $+bacd - cabd - badc - dacb + dabc + cadb$
    * Integrale
      $+D - \frac{1}{2} \cdot (ac|ca) - 1 \cdot (cd|dc) - \frac{1}{2} \cdot (ad|da) + 1 \cdot (ab|ba) - \frac{1}{2} \cdot (bc|cb) - \frac{1}{2} \cdot (bd|db)$

- $[2^2]$
  - $\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 & 4 \\ \hline\end{array}$
    * $\hat{A}(13 + 31)(24 + 42) = \left[\hat{A}(13 + 31)24\right] - \left[\hat{A}(13 + 31)42\right]$
      $= 1234 - 2134 - 1243 + 2143 + 3214 - 3124 - 4213 + 4123$
      $+1432 - 2431 - 1342 + 2341 + 3412 - 3421 - 4312 + 4321$
      bzw. $abcd - bacd - abdc + badc + cbad - bcad - cbda + bcda$
      $+adcb - dacb - adbc + dabc + cdab - dcab - cdba + dcba$
    * Integrale
      $+D - \frac{1}{2} \cdot (ab|ba) - \frac{1}{2} \cdot (cd|dc) + 1 \cdot (ac|ca) + 1 \cdot (bd|db) - \frac{1}{2} \cdot (bc|cb) - \frac{1}{2} \cdot (ad|da)$
  - $\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array}$
    * $\hat{A}(12 + 21)(34 + 43) = \left[\hat{A}(12 + 21)34\right] - \left[\hat{A}(12 + 21)43\right]$
      $= 1234 - 3214 - 1432 + 3412 + 2134 - 2314 - 4132 + 4312$
      $+1243 - 3241 - 1423 + 3421 + 2143 - 2341 - 4123 + 4321$
      bzw. $abcd - cbad - adcb + cdab + bacd - cabd - bdca + cdba$
      $+abdc - dbac - acdb + dcab + badc - dabc - bcda + dcba$
    * Integrale
      $+D - \frac{1}{2} \cdot (ac|ca) - \frac{1}{2} \cdot (bd|db) + 1 \cdot (ab|ba) + 1 \cdot (cd|dc) - \frac{1}{2} \cdot (bc|cb) - \frac{1}{2} \cdot (ad|da)$

- $[3 \quad 1]$:
  - $\begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline 4 & & \\ \cline{1-1}\end{array}$:
    * $\hat{A}\,(123 + 312 + 231 + 213 + 132 + 321)\,4$
      $= 1234 - 4231 + 3124 - 3421 + 2314 - 2341$
      $+2134 - 2431 + 1324 - 4321 + 3214 - 3241$
  - $\begin{array}{|c|c|c|}\hline 1 & 3 & 4 \\ \hline 2 & & \\ \cline{1-1}\end{array}$:

    * $\hat{A}\,(134 + 413 + 341 + 314 + 143 + 431)\,2$
      $= 1234 - 2134 + 4213 - 4123 + 3241 - 3142$
      $+3214 - 3124 + 1243 - 2143 + 4231 - 4132$

  - $\begin{array}{|c|c|c|}\hline 1 & 2 & 4 \\ \hline 3 \\ \cline{1-1} \end{array}$:

    * $\hat{A}\,(124 + 412 + 241 + 214 + 142 + 421)\,3$
      $= 1234 - 3214 + 4132 - 4312 + 2431 - 2413$
      $+2134 - 2314 + 1432 - 3412 + 4231 - 4213$

- $[4]$:

  - $\begin{array}{|c|c|c|c|}\hline 1 & 2 & 3 & 4 \\ \hline \end{array}$:

    * $1234 + 1243 + 1324 + 1342 + 1423 + 1432$
      $+2134 + 2143 + 2314 + 2341 + 2413 + 2431$
      $+3124 + 3142 + 3214 + 3241 + 3412 + 3421$
      $+4123 + 4132 + 4213 + 4231 + 4312 + 4321$

3 Integrale

3.1 Überlappungsmatrixelemente

3.1.1 1. Antisymmetrisieren, 2. Symmetrisieren

3.1.1.1 Spin

Überlappung gl. Tableaus $\rightarrow 1$

$\sigma_{12} = \sigma_{21} = \left\langle \left| \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 & 4 \\ \hline \end{array} \right|_{\sigma} \middle| \left| \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} \right|_{\sigma} \right\rangle$
$= \frac{1}{\sqrt{4}} \cdot \frac{1}{\sqrt{4}} \cdot \langle 4\alpha\alpha\beta\beta - 4\beta\alpha\alpha\beta - 4\alpha\beta\beta\alpha - 4\beta\beta\alpha\alpha | \beta\alpha\alpha\beta + \alpha\beta\beta\alpha - \alpha\beta\alpha\beta - \beta\alpha\beta\alpha \rangle$
$= \frac{1}{4} \cdot (-4 \langle \beta\alpha\alpha\beta | \beta\alpha\alpha\beta \rangle - 4 \langle \alpha\beta\beta\alpha | \alpha\beta\beta\alpha \rangle) = -2$

3.1.1.2 Ortsanteile

3.1.2 1. Symmetrisieren, 2. Antisymmetrisieren

3.1.2.1 Spin

Überlappung gl. Tableaus $\rightarrow 1$

(Err: 0-Wert bei Spinfunktionen)

3.1.2.2 Ortsanteile

3.2 Hamiltonmatrixelemente

3.2.1 1. Antisymmetrisieren, 2. Symmetrisieren

3.2.1.1 Spin

s. Überlappung

3.2.1.2 Ortsanteile

3.2.2 1. Symmetrisieren, 2. Antisymmetrisieren

3.2.2.1 Spin

s. Überlappung

3.2.2.2 Ortsanteile

$$\Phi_{11} = \left\langle \left| \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} \right|_{\Phi} \middle| \hat{H} \middle| \left| \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} \right|_{\Phi} \right\rangle \tag{1}$$

$$= +D - \frac{1}{2} \cdot (ac|ca) - \frac{1}{2} \cdot (bd|db) + 1 \cdot (ab|ba) + 1 \cdot (cd|dc) - \frac{1}{2} \cdot (bc|cb) - \frac{1}{2} \cdot (ad|da) \tag{2}$$

$$\Phi_{12} = \left\langle \left| \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} \right|_{\Phi} \hat{H} \left| \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & 4 \\ \hline \end{array} \right|_{\Phi} \right\rangle \tag{3}$$

$$= -\frac{1}{4} \cdot D - \frac{1}{4} \cdot (ab|ba) - \frac{1}{4} \cdot (cd|dc) - \frac{1}{4} \cdot (ac|ca) - \frac{1}{4} \cdot (bd|db) + \frac{1}{2} \cdot (bc|cb) + \frac{1}{2} \cdot (ad|da) \tag{4}$$

$$\Phi_{22} = \left\langle \left| \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & 4 \\ \hline \end{array} \right|_{\Phi} \hat{H} \left| \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & 4 \\ \hline \end{array} \right|_{\Phi} \right\rangle \tag{5}$$

$$= +D - \frac{1}{2} \cdot (ab|ba) - \frac{1}{2} \cdot (cd|dc) + 1 \cdot (ac|ca) + 1 \cdot (bd|db) - \frac{1}{2} \cdot (bc|cb) - \frac{1}{2} \cdot (ad|da) \tag{6}$$