# SKLAPLJANJE VRTILNIH KOLIČIN

## (GRADNJA LASTNIH STANJ IN SKLOPLJENIH OPERATORJEV)

Pri večini realnih sistemov je treba upoštevati več vrtilnih količin: Vsak $e^-$ ima tirno in spinsko vrtilno količino, ki sta sklopljeni preko interakcije spin-tir in v večelektronskih sistemih se vrtilne količine sklapljajo na različne načine, odvisno od situacije, ki jo opisujemo.

- SKLOPITEV DVEH VRTILNIH KOLIČIN

2 neodvisna dela

1 2

$k = 1,2$

$$\hat{j}^2(k)\,|j_k m_k\rangle = j_k(j_k+1)\,|j_k m_k\rangle$$

$$\hat{j}_z(k)\,|j_k m_k\rangle = m_k\,|j_k m_k\rangle$$

$$\hat{\vec{J}} = \hat{\vec{j}}(1) + \hat{\vec{j}}(2)$$

Komponente vrtilnih količin neodvisnih podsistemov med seboj komutirajo

$$[\hat{j}_x(1), \hat{j}_y(2)] = 0 \longrightarrow [\hat{J}_x, \hat{J}_y] = i\hat{J}_z$$

$\hat{\vec{J}}$ ima enake lastnosti kot $\hat{\vec{j}}(1)$ in $\hat{\vec{j}}(2)$: je vrtilna količina

$$\hat{J}^2\,|(j_1 j_2)JM\rangle = J(J+1)\,|(j_1 j_2)JM\rangle$$

$$\hat{J}_z\,|(j_1 j_2)JM\rangle = M\,|(j_1 j_2)JM\rangle$$

← lastna funkcija $\hat{J}^2$ in $\hat{J}_z$

$-J \leq M \leq J$

Produkt enodelčnih valovnih funkcij $|j_1 m_1, j_2 m_2\rangle = |j_1 m_1\rangle |j_2 m_2\rangle$ je lastna funkcija $\hat{J}_z$:

$$\hat{J}_z\,|j_1 m_1, j_2 m_2\rangle = (\hat{j}_z(1) + \hat{j}_z(2))\,|j_1 m_1, j_2 m_2\rangle$$

$$= (m_1 + m_2)\,|j_1 m_1, j_2 m_2\rangle$$

ne pa $\hat{J}^2$.

To konstruiramo z linearno kombinacijo produktnih funkcij, tako da je ves čas $M = m_1 + m_2$.

$$|(j_1 j_2)JM\rangle = \sum_{m_1,m_2} |j_1 m_1, j_2 m_2\rangle \langle j_1 m_1, j_2 m_2 | JM\rangle \leftarrow \text{uteži}$$

$\langle j_1 m_1\, j_2 m_2 | JM\rangle \equiv \langle j_1 m_1, j_2 m_2 | (j_1 j_2) JM\rangle$ Clebsh-Gordanov koeficient je $\neq 0$, ko je $m_1 + m_2 = M$

ker tvorijo produktne funkcije $|j_1 m_1\rangle |j_2 m_2\rangle$ ortonormalni set

Absolutna faza koeficientov CG je določena z dogovorom: pri danih $j_1, j_2$ in $J$ ter maksimalni vrednosti $m_1$ in $M$ (se pravi $m_1 = j_1$, $M = J$) je koeficient realen in nenegativen.

$\rightarrow$ vsi CG so REALNI.

– INVERZNA TRANSFORMACIJA:

$$|j_1 m_1, j_2 m_2\rangle = \sum_{J,M} |(j_1 j_2) JM\rangle \langle JM | j_1 m_1, j_2 m_2\rangle$$

$$\langle JM | j_1 m_1 j_2 m_2\rangle = \langle (j_1 j_2) JM | j_1 m_1, j_2 m_2\rangle = \langle j_1 m_1\, j_2 m_2 | JM\rangle^*$$

$$\rightarrow \quad \langle j_1 m_1\, j_2 m_2 | JM\rangle = \langle JM | j_1 m_1 j_2 m_2\rangle$$

PRIMER: KAKŠNA SO LASTNA STANJA SKUPNE VRTILNE KOLIČINE ZA 2 ELEKTRONA S TIRNO VRTILNO KOLIČINO 1?

$l_1 = 1$, $l_2 = 1$ $\quad |1 m_1\, 1 m_2\rangle \quad m_1, m_2 = -1, 0, 1$

$|11,11\rangle \to M_L = m_1 + m_2 = 2$ edino stanje $J=2$

$|(11)22\rangle = |11,11\rangle$ ostala stanja z $J=2$ dobimo z operatorjem $\hat{L}_- = \hat{\ell}_-(1) + \hat{\ell}_-(2)$

$$|(11)21\rangle = \frac{1}{\sqrt{2}}\left(|11,10\rangle + |10,11\rangle\right)$$

$$|(11)20\rangle = \frac{1}{\sqrt{6}}\left(|11,1{-1}\rangle + 2|10,10\rangle + |1{-1},11\rangle\right)$$

$$|(11),2{-1}\rangle = \frac{1}{\sqrt{2}}\left(|10,1{-1}\rangle + |1{-1},10\rangle\right)$$

$$|(11)2{-2}\rangle = |1{-1},1{-1}\rangle$$

Obstaja še ena linearna kombinacija $a|11,10\rangle + b|10,11\rangle$, ki ima $M_L = 1$, ta ustreza $J=1$. Ortogonalnost $|(11)21\rangle$ in $|(11)11\rangle$ privede do $a+b=0$. Normalizirano stanje $|(11)11\rangle = \frac{1}{\sqrt{2}}\left(|11,10\rangle - |10,11\rangle\right)$. Ostala $J=1$ stanja z aplikacijo $\hat{L}_-$. Podobno dobimo še stanje z $J=0$: $|(11)00\rangle$. ~~za~~ katero zahtevamo, da je ortogonalno na $|(11)20\rangle$ in $|(11)10\rangle$.

Očitno lahko konstrukcijski pristop posplošimo.

Wigner 1931: $\hat{J}_+ |(j_1 j_2)JJ\rangle = \hat{J}_+ \sum_{m_1 m_2} |j_1 m_1, j_2 m_2\rangle\langle j_1 m_1 j_2 m_2 | JJ\rangle = 0$

privede do rekurzijskih relacij med CG ....

in izraza za CG koeficient:

(4) $$\langle j_1 m_1 j_2 m_2 | J M\rangle = \delta(m_1+m_2, M)\sqrt{\frac{(2J+1)(j_1+j_2-J)!(j_1-m_1)!(j_2-m_2)!(J+M)!(J-M)!}{(j_1+j_2+J+1)!(J+j_1-j_2)!(J+j_2-j_1)!(j_1+m_1)!(j_2+m_2)!}}$$

$$\times \sum_r (-1)^{j_1-m_1+r}\frac{(j_1+m_1+r)!(j_2+J-m_1-r)!}{r!(J-M-r)!(j_1-m_1-r)!(j_2-J+m_1+r)!}$$

– ŠE EN PRIMER: VRTILNA KOLIČINA ELEKTRONA, SESTAVLJENA IZ TIRNE IN SPINSKE.

$\vec{j} = \vec{l} + \vec{s}$ $\qquad s = \frac{1}{2}$

| $J \backslash m_s$ | $\frac{1}{2}$ | $-\frac{1}{2}$ |
|---|---|---|
| $l+\frac{1}{2}$ | $\sqrt{\frac{l+m_j+1/2}{2l+1}}$ | $\sqrt{\frac{l-m_j+1/2}{2l+1}}$ |
| $l-\frac{1}{2}$ | $\sqrt{\frac{l-m_j+1/2}{2l+1}}$ | $-\sqrt{\frac{l+m_j+1/2}{2l+1}}$ |

$$|(l\tfrac{1}{2})\, l+\tfrac{1}{2}\; m_j\rangle = \sqrt{\frac{l+m_j+1/2}{2l+1}}\,|l\, m_j-\tfrac{1}{2}, \tfrac{1}{2}\,\tfrac{1}{2}\rangle + \sqrt{\frac{l-m_j+1/2}{2l+1}}\,|l\, m_j+\tfrac{1}{2}, \tfrac{1}{2}\,-\tfrac{1}{2}\rangle$$

$$|(l\tfrac{1}{2})\, l-\tfrac{1}{2}\; m_j\rangle = \sqrt{\frac{l-m_j+1/2}{2l+1}}\,|l\, m_j-\tfrac{1}{2}, \tfrac{1}{2}\,\tfrac{1}{2}\rangle - \sqrt{\frac{l+m_j+1/2}{2l+1}}\,|l\, m_j+\tfrac{1}{2}, \tfrac{1}{2}\,-\tfrac{1}{2}\rangle$$

ŠE NEKAJ LASTNOSTI CG:

$$\langle j_2 m_2\, j_1 m_1 | JM\rangle = (-1)^{j_1+j_2-J}\langle j_1 m_1\, j_2 m_2 | JM\rangle$$

$$\langle J\, -M\, j_2 m_2 | j_1 m_1\rangle = (-1)^{j_2+m_2}\sqrt{\frac{2j_1+1}{2J+1}}\,\langle j_1 m_1\, j_2 m_2 | JM\rangle$$

$$\langle j_1\, -m_1\, j_2\, -m_2 | J\, M\rangle = (-1)^{j_1+j_2-J}\langle j_1 m_1\, j_2 m_2 | JM\rangle$$

NI SIMETRIJE MED CG ZA MENJAVO VRSTNEGA REDA TREH VRTILNIH KOLIČIN.
ZATO OBIČAJNO RAJE UPORABLJAMO <u>WIGNERJEV 3-j SIMBOL</u>:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \equiv \frac{(-1)^{j_1-j_2-m_3}}{\sqrt{2j_3+1}}\langle j_1 m_1\, j_2 m_2 | j_3\, -m_3\rangle \qquad \neq 0 \quad \begin{matrix} m_1+m_2+m_3=0 \\ |j_1-j_2|\le j_3\le j_1+j_2 \end{matrix}$$

LASTNOSTI 3-j SIMBOLOV:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix}$$

SODA PERMUTACIJA NE SPREMENI VREDNOSTI,

$$\begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

LIHA PA UVEDE FAZNI FAKTOR

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

KER LASTNA STANJA TVORIJO ORTONORMALNI SET: (6)

$$\langle j_1 m_1, j_2 m_2 | j_1 m_1', j_2 m_2' \rangle = \delta(m_1, m_1')\delta(m_2, m_2')$$

$$\langle (j_1 j_2) j_3 m_3 | (j_1 j_2) j_3' m_3' \rangle = \delta(j_3, j_3')\delta(m_3, m_3')$$

VELJAJO ŠE ZVEZE MED CG OZIROMA 3-j SIMBOLI:

① $$\sum_{j_3 m_3} \langle j_1 m_1 j_2 m_2 | j_3 m_3 \rangle \langle j_3 m_3 | j_1 m_1' j_2 m_2' \rangle = \delta(m_1, m_1')\delta(m_2, m_2')$$

OZ. $$\sum_{j_3 m_3} (2j_3+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3 \end{pmatrix} = \delta(m_1, m_1')\delta(m_2, m_2')$$

② $$\sum_{m_1 m_2} \langle j_3' m_3' | j_1 m_1 j_2 m_2 \rangle \langle j_1 m_1 j_2 m_2 | j_3 m_3 \rangle = \delta(j_3, j_3')\delta(m_3, m_3')$$

OZ. $$\sum_{m_1, m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{\delta(j_3, j_3')\delta(m_3, m_3')}{\sqrt{2j_3+1}}$$

SKLOPITEV SFERNIH TENZORSKIH OPERATORJEV (STO): TENZORSKI PRODUKT STO $\hat{X}^K$ S KOMPONENTAMI $\hat{X}^K_Q$

$$\hat{X}^K_Q = \{\hat{t}^{k_1}(1)\, \cancel{\hat{u}}^{k_2}(2)\}^K_Q = \sum_{q_1, q_2} \hat{t}^{k_1}_{q_1}(1)\, \hat{u}^{k_2}_{q_2}(2) \langle k_1 q_1 k_2 q_2 | KQ \rangle$$

$\hat{t}^{k_1}$ in $\hat{u}^{k_2}$ delujeta na različne prostostni stopnji sistema, recimo (1) na spinski del, (2) na tirni del elektrona, ali v dvoelektronskem sistemu $\hat{t}^{k_1}(1)$ deluje na koordinato prvega, $\hat{u}^{k_2}(2)$ pa drugega elektrona.

(7) Operator $\hat{X}^K_Q$ se pri rotacijah transformira kot stanje vrtilne količine $|(k_1 k_2)KQ\rangle$ in je torej STO reda K. $\hat{X}^K_Q$ je <u>tenzorski produkt</u> operatorjev $\hat{t}^{k_1}$ in $\hat{u}^{k_2}$, ki sta tenzorska operatorja reda $k_1$ in $k_2$ in se transformirata kot stanja vrtilne količine $|k_1 q_1\rangle$ in $|k_2 q_2\rangle$.

Dva tenzorska operatorja istega reda lahko sestavimo v tenzorski produkt reda 0 (skalarni operator).

$$\hat{X}^0_0 = \{\hat{t}^k_{(1)}\hat{u}^k(2)\}^0_0 = \sum_q t^k_q(1)\, u^k_{-q}(2) \langle k q\, k\, {-q} | 00\rangle$$

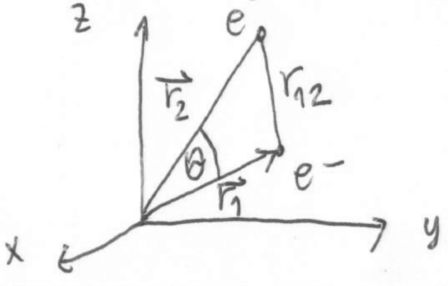
$$= \sum_q \begin{pmatrix} k & k & 0 \\ q & -q & 0 \end{pmatrix} \hat{t}^k_q(1)\,\hat{u}^k_{-q}(2) = \frac{(-1)^k}{\sqrt{2k+1}} \sum_q (-1)^q \hat{t}^k_q(1)\,\hat{u}^k_{-q}(2)$$

$$\equiv \frac{(-1)^k}{\sqrt{2k+1}} \hat{\vec{t}}^k \cdot \hat{\vec{u}}^k$$

$\Leftarrow$ tradicionalna definicija SKALARNEGA PRODUKTA 2 TENZORJEV: $\hat{\vec{t}}^k(1)\cdot\hat{\vec{u}}^k(2) \equiv \sum_q (-1)^q \hat{t}^k_q(1)\,\hat{u}^k_{-q}(2)$

PRIMER!!

COULOMBSKA INTERAKCIJA MED 2 ELEKTRONOMA:




$$\frac{1}{r_{12}} = \sum_k \frac{r_<^k}{r_>^{k+1}} P_k(\cos\theta)$$

$$r_< = \begin{cases} r_1, & r_1 \le r_2 \\ r_2, & \text{sicer} \end{cases}$$

$$r_> = \begin{cases} r_2, & r_1 \le r_2 \\ r_1, & \text{sicer} \end{cases}$$

ADICIJSKI IZREK ZA SFERNE HARMONIKE:

$$P_k(\cos\theta) = \frac{4\pi}{2k+1}\sum_q Y_q^k(\theta_1,\varphi_1)\,Y_q^{k*}(\theta_2,\varphi_2)$$

DEFINIRAJMO C-tenzor $\hat{C}^k$ S KOMPONENTAMI $\hat{C}_q^k = \sqrt{\frac{4\pi}{2k+1}}\,Y_q^k(\theta,\varphi)$:

$$P_k(\cos\theta) = \hat{C}^k(1)\cdot\hat{C}^k(2) \longrightarrow \frac{1}{r_{12}} = \sum_k \frac{r_<^k}{r_>^{k+1}}\,\hat{C}^k(1)\cdot\hat{C}^k(2)$$

COULOMBSKA INTERAKCIJA JE INVARIANTNA NA VRTENJE OBEH $e^-$ HKRATI. ZATO MORATA BITI $\hat{C}^k(1)$ IN $\hat{C}^k(2)$ SKLOPLJENA TAKO, DA FORMIRATA TENZORSKI PRODUKT REDA 0 $\longrightarrow$ SKALARNI OPERATOR

## WIGNER-ECKARTOV TEOREM

OBRAVNAVALI SMO ŽE TRANSFORMACIJSKE LASTNOSTI (SKLOPLJENIH) LASTNIH STANJ VRTILNE KOLIČINE IN STO: OBE SKUPINI SE TRANSFORMIRATA NA ENAK NAČIN, PAČ TAKO KOT VELEVAJO IREDUCIBILNE REPREZENTACIJE ROTACIJSKIH GRUP.

ZDAJ NAS ZANIMA UČINEK SIMULTANEGA VRTENJA TENZORSKIH OPERATORJEV IN LASTNIH STANJ V MATRIČNIH ELEMENTIH. IZKAŽE SE, DA JE MOGOČE MATRIČNE ELEMENTE STO FAKTORIZIRATI NA PRODUKT DVEH DELOV, OD KATERIH JE SAMO EN DEL (TRIVIALNO) ODVISEN OD MAGNETNIH KVANTNIH ŠTEVIL!

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$$P(\omega)\hat{t}^{k}_{q}|\gamma jm\rangle = P(\omega)\hat{t}^{k}_{q}P^{-1}(\omega)P(\omega)|\gamma jm\rangle$$
$$= \sum_{q'm'} \hat{t}^{k}_{q'} \underbrace{D^{k}_{q'q}(\omega)\,|\gamma jm'\rangle\, D^{j}_{m'm}(\omega)}_{\text{transformacija kot } \vec{D}^{k} \otimes \vec{D}^{j} \text{ direktni produkt}}$$

Funkcija $\hat{t}^{k}_{q}|\gamma jm\rangle$ se torej transformira kot produktna funkcija $|\gamma_1 kq\rangle|\gamma_2 jm\rangle$.

$$\phi(\beta JM) = \sum_{q,m} t^{k}_{q}|\gamma jm\rangle\langle kq\, jm|JM\rangle = \sum_{\gamma''} c(\gamma'', J)\,|\gamma'' JM\rangle$$

INVERZNA TRANSFORMACIJA

$$\hat{t}^{k}_{q}|\gamma jm\rangle = \sum_{JM}\phi(\beta JM)\langle JM|kq\, jm\rangle = \sum_{\gamma'' JM} c(\gamma'', J)\,|\gamma'' JM\rangle\langle JM|kq\, jm\rangle \quad \Big\{ \cdot \langle \gamma' j' m'|$$

$$\langle \gamma' j' m'|\hat{t}^{k}_{q}|\gamma jm\rangle = c(\gamma' j')\langle j' m'|kq\, jm\rangle = c(\gamma', j')\begin{pmatrix} j' & k & j \\ -m' & q & m \end{pmatrix}\sqrt{2j'+1}\,(-1)^{-k+j'-m'}$$

$j \leftrightarrow j'$

$$\boxed{\langle \gamma j m|\hat{t}^{k}_{q}|\gamma' j' m'\rangle = (-1)^{j-m}\begin{pmatrix} j & k & j' \\ -m & q & m' \end{pmatrix}\left[(-1)^{-k+j'-j}\sqrt{2j+1}\; c(\gamma, j)\right]}$$

$$\boxed{\equiv (-1)^{j-m}\begin{pmatrix} j & k & j' \\ -m & q & m' \end{pmatrix}\langle \gamma j\|\hat{t}^{k}\|\gamma' j'\rangle}$$

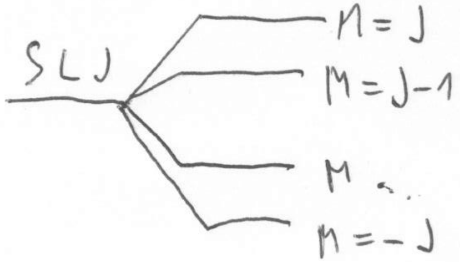
REDUCIRANI MATRIČNI ELEMENT

PRIMER: ZEEMANOV EFEKT, INTERAKCIJA MAGNETNEGA MOMENTA ATOMA S ŠIBKIM ZUNANJIM MAGNETNIM POLJEM. z-OS VZDOLŽ SMERI $\vec{B}$.

$$\hat{H}_m = -\hat{\vec{\mu}}\cdot\vec{B} = \mu_B B\,(\hat{L}_z + g_s \hat{S}_z)$$

orbitalni del — giromagnetno razmerje — spinski del

MAGNETNI MOMENT JE POSLEDICA VRTILNE KOLIČINE ELEKTRONA




$$\Delta E_M = \langle (LS)JM|\hat{H}_m|(LS)JM\rangle$$

$$\hat{H}_m = \mu_B B g_J \hat{J}_z$$

↑ Landé-jev g faktor

W-E:

$$\frac{\langle (LS)JM|\hat{J}_q|(LS)JM'\rangle}{\langle (LS)J\|\hat{\vec{J}}\|(LS)J\rangle} = \frac{\langle (LS)JM|\hat{L}_q|(LS)JM'\rangle}{\langle (LS)J\|\hat{\vec{L}}\|(LS)J\rangle}$$

ZA POLJUBNO KOMPONENTO $q$

$$\rightarrow \langle (LS)JM|\hat{L}_q|(LS)JM'\rangle = \underbrace{\frac{\langle (LS)J\|\hat{\vec{L}}\|(LS)J\rangle}{\langle (LS)J\|\hat{\vec{J}}\|(LS)J\rangle}}_{\equiv \alpha_L}\langle (LS)JM|\hat{J}_q|(LS)JM'\rangle$$

PODOBNO ZA SPIN

$$\langle (LS)JM|\hat{S}_q|(LS)JM'\rangle = \underbrace{\frac{\langle (LS)J\|\hat{\vec{S}}\|(LS)J\rangle}{\langle (LS)J\|\hat{\vec{J}}\|(LS)J\rangle}}_{\equiv \alpha_S}\langle (LS)JM|\hat{J}_q|(LS)JM'\rangle$$

$$\left.\right\}\quad \vec{L} = \alpha_L \cdot \vec{J},\qquad \vec{S} = \alpha_S \cdot \vec{J}$$

$g_J = \alpha_L + g_s \alpha_S$ (neodvisen od M), $\hat{J}_q = \hat{S}_q + \hat{L}_q \rightarrow \alpha_S + \alpha_L = 1$

MAGNETNA INTERAKCIJA RAZCEPI NIVO SLJ NA PODNIVOJE, KI SO ENAKOMERNO RAZMAKNJENI. NJIMOV RAZMIK NARAŠČA SORAZMERNO Z VELIKOSTJO $\vec{B}$ IN JE ODVISEN OD SLJ PREKO LANDÉ-JEVEGA $g$ FAKTORJA



IZRAČUNAJMO $g_J$:

$$\hat{L}^2 = (\hat{\vec{J}} - \hat{\vec{S}})^2 = \hat{J}^2 + \hat{S}^2 - 2\hat{\vec{J}}\cdot\hat{\vec{S}} = \hat{J}^2 + \hat{S}^2 - 2\alpha_S \hat{J}^2$$

$$\langle (LS)JM | \hat{L}^2 | (LS)JM \rangle = L(L+1) = J(J+1) + S(S+1) - 2\alpha_S J(J+1)$$

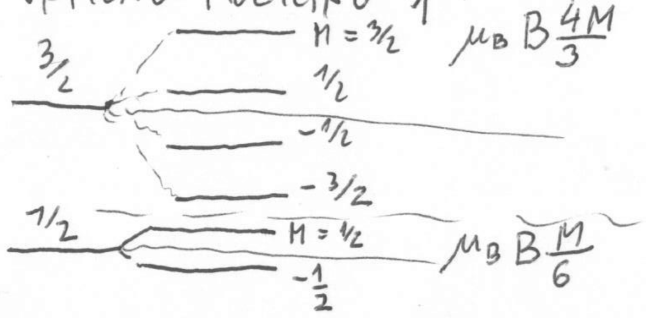
$$\rightarrow \quad \alpha_S = \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

$$\alpha_L = 1 - \alpha_S = \frac{J(J+1) - S(S+1) + L(L+1)}{2J(J+1)}$$

$$g_J(g_S = 2) = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

PRIMER: ELEKTRON V STANJU Z ORBITALNO VRTILNO KOLIČINO 1:
(S SPINOM 1/2)

$$g_{1/2} = \frac{1}{6}, \quad g_{3/2} = \frac{4}{3} \quad \rightarrow$$



IZRAZIMO MATRIČNI ELEMENT COULOMBSKE INTERAKCIJE MED DVEMA ELEKTRONOMA.
POKAZALI SMO ŽE: 12

$$\frac{1}{r_{12}} = \sum_k \frac{r_<^k}{r_>^{k+1}} \hat{C}^k(1)\cdot\hat{C}^k(2) = \sum_k \frac{(-1)^k}{\sqrt{2k+1}} \frac{r_<^k}{r_>^{k+1}} \left\{\hat{C}^k(1)\hat{C}^k(2)\right\}_0^0$$

SPADA V MNOŽICO OPERATORJEV OBLIKE

$$g_{12} = \gamma(r_1,r_2)\left\{\hat{t}^{k_1}(1)\,\hat{u}^{k_2}(2)\right\}_Q^K \quad , \hat{t}^{k_1} \text{ in } \hat{u}^{k_2}$$

neodvisna od spina

IZRAZIMO MATRIČNI ELEMENT

$$\langle ab|\gamma(r_1,r_2)\left\{\hat{t}^{k_1}(1)\,\hat{u}^{k}(2)\right\}_Q^K|cd\rangle$$

MED NESKLOPLJENIMI ENOELEKTRONSKIMI STANJI (ORBITALAMI) $|a\rangle = |n_a l_a m_s^a m_l^a\rangle$

$$|n l m_s m_l\rangle = \frac{1}{r} P_{nl}(r)\, Y_{m_l}^{l}(\theta,\varphi)\, \chi_{m_s}$$

← SPINSKA FUNKCIJA S PROJEKCIJO $m_s$

radialna funkcija

SF. HARMONIK

$$\langle ab|\gamma(r_1,r_2)\left\{\hat{t}^{k_1}(1)\,\hat{u}^{k_2}(2)\right\}_Q^K|cd\rangle = \iint P_a(r_1)P_b(r_2)\gamma(r_1,r_2)P_c(r_1)P_d(r_2)\,dr_1\,dr_2$$

$$\cdot\sum_{q_1 q_2} \langle a|\hat{t}_{q_1}^{k_1}|c\rangle\langle b|\hat{u}_{q_2}^{k_2}|d\rangle\langle k_1 q_1 k_2 q_2|KQ\rangle \times \delta(m_s^a, m_s^c)\,\delta(m_s^b, m_s^d)$$

INTEGRAL ČEZ KOTNE KOORDINATE 1

INTEGRAL ČEZ KOTNE KOORD. 2

$$(-1)^{k_1-k_2+Q}\begin{pmatrix} k_1 & k_2 & K \\ q_1 & q_2 & -Q \end{pmatrix}\sqrt{2K+1}$$

W.E.: $\langle a | \hat{t}^{k_1}_{q_1} | c \rangle = (-1)^{l_a - m_l^a} \begin{pmatrix} l_a & k_1 & l_c \\ -m_l^a & q_1 & m_l^c \end{pmatrix} \langle a \| \hat{t}^{k_1} \| c \rangle$

$$\langle b | \hat{u}^{k_2}_{q_2} | d \rangle = (-1)^{l_b - m_l^b} \begin{pmatrix} l_b & k_2 & l_d \\ -m_l^b & q_2 & m_l^d \end{pmatrix} \langle b \| \hat{u}^{k_2} \| d \rangle$$

$$\rightarrow \langle ab | \gamma(r_1,r_2) \{ \hat{t}^{k_1}_{(1)}, \hat{u}^{k_2}_{(2)} \}^K_Q | cd \rangle = \iint P_a(r_1) P_b(r_2) \gamma(r_1,r_2) P_c(r_1) P_d(r_2) dr_1 dr_2$$

$$\times (-1)^{l_a + l_b + k_1 - k_2 + Q - m_l^a - m_l^b} \sqrt{2K+1} \langle a \| \hat{t}^{k_1} \| c \rangle \langle b \| \hat{u}^{k_2} \| d \rangle \delta(m_s^a, m_s^c) \delta(m_s^b, m_s^d)$$

$$\sum_{q_1 q_2} \begin{pmatrix} l_a & k_1 & l_c \\ -m_l^a & q_1 & m_l^c \end{pmatrix} \begin{pmatrix} l_b & k_2 & l_d \\ -m_l^b & q_2 & m_l^d \end{pmatrix} \begin{pmatrix} k_1 & k_2 & K \\ q_1 & q_2 & -Q \end{pmatrix}$$

COULOMBSKI PRIMER: $K = 0 = Q \quad k_1 = k_2 = k \quad + \sum \text{po } k$

$$\langle ab | \frac{1}{r_{12}} | cd \rangle = \sum_{k=0} \iint P_a(r_1) P_b(r_2) \frac{r_<^k}{r_>^{k+1}} P_c(r_1) P_d(r_2) dr_1 dr_2 \, (-1)^{l_a + l_b - m_l^a - m_l^b}$$

$$\langle a \| C^k \| c \rangle \langle b \| C^k \| d \rangle \delta(m_s^a, m_s^c) \delta(m_s^b, m_s^d)$$

$$\sum_q \begin{pmatrix} l_a & k & l_c \\ -m_l^a & q & m_l^c \end{pmatrix} \begin{pmatrix} l_b & k & l_d \\ -m_l^b & -q & m_l^d \end{pmatrix} \begin{pmatrix} k & k & 0 \\ q & -q & 0 \end{pmatrix} \leftarrow \frac{(-1)^{k-q}}{\sqrt{2k+1}}$$

Slaterjev integral $R^k(ab,cd)$

REDUCIRANI MATRIČNI ELEMENT TENZORJA "C": 14

$$\langle lm | C^k_q | l'm' \rangle = \sqrt{\frac{4\pi}{2k+1}} \int Y^{l*}_m(\Omega) Y^k_q(\Omega) Y^{l'}_{m'}(\Omega)\, d\Omega \overset{W.E.}{=} (-1)^{l-m} \begin{pmatrix} l & k & l' \\ -m & q & m' \end{pmatrix} \underbrace{\langle l \| \hat{C}^k \| l' \rangle}_{?}$$

$$Y^k_q(\Omega) Y^{l'}_{m'}(\Omega) = \sum_{lm} a_{lm} Y^l_m(\Omega), \quad a_{lm} = \int Y^{l*}_m(\Omega) Y^k_q(\Omega) Y^{l'}_{m'}(\Omega)\, d\Omega$$

$$Y^k_q(\Omega) Y^{l'}_{m'}(\Omega) = \sqrt{\frac{2k+1}{4\pi}} \sum_{lm} (-1)^{l-m} \begin{pmatrix} l & k & l' \\ -m & q & m' \end{pmatrix} \langle l \| \hat{C}^k \| l' \rangle Y^l_m(\Omega)$$

$$\sum_{qm'} \begin{pmatrix} l'' & k & l' \\ -m'' & q & m' \end{pmatrix} Y^k_q(\Omega) Y^{l'}_{m'}(\Omega) = \sqrt{\frac{2k+1}{4\pi}} \sum_{lm} (-1)^{l-m} \langle l \| \hat{C}^k \| l' \rangle Y^l_m(\Omega) \sum_{qm'} \begin{pmatrix} l'' & k & l' \\ -m'' & q & m' \end{pmatrix} \begin{pmatrix} l & k & l' \\ -m & q & m' \end{pmatrix}$$

UPORABIM

$$\sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{1}{(2j_3+1)} \delta(j_3, j_3') \delta(m_3, m_3')$$

$$= \sqrt{\frac{2k+1}{4\pi}} (-1)^{l''-m''} \langle l'' \| \hat{C}^k \| l' \rangle \frac{1}{2l''+1} Y^{l''}_{m''}(\Omega)$$

Enačba velja za vse kote, torej tudi za $\theta = 0$: $Y^l_m(\theta,\varphi) \to \sqrt{\frac{2l+1}{4\pi}} P^m_l(1)\, e^{im\varphi} = \sqrt{\frac{2l+1}{4\pi}} \delta(m,0)$

$$\begin{pmatrix} l'' & k & l \\ 0 & 0 & 0 \end{pmatrix} \frac{\sqrt{(2k+1)(2l+1)}}{4\pi} = (-1)^{l''} \frac{1}{4\pi} \sqrt{\frac{2k+1}{2l''+1}} \langle l'' \| \hat{C}^k \| l' \rangle$$

$$\Rightarrow \boxed{\langle l \| \hat{C}^k \| l' \rangle = (-1)^l \sqrt{(2l+1)(2l'+1)} \begin{pmatrix} l & k & l' \\ 0 & 0 & 0 \end{pmatrix}}$$

NADALJUJEM Z MATRIČNIM ELEMENTOM:

$$\langle ab | \frac{1}{r_{12}} | cd \rangle = \sum_k \Big[ R^k(ab, cd) \sqrt{\frac{(2l_a+1)(2l_b+1)(2l_c+1)(2l_d+1)}{2k+1}} (-1)^k \begin{pmatrix} l_a & k & l_c \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_b & k & l_d \\ 0 & 0 & 0 \end{pmatrix}$$

$$(-1)^{m_l^a + m_l^b} \delta(m_s^a, m_s^c) \delta(m_s^b, m_s^d) \sum_{q=-k}^{k} (-1)^q \begin{pmatrix} l_a & k & l_c \\ -m_l^a & q & m_l^c \end{pmatrix} \begin{pmatrix} l_b & k & l_d \\ -m_l^b & -q & m_l^d \end{pmatrix} \Big]$$

SKLAPLJANJE 3 VRTILNIH KOLIČIN