

# Barimpuls moment koppling

- Givet 2 elektroner med spinn  $S_1$  och  $S_2$  kan vi skapa fyra olika totala spinnfunktioner:

$$\sigma_{-(1,2)} = \frac{1}{\sqrt{2}} (\alpha\beta - \beta\alpha) \quad S=0 \quad \text{anti-sym}$$

$$\sigma_{+(1,2)} = \frac{1}{\sqrt{2}} (\alpha\beta + \beta\alpha), \quad \alpha\alpha, \beta\beta \quad S=1 \quad \text{symmett}$$

- ~~Den~~  $S=0$  har bara en komponent och kallas för en singlett funktion

- Medan  $S=1$  har 3 komponenter och kallas för en triplet.

- Gemensamt kallas dessa tillstånd för multiplicitet, pga. antalet linjer de kan ge upphov i ett spektrum

- Med 2 oparade elektroner ligger tripletten oftast lägst i energi (Hund) pga. exchange bidraget.

- Men, medan barimpulsmomentet hos elektronen förändras i en transition ( $S=1$  hos  $S=0$  eller tvärtom), är det inget som pareras spinnnet! Singlet-triplet trans. sker ej (normalt) jfr. ortho-pura Helium.

Alins  
beräkningsfysik

3101  
3102

- Spin och banimpuls moment är i princip två oberoende storheter:

Men: spinnet ~~är~~ ger upphov till ett inneboende magnetiskt moment hos elektronen, medan elektronens banimpuls moment kan tolkas som en ström (laddning i rörelse) vilket inducerar ett annat magnetiskt moment. Spin och banimpuls-moment kan således koppla till varandra:  
Spin - bankoppling

- Spin-bankoppling kallas ofta för en relativistisk effekt, men detta stämmer inte. S.E. saknar spin och därmed också SO-koppling. Dirac ekvationen tar hen med naturligt!

- SO-kopplingen är starkast i närheten av kärnan där elektroner rör sig fortast! Störst effekt på p-elektroner i tunga element! Core-valens polarisering påverkar alla orbitaler!

3

- Vi kan koppla spinnet och banimpulsmomentet hos en elektron till ett nytt totalt impulsmomentkvanttal

$$j = l + s = |l \pm \frac{1}{2}|$$

för en p-elektron  $j = \left\{ \frac{1}{2}, \frac{3}{2} \right\}$

- I fall spinn-bankopplingen är noll har det ingen betydelse om en elektron har  $\alpha$ - eller  $\beta$ -spinn.

- I fall vi har spinn-bankoppling har olika  $j$ -nivåer olika energi:

$$E_{l, s, j} = \frac{1}{2} hc A [j(j+1) - l(l+1) - s(s+1)]$$

växelvärdet Energiu mellan ett magnetiskt moment och ett externt fält är  $E = -\mu \cdot B$

I fall vi betraktar magnetfältet från endera momentet som "externt" får vi

$$E \propto s \cdot l \quad (\text{vid } \sigma\text{-SO-koppling } s \perp l)$$

S · l :

$$\begin{aligned} \mathbf{j} &= \mathbf{l} + \mathbf{s} & \mathbf{j} \cdot \mathbf{j} &= (\mathbf{l} + \mathbf{s}) \cdot (\mathbf{l} + \mathbf{s}) \\ & & &= \mathbf{l} \cdot \mathbf{l} + \mathbf{s} \cdot \mathbf{s} + 2 \mathbf{s} \cdot \mathbf{l} \end{aligned}$$

$$\Rightarrow \mathbf{s} \cdot \mathbf{l} = \frac{1}{2} (\mathbf{j} \cdot \mathbf{j} - \mathbf{l} \cdot \mathbf{l} - \mathbf{s} \cdot \mathbf{s}) = \frac{1}{2} (j^2 - l^2 - s^2)$$

i operatorform:

$$\hat{\mathbf{s}} \cdot \hat{\mathbf{l}} = \frac{1}{2} (\hat{\mathbf{j}}^2 - \hat{\mathbf{l}}^2 - \hat{\mathbf{s}}^2)$$

$$\langle \psi_{l,s,j} | \hat{\mathbf{s}} \cdot \hat{\mathbf{l}} | \psi_{l,s,j} \rangle = \frac{1}{2} \langle \psi_{l,s,j} | \hat{\mathbf{j}}^2 - \hat{\mathbf{l}}^2 - \hat{\mathbf{s}}^2 | \psi_{l,s,j} \rangle$$

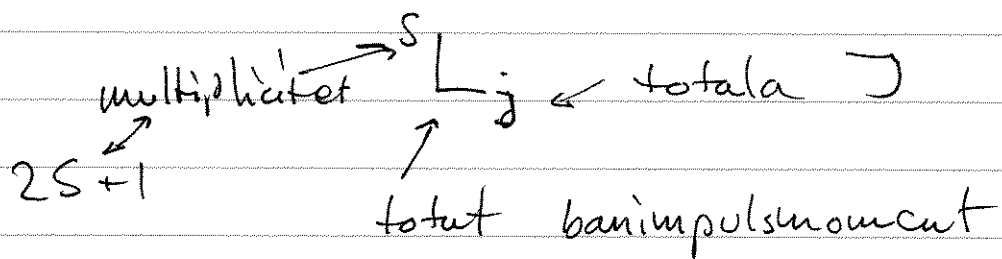
$$= \frac{1}{2} [j(j+1) - l(l+1) - s(s+1)] \quad \square$$

dvs det totala momentet minus  
 spinnet och banimpuls momentet!  
 → styrkan på kopplingen.

- Spin-ban kopplingen kan ses tydligt t.ex. i emissions-spektrat till Na (gula gatulampor, nm).

- Na har en oparad 2s - elektron som kan vara  $\alpha$  eller  $\beta$ : vid excitation får vi  $l=1 \rightarrow j = \frac{1}{2}$  eller  $j = \frac{3}{2}$ .  
I Na är denna splitning ca.  $17 \text{ cm}^{-1}$ !  
(0.12 nm)

- Elektroniska tillstånd i atomer kan klassificeras precist med sk-termsymboler:



t.ex. Na  $^2S_{1/2}$ , exiterat  $^2P_{3/2} / ^2P_{1/2}$

5

- I fall vi har fler än en oparad elektron kan vi konstruera totala impulsmoment:  $L, S, J$  med komponenterna  $M_L, M_S$  och  $M_J$ , samt längdena  $\{J(J+1)\}^{1/2} \hbar \dots$

- Två impulsmoment kopplas genom Clebsch-Gordan serien:

$$L = l_1 + l_2, l_1 + l_2 - 1 \dots |l_1 - l_2|$$

-  $L$ : 0      1      2      3      4      5      ...  
      S      P      D      F      G      H      ...

ex. 2 d-elektroner  $l_1 = 2, l_2 = 2$

$$\rightarrow L = 4, 3, 2, 1, 0$$

- Fler än 2 impulsmoment kopplas genom att först koppla 2, och sedan koppla det 3:je till alla existerande termer. Dessa blir väldigt många väldigt fort!

ex.  $p^3: p^2 = L = 2, 1, 0$

$L=2 + p^1 \rightarrow L=3, 2, 1$

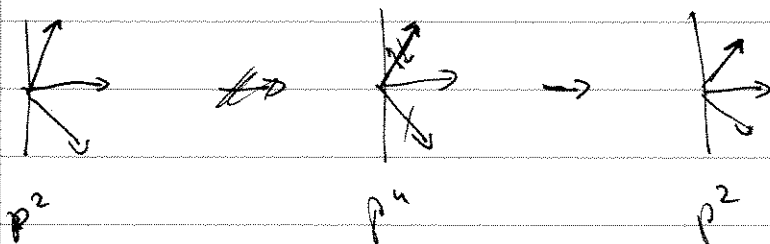
$L=1 + p^1 \rightarrow L=2, 1, 0$

$L=0 + p^1 \rightarrow L=1, 0$

$\Rightarrow L = 3, 2, 2, 1, 1, 1, 0$

notera att samma tillstånd kan nås på flera olika sätt! Detta har stor betydelse för ensambler av impulsmomentsystem.

- notera att max komplikation fås för ide. ekvivalenta elektroner, och för halvfulla skal av ekvivalenta elektroner



- vi kan alltså räkna "hål" istället!

$d^9$  är m.a.o. inget problem :)

- Det totala spinnet kopplas precis på samma vis!

$$S = s_1 + s_2, s_1 + s_2 - 1, \dots, |s_1 - s_2|$$

- Multipliciteten (antalet spinntermer)  
 $2s + 1$

dvs:  $s = 0$  ~~1~~ ~~2~~ ~~3~~ ~~4~~ ~~5~~ ~~6~~ ~~7~~ ~~8~~ ~~9~~ ~~10~~ ~~11~~ ~~12~~ ~~13~~ ~~14~~ ~~15~~ ~~16~~ ~~17~~ ~~18~~ ~~19~~ ~~20~~ ~~21~~ ~~22~~ ~~23~~ ~~24~~ ~~25~~ ~~26~~ ~~27~~ ~~28~~ ~~29~~ ~~30~~ ~~31~~ ~~32~~ ~~33~~ ~~34~~ ~~35~~ ~~36~~ ~~37~~ ~~38~~ ~~39~~ ~~40~~ ~~41~~ ~~42~~ ~~43~~ ~~44~~ ~~45~~ ~~46~~ ~~47~~ ~~48~~ ~~49~~ ~~50~~ ~~51~~ ~~52~~ ~~53~~ ~~54~~ ~~55~~ ~~56~~ ~~57~~ ~~58~~ ~~59~~ ~~60~~ ~~61~~ ~~62~~ ~~63~~ ~~64~~ ~~65~~ ~~66~~ ~~67~~ ~~68~~ ~~69~~ ~~70~~ ~~71~~ ~~72~~ ~~73~~ ~~74~~ ~~75~~ ~~76~~ ~~77~~ ~~78~~ ~~79~~ ~~80~~ ~~81~~ ~~82~~ ~~83~~ ~~84~~ ~~85~~ ~~86~~ ~~87~~ ~~88~~ ~~89~~ ~~90~~ ~~91~~ ~~92~~ ~~93~~ ~~94~~ ~~95~~ ~~96~~ ~~97~~ ~~98~~ ~~99~~ ~~100~~ ~~101~~ ~~102~~ ~~103~~ ~~104~~ ~~105~~ ~~106~~ ~~107~~ ~~108~~ ~~109~~ ~~110~~ ~~111~~ ~~112~~ ~~113~~ ~~114~~ ~~115~~ ~~116~~ ~~117~~ ~~118~~ ~~119~~ ~~120~~ ~~121~~ ~~122~~ ~~123~~ ~~124~~ ~~125~~ ~~126~~ ~~127~~ ~~128~~ ~~129~~ ~~130~~ ~~131~~ ~~132~~ ~~133~~ ~~134~~ ~~135~~ ~~136~~ 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- Det totala <sup>ban</sup> impulsmomentet kan skapas på två icke-ekvivalenta sätt!

- I fall man kan anse att spinn-bankopplingen hos en elektron och dess l är liten (lätta element), dvs. l och s var för sig beskriver banimpulsmomenten (goda kvanttal), är det korrekt att använda Russel-Saunders koppling:

$$J = L + S, L + S - 1, \dots |L - S|$$

Dvs, Clebsch-Gordan serien för par av totala L och S

- I tunga element är SO-kopplingen stark och endast j är ett gott kvanttal. I dessa system måste man använda jj-koppling

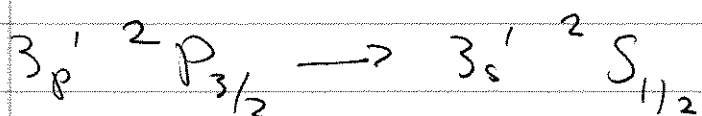
$$J = j_1 + j_2, j_1 + j_2 - 1, \dots |j_1 - j_2|$$

(vi kan tänka på elektroner med lex spin 3/2, 1/2 (p))

$$\begin{aligned} j_1 = 3/2 \quad j_2 = 3/2 &\rightarrow J = 3, 2, 1, 0 \\ j_1 = 3/2 \quad j_2 = 1/2 &\rightarrow J = 2, 1 \end{aligned}$$

## Urvalsregler

- Spektroskopiska transitioner i atomer kan nu precis specificeras med hjälp av termer:



↑  
övre tillstånd

↑  
nedre tillstånd

- För absorption byter vi riktning på pilen inte ordning!

- Urvalsreglerna är:

$$\Delta S = 0 \quad \left[ \begin{array}{l} \Delta L = 0, \pm 1 \\ \Delta l = \pm 1 \end{array} \right. \quad \Delta J = 0, \pm 1$$

$$\neq 0 \leftrightarrow 0$$

- I (nästan av) tunga element är S inte ett gott kvanttal och således är spin-flips (singlet - triplet transitioner) möjliga!

## Clebsch - Gordan koefficienter:

- För en elektron vet vi att kärnimpuls-  
moment funktioner beskrivs av  $Y_{l,m}(\theta, \varphi)$

$$\hat{L}^2 |l, m\rangle = l(l+1) |l, m\rangle$$

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

- Men hur konstruera en kärnimpulsmoment-  
eigenfunktion för två eller fler elektroner  
som är kopplade?

$|L, M\rangle = Y_{l_1, m_1}^{(1)} Y_{l_2, m_2}^{(2)}$  är normalt inte  
en egenfunktion  
till  $\hat{L}^2, \hat{L}_z$ !

$$\langle l_1, m_1; l_2, m_2 | L, M \rangle$$

- Med hjälp av grupp teori kan man härleda  
sh. Clebsch - Gordan koefficienter (3 j -  
symboler / 6-j / 9-j-) som finns tabellerade.

- Vi kan spänna  $\psi_{jm}$  som

$$\psi_{jm} = \sum C(jm; l_1, m_1, l_2, m_2) | Y_{l_1, m_1}^{(1)} Y_{l_2, m_2}^{(2)} \rangle$$

- om det finns många sätt att uppnå en viss  
 $L$ , så är antalet sätt att uppnå ett  
visst  $M_L$  mycket större... :)