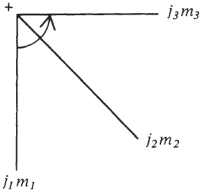
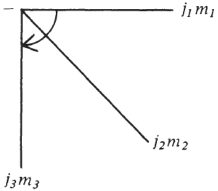
ANGULAR MOMENTUM GRAPHS



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



- change from $+ \to -$ gives a phase $(-1)^{j_1+j_2+j_3}$

$$\underline{jm \qquad\quad j'm'} = \delta(j,j')\,\delta(m,m')$$

$$\xleftarrow{jm \qquad\quad j'm'} = (-1)^{j-m}\,\underline{jm \qquad\quad j' \ -m'} = (-1)^{j-m}\,\delta(j,j')\,\delta(m,-m')$$

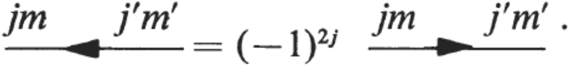
$$\xrightarrow{jm \qquad\quad j'm'} = (-1)^{j'-m'}\,\underline{jm \qquad\quad j' \ -m'} = (-1)^{j+m}\,\delta(j,j')\,\delta(m,-m').$$

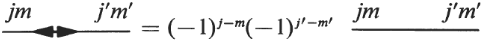
- phases are indicated with arrows (note where it points!)

ANGULAR MOMENTUM GRAPHS

$$(-1)^{j-m}\delta(j,j')\delta(m,-m')$$

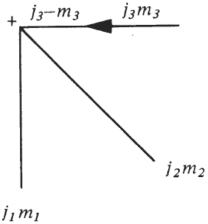
$$(-1)^{j'-m'}\delta(j,j')\delta(m,-m') = (-1)^{j+m}\delta(j,j')\delta(m,-m')$$



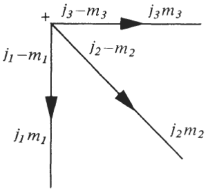


$$= \delta(j,j')\delta(m,m')$$

Angular momentum Graphs



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



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

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

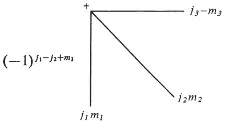
free to add/remove
3 arrows at a vertex
($j_1 + j_2 + j_3 = \text{int}$)

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

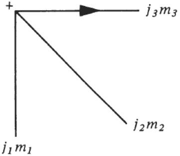
VECTOR COUPLING COEFFICIENTS

CLEBSCH-GORDAN COEFFICIENTS

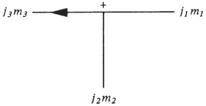
$$\langle j_1 m_1 j_2 m_2 \mid j_3 m_3 \rangle = (-1)^{j_1 - j_2 + m_3} \sqrt{2j_3 + 1} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} \quad (2.81)$$



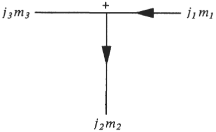
$= (-1)^{j_1 - j_2 + j_3}$



$= (-1)^{2j_2}$

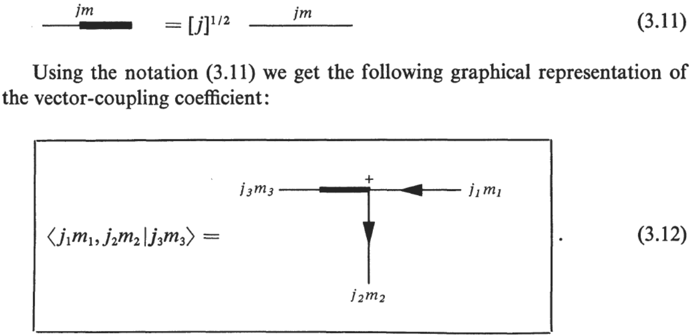


$=$



VECTOR COUPLING COEFFICIENTS

CLEBSCH-GORDAN COEFFICIENTS



$= [j]^{1/2}$ (3.11)

Using the notation (3.11) we get the following graphical representation of the vector-coupling coefficient:

$\langle j_1m_1, j_2m_2 | j_3m_3 \rangle =$. (3.12)

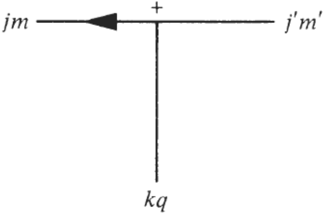
$$[j] = 2j + 1$$

WIGNER-ECKART'S THEOREM

$$\langle \gamma j m \mid t^k_q \mid \gamma' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & k & j' \\ -m & q & m' \end{pmatrix} \langle \gamma j \parallel \mathbf{t}^k \parallel \gamma' j' \rangle$$

- the reduced matrix element independent of all the magnetic quantum numbers

$$\langle \gamma j m | t^k_q | \gamma' j' m' \rangle =$$



$$\langle \gamma j \| t^k \| \gamma' j' \rangle$$

COUPLING OF TWO ELECTRONS

THE STRAIGHT FORWARD WAY

LS - coupling: $\mathbf{L} = \sum_i \ell_i$, $\mathbf{S} = \sum_i s_i$ gives the LS-terms
Example: $2p^2$

$$\mid n\ell m_\ell m_s\rangle = \mid 21 m_\ell m_s\rangle$$

- $2 \cdot 3 = 6$ possible combinations
- two electrons $6 \cdot 5 = 30$ combinations
- The electrons are indistinguishable → 15 combinations
- we are looking for 15 micro states

COUPLING OF TWO ELECTRONS

THE STRAIGHT FORWARD WAY - 15 STATES AS EXPECTED

	$M_S = -1$	$M_S = 0$	$M_S = 1$
$M_L = -2$		$(-1^+ - 1^-)$	
$M_L = -1$	$(0^- - 1^-)$	$(0^+ - 1^-)$ $(-1^+ 0^-)$	$(0^+ - 1^+)$
$M_L = 0$	$(1^- - 1^-)$	$(1^+ - 1^-)$ $(0^+ 0^-)$ $(-1^+ 1^-)$	$(1^+ - 1^+)$
$M_L = +1$	$(0^- 1^-)$	$(0^+ 1^-)$ $(1^+ 0^-)$	$(0^+ 1^+)$
$+M_L = 2$		$(1^+ 1^-)$	

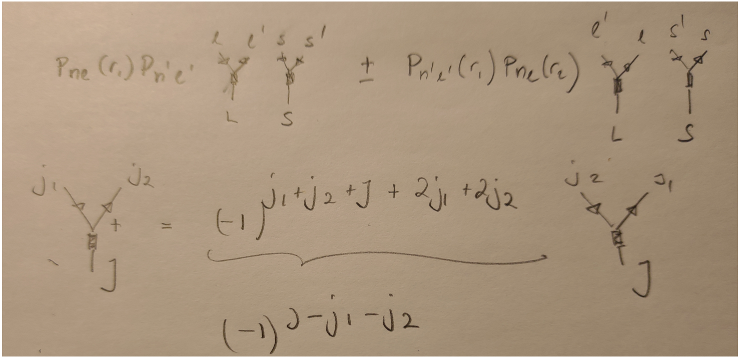
COUPLING OF TWO ELECTRONS

THE STRAIGHT FORWARD WAY

- Maximum $M_L = 2$, only in combination with $M_S = 0 \rightarrow$ there is a ${}^1D$ -term. $M_L = 2, 1, 0, -1, -2 \rightarrow$ five terms.
- Maximum $M_S = 1$, for $M_L \leq 1 \rightarrow$ a ${}^3P$ -term. $3 \cdot 3 = 9$ states belongs to this term.
- $9 + 5 = 14$ states. One is missing?
- Three states with $M_L = 0, M_S = 0$. One belongs to ${}^3P$. One belongs to ${}^1D$. The third is the the single member of a third term $\rightarrow$ must be ${}^1S$.

$2p^2$ can couple to ${}^1S, {}^3P, {}^1D$

COUPLING OF TWO ELECTRONS



- Singlet $(-1)^{0-1/2-1/2}) = -1$
- Triplet $(-1)^{1-1/2-1/2}) = 1$

- $L = 0 \rightarrow (-1)^{0-1-1} = 1$
- $L = 1 \rightarrow (-1)^{1-1-1} = -1$
- $L = 2 \rightarrow (-1)^{2-1-1} = 1$

THE COULOMB INTERACTION

We can expand the Coulomb Interaction using Legendre polynomials (discussed in for example Jackson or Arfken)

$$\frac{1}{r_{12}} = \sum_k \frac{r_<^k}{r_>^{k+1}} P_k(\cos\gamma) = \sum_k \frac{r_<^k}{r_>^{k+1}} \frac{4\pi}{2k+1} \sum_q Y_q^k(\theta,\phi)\, Y_q^{k*}(\theta,\phi)$$

- C-tensors

$$C_q^k = \sqrt{\frac{4\pi}{2k+1}}\, Y_q^k(\theta,\phi)$$

- gives

$$P_k(\cos\gamma) = \mathbf{C}^k(1)\cdot\mathbf{C}^k(2) \rightarrow \frac{1}{r_{12}} = \sum_k \frac{r_<^k}{r_>^{k+1}} \mathbf{C}^k(1)\cdot\mathbf{C}^k(2)$$

- radial part times angular contribution

COUPLING OF TENSOR OPERATORS

$$\mathbf{C}^{k}(1)\cdot\mathbf{C}^{k}(2)$$

- $\mathbf{C}^{k}$ tensor operator of rank k
- two tensor operators of the same rank can couple to rank zero
- above we have a scalar product

The **general form** - as we couple angular momenta:

$$\left\{\mathbf{t}^{k_1}(1)\,\mathbf{u}^{k_2}(2)\right\}^{K}_{Q}=\sum_{q_1,q_2}t^{k_1}_{q_1}u^{k_2}_{q_2}\langle k_1q_1k_2q_2\mid KQ\rangle$$

- i.e. with a Clebsch-Gordan coefficient
- $\mathbf{t}^{k_1}$ and $\mathbf{u}^{k_2}$ work on different parts of the system
- Coulomb interaction - different particles
- Spin-orbit interaction $(\mathbf{l}\cdot\mathbf{s})$ spin part - spatial part
- Breit interaction - all of it.

COUPLING OF TENSOR OPERATORS

Couple to zero rank

$$\left\{\mathbf{t}^{k}(1)\,\mathbf{u}^{k}(2)\right\}_{0}^{0} = \sum_{q} t_{q}^{k}(1)\,u_{-q}^{k}(2)\,\langle kq, k-q \mid 00\rangle =$$

$$\sum_{q} t_{q}^{k}(1)\,u_{-q}^{k}(2) \begin{pmatrix} k & k & 0 \\ q & -q & 0 \end{pmatrix} = \frac{(-1)^{k}}{\sqrt{2k+1}} \sum_{q} (-1)^{q} t_{q}^{k}(1)\,u_{-q}^{k}(2)$$

- compare 2.82 - here the phase $(-1)^{k-k-0} = 1$
- The expression for the 3j-symbol is calculated in Problem 2.14.

Scalar product defined slightly differently

$$\mathbf{t}^{k}(1) \cdot \mathbf{u}^{k}(2) = \sum_{q} (-1)^{q} t_{q}^{k}(1)\,u_{-q}^{k}(2) =$$

$$(-1)^{k}\sqrt{2k+1}\left\{\mathbf{t}^{k}(1)\,\mathbf{u}^{k}(2)\right\}_{0}^{0}$$

THE COULOMB INTERACTION

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

We want to evaluate it between **orbitals**:

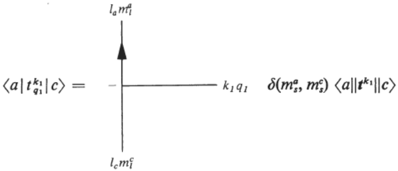
$$\langle ab \mid \frac{1}{r_{12}} \mid cd \rangle, \text{with} \mid a \rangle = \mid n_a \ell_a m_{\ell_a} m_{s_a} \rangle,\ P_{n_a \ell_a}(r)\, Y_{\ell_a, m_a}(\theta, \phi)\, \chi(m_{s_a}) \, \text{etc.}$$

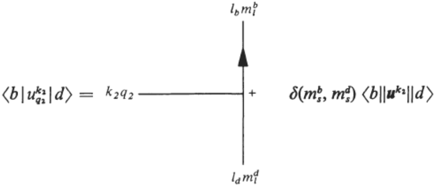
Special case of the general expression:

$$\begin{aligned} \langle ab \mid \gamma(r_1, r_2) \left\{ \mathbf{t}^{k_1}(1)\, \mathbf{u}^{k_2}(2) \right\}_Q^K \mid cd \rangle = \\ \int \int P_a(r_1) P_b(r_2) \gamma(r_1, r_2) P_c(r_1) P_d(r_2) \, dr_1 dr_2 \\ \times \sum_{q_1, q_2} \langle a \mid t_{q_1}^{k_1} \mid c \rangle \langle k_1 q_1 k_2 q_2 \mid KQ \rangle \langle b \mid u_{q_2}^{k_2} \mid d \rangle \end{aligned}$$

USE WIGNER-ECKART

$$\langle a \mid t^{k_1}_{q_1} \mid c \rangle \langle k_1 q_1 k_2 q_2 \mid KQ \rangle \langle b \mid u^{k_2}_{q_2} \mid d \rangle$$

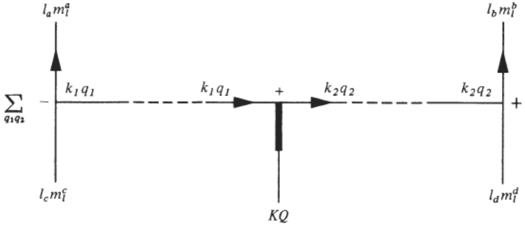




- no spin dependence assumed → $\delta\left(m_{s_a}, m_{s_c}\right), \delta\left(m_{s_b}, m_{s_d}\right)$

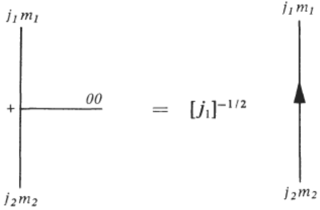
USE WIGNER-ECKART -AND COUPLE THE OPERATORS

$$\langle a \mid t^{k_1}_{q_1} \mid c\rangle\langle k_1 q_1 k_2 q_2 \mid KQ\rangle\langle b \mid u^{k_2}_{q_2} \mid d\rangle$$



- If $K = 0$ (Coulomb case) the zero line can be removed (3.18)

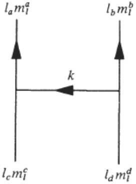
$$\begin{pmatrix} k & k & 0 \\ q & -q & 0 \end{pmatrix} = \frac{(-1)^{k-q}}{\sqrt{2k+1}}$$



THE COULOMB INTERACTION

$$\langle ab \mid \frac{1}{r_{12}} \mid cd \rangle = \sum_k \int \int P_a(r_1) P_b(r_2) \frac{r_<^k}{r_>^{k+1}} P_c(r_1) P_d(r_2) dr_1 dr_2$$
$$\times (-1)^k \langle \ell_a \parallel \mathbf{C}^k \parallel \ell_c \rangle \langle \ell_b \parallel \mathbf{C}^k \parallel \ell_d \rangle$$

times



$$\times \delta(m_{s_a}, m_{s_c}) \delta(m_{s_b}, m_{s_d})$$

- Reduced Matrix Elements: $\ell_a + k + \ell_c = \text{even}$, $\mid \ell_a - \ell_c \mid \leq k \leq \ell_a + \ell_c$ and same for ℓ_b, ℓ_d
- Rule: the internal m/q quantum numbers are summed over.
- Typically the diagrams can -eventually- be evaluated analytically.
- Next time we will couple to total LM and see how all the m :s can easily! be taken care of.