September 25

Lecture #6

Addition of the angular momentum states

Clebsch-Gordon coefficients & 3j symbols

Irreducible tensor operators

Wigner-Eckart theorem

Graphical representation

6j symbols

Chapter 1, pages 11-20, 95-98 of the Lectures on Atomic Physics

Chapter 6, pages 223-228 of QM by Jasprit Singh

Atomic many-body theory, Lindgren & Morrison, pages 29-37,39

Quantum mechanics of the angular momentum: SUMMARY

$$\left[J_i, J_j\right] = i\varepsilon_{ijk} J_k \Rightarrow \begin{array}{l} J^2 |jm\rangle = j(j+1)|jm\rangle \\ J_z |jm\rangle = m|jm\rangle \end{array}$$

$$\lambda = j(j+1)$$

$$m = -j, -j+1, \ldots, j-1, j: \ (2j+1) \textit{ eigenfunctions for each value of } j$$

$$j: 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$$

$$J_+ = J_x + iJ_y$$
$$J_- = J_x - iJ_y$$

$$J_+ |j,m\rangle = \sqrt{j(j+1) - m(m+1)}\,|j,m+1\rangle$$
$$J_- |j,m\rangle = \sqrt{j(j+1) - m(m-1)}\,|j,m-1\rangle$$

Addition of the angular momentum states

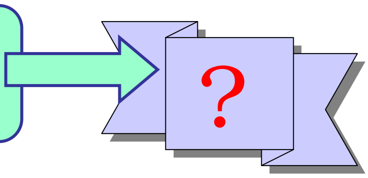
$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$$

$$J_1^2 | j_1 m_1 \rangle = j_1(j_1+1) | j_1 m_1 \rangle \qquad J_2^2 | j_2 m_2 \rangle = j_2(j_2+1) | j_2 m_2 \rangle$$

$$J_{1z} | j_1 m_1 \rangle = m_1 | j_1 m_1 \rangle \qquad J_{2z} | j_2 m_2 \rangle = m_2 | j_2 m_2 \rangle$$

$$J^2 | jm \rangle = j(j+1) | jm \rangle$$

$$J_z | jm \rangle = m | jm \rangle$$



Addition of the angular momentum states

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$$

What do we want to find?

$$J^2 | jm \rangle = j(j+1) | jm \rangle$$

$$J_z | jm \rangle = m | jm \rangle$$

- How many states?
- What are the values of j and m?
- How to build $|jm\rangle$?

$$|(j_1 j_2) JM \rangle = \sum_{m1,m2} | j_1 m_1 j_2 m_2 \rangle \langle j_1 m_1 j_2 m_2 | JM \rangle$$

Clebsch-Gordon coefficients

$$\mathbf{L} = \boldsymbol{l}_1 + \boldsymbol{l}_2$$

Example: two p electrons

Strategy:

$l_1=1 \; |l_1 m_1\rangle$
$l_2=1 \; |l_2 m_2\rangle$

$L = ?$
$M = ?$
$|LM\rangle = ?$

1. Find the state with maximum M_{max}
2. Use lowering operator L_ to find all states with L_{max}, M where $M=L_{max} \ldots -L_{max}$. Note: one can combine M_{max}, L_ and M_{max}, L_+.
3. Find state with $L=L_{max}-1$ and corresponding maximum value of M. Use orthogonality condition or $L_+| L_{max}-1, M_{max}-1\rangle=0$

Rename $L_{max}=L_{max}-1$ and repeat until all of the $(2l_1+1)(2l_2+1)$ functions are obtained

Note: need phase convention

$$L_- |LM\rangle = \sqrt{L(L+1) - M(M-1)}\, |L, M-1\rangle$$

$l_1=1 \; |l_1 m_1\rangle$
$l_2=1 \; |l_2 m_2\rangle$

Example: two p electrons

1. Find the state with maximum M_{max}: $M_{max}=2$

$$|(l_1 l_2)LM\rangle = |l_1 m_1, l_2 m_2\rangle$$
$$|(11)22\rangle = |11,11\rangle$$

2. Use lowering operator L_ to find all states with L_{max}, M where $M=L_{max} \ldots -L_{max}$. Note: one can combine M_{max}, L_ and M_{max}, L_+.

$$L_- = l_-(1) + l_-(2)$$

$$L_- |(11)22\rangle = 2|(11)21\rangle = L_- |11,11\rangle = \sqrt{2}\,|10,11\rangle + \sqrt{2}\,|11,10\rangle$$
$$|(11)21\rangle = \frac{1}{\sqrt{2}}\{|10,11\rangle + |11,10\rangle\}$$

$$L_-|LM\rangle = \sqrt{L(L+1)-M(M-1)}\,|L,M-1\rangle$$
$$L_+|LM\rangle = \sqrt{L(L+1)-M(M+1)}\,|L,M+1\rangle$$

Example: two p electrons

2. Keep use lowering operator L_ to find all states with L_{max}, M

$$L_-|(11)21\rangle = \sqrt{6}|(11)20\rangle = \frac{1}{\sqrt{2}} L_-\{|10,11\rangle + |11,10\rangle\} =$$

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

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

2′. One can keep use lowering operator L_ to find all states with L_{max}=2 or use M_{min} state and L_+.

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

$$L_+|(11)2-2\rangle = 2|(11)2-1\rangle = L_+|1-1,1-1\rangle$$

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

Example: two p electrons
Summary so far: L=2, M=2,1,0,-1,-2

$$|(11)22\rangle = |11,11\rangle$$

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

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

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

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

Example: two p electrons
Next step: L=1, M=1

3. Find state with $L=L_{max}-1$ and corresponding maximum value of M. Use orthogonality condition or $L_+| L_{max}-1,M_{max}-1>=0$

$$|(11)11\rangle = a|11,10\rangle + b|10,11\rangle$$

$$\langle(11)11|(11)21\rangle = 0 \; or \; L_+|(11)11\rangle = 0 \Rightarrow a+b=0$$

Phase convention: positive coefficient for the term with maximum m_1

$$|(11)11\rangle = a|11,10\rangle + b|10,11\rangle$$

Maximum $m_1 \Rightarrow a$ is positive

Example: two p electrons
Next step: L=1, M=1,0,-1

$$|(11)11\rangle = a|11,10\rangle - a|10,11\rangle$$

Use normalization condition to find a

$$\langle(11)11|(11)11\rangle = 1 \rightarrow a = \frac{1}{\sqrt{2}}$$

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

2 (repeat). Use lowering operator L_ to find all states with L_{max}, M

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

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

Example: two p electrons
Next step: L=0, M=0

3(again). Use orthogonality condition to get |(11)00>

$$|(11)00\rangle = a|10,10\rangle + b|1-1,11\rangle + c|11,1-1\rangle$$

$$\langle(11)10|(11)00\rangle = 0 \rightarrow b = c$$

$$\langle(11)20|(11)00\rangle = 0 \rightarrow a = -b$$

Phase convention : c must be positive.

$$|(11)00\rangle = -a|10,10\rangle + a|1-1,11\rangle + a|11,1-1\rangle$$

Use normalization condition to find a $\langle(11)00|(11)00\rangle = 1 \rightarrow a = \frac{1}{\sqrt{3}}$

$$|(11)00\rangle = \frac{1}{\sqrt{3}}\{|1-1,11\rangle - |10,10\rangle + |11,1-1\rangle\}$$

Note: we also calculated all relevant Clebsch-Gordon coefficients

Clebsch-Gordon coefficients

$$|(j_1 j_2)JM\rangle = \sum_{m1,m2} |j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2|JM\rangle$$

$$|(11)22\rangle = |11,11\rangle \quad \rightarrow \quad \langle 11,11|22\rangle = 1$$

$$|(11)21\rangle = \frac{1}{\sqrt{2}}\{|10,11\rangle + |11,10\rangle\} \quad \rightarrow \quad \langle 10,11|21\rangle = \langle 11,10|21\rangle = \frac{1}{\sqrt{2}}$$

$$|(11)20\rangle = \frac{1}{\sqrt{6}}\{|1-1,11\rangle + 2|10,10\rangle + |11,1-1\rangle\} \rightarrow \langle 10,10|20\rangle = \sqrt{\frac{2}{3}}, \ldots$$

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$$

Addition of the angular momentum states

What do we want to find?

$$J^2 | jm \rangle = j(j+1) | jm \rangle$$
$$J_z | jm \rangle = m | jm \rangle$$

- How many states?
- What are the values of j and m?
- How to build $| jm \rangle$?

Clebsch-Gordon coefficients

$$|(j_1 j_2) JM \rangle = \sum_{m1,m2} | j_1 m_1 j_2 m_2 \rangle \langle j_1 m_1 j_2 m_2 | JM \rangle$$

General case

$$|(j_1 j_2) JM \rangle = \sum_{m1,m2} | j_1 m_1 j_2 m_2 \rangle \langle j_1 m_1 j_2 m_2 | JM \rangle$$

$$J_z = J_{1z} + J_{2z} \quad \rightarrow \quad M = m_1 + m_2$$

"Maximally extended" state $| j_1 j_1, j_2 j_2 \rangle$

$$J^2 = J_1^2 + J_2^2 + 2 J_{1z} J_{2z} + J_{1+} J_{2-} + J_{1-} J_{2+}$$
$$J^2 | j_1 j_1, j_2 j_2 \rangle = \left(j_1(j_1+1) + j_2(j_2+1) + 2 j_1 j_2 \right) | j_1 j_1, j_2 j_2 \rangle$$
$$= (j_1 + j_2)(j_1 + j_2 + 1) | j_1 j_1, j_2 j_2 \rangle$$

$$J_{\max} = j_1 + j_2$$

$J_{max}=j_1+j_2$, $J_{min}=?$

$$J_{max} = j_1 + j_2$$

Total number of states: $(2j_1+1)(2j_2+1)$

$$-J \le M \le J$$

$$\sum_{m=1}^{n} m = \frac{1}{2}n(n+1)$$

$$\sum_{j=J_{min}}^{j_1+j_2} (2j+1) = (2j_1+1)(2j_2+1) \leftarrow \sum_{m=J_{min}}^{J_{max}} m = \sum_{m=1}^{J_{max}} m - \sum_{m=1}^{J_{min}-1} m$$

$$\sum_{j=J_{min}}^{J_{max}=j_1+j_2} (2j+1) = J_{max}(J_{max}+1) - J_{min}(J_{min}+1) + J_{max} - J_{min} + 1 =$$

$$= (2j_1+1)(2j_2+1)$$

$$J_{min} = |j_1 - j_2|$$

$$|j_1 - j_2| \le J \le j_1 + j_2$$ ← Triangular condition

Clebsch-Gordon coefficients: general formula

Wigner (1931)
Racah (1942)

$$\langle j_1 m_1 j_2 m_2 | jm \rangle = \delta_{m_1+m_2,m} \sqrt{\frac{(j_1+j_2-j)!(j+j_1-j_2)!(j+j_2-j_1)!(2j+1)}{(j+j_1+j_2+1)!}}$$

$$\times \sum_k \frac{(-1)^k \sqrt{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j+m)!(j-m)!}}{k!(j_1+j_2-j-k)!(j_1-m_1-k)!(j_2+m_2-k)!(j-j_2+m_1+k)!(j-j_1-m_2+k)!}$$

Clebsch-Gordon coefficients: symmetry relations

Neither transparent or convenient!

$$\langle j_1 - m_1 j_2 - m_2 | j - m \rangle = (-1)^{j_1 + j_2 - j} \langle j_1 m_1 j_2 m_2 | jm \rangle$$

$$\langle j_2 m_2 j_1 m_1 | jm \rangle = (-1)^{j_1 + j_2 - j} \langle j_1 m_1 j_2 m_2 | jm \rangle$$

$$\langle j - m j_2 m_2 | j_1 - m_1 \rangle = (-1)^{j_2 + m_2} \sqrt{\frac{2j_1 + 1}{2J + 1}} \langle j_1 m_1 j_2 m_2 | jm \rangle$$

Three-j symbols

3-j symbol

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

$$m_1 + m_2 + m_3 = 0$$

Three-j symbols: symmetry relations

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

312 − 231 − 123 : *no change with even permutations*

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

213-132-321: *phase change with odd permutations*

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

Three-j symbols: orthogonality relations

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

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

Irreducible tensor operators

Irreducible tensor operators: a family of $2k+1$ operators with q=-k,-k+1, …, k satisfying the commutation relations

$$\left[J_z, T_q^k\right] = qT_q^k$$

$$\left[J_\pm, T_q^k\right] = \sqrt{(k \pm q+1)(k \mp q)}\,T_{q\pm 1}^k$$

How to calculate their matrix elements?

Wigner-Eckart theorem

Matrix elements of irreducible tensor operators between angular momentum states are evaluated using **Wigner-Eckart theorem**

$$\left\langle j_1 m_1 \middle| T_q^k \middle| j_2 m_2 \right\rangle = (-1)^{j_1-m_1} \begin{pmatrix} j_1 & k & j_2 \\ -m_1 & q & m_2 \end{pmatrix} \left\langle j_1 \middle\| T^k \middle\| j_2 \right\rangle$$

Reduced matrix elements: no dependence on the magnetic quantum numbers

$$\left\langle j_1 m_1 \middle| T_q^k \middle| j_2 m_2 \right\rangle \neq 0 \text{ if}$$

$$q = m_1 - m_2$$

$$\left|j_1 - j_2\right| \le k \le j_1 + j_2$$

Transition selection rules