Lecture - 12 + 13

Calculation of $\alpha(k,j)$, Lande g-factor

Generalisation to irreducible spherical tensors.

Recall

$$\langle kjm|\vec{V}|k'j'm'\rangle_{kj} = \alpha(k,j)\ \langle kjm|\vec{J}|k'j'm'\rangle_{kj}$$

This implies the following

$$\boxed{\begin{aligned}\langle kjm|\vec{J}\cdot\vec{V}|k'j'm'\rangle_{kj} &= \alpha(k,j)\langle kjm|\vec{J}^2|k'j'm'\rangle_{kj} \\ &= \delta_{kk'}\, j(j+1)\hbar^2\,\alpha(k,j)\,\delta_{jj'}\delta_{mm'}\end{aligned}}$$

$\downarrow$

In fact this statement can be proved by using projection theorem.

$$\therefore \langle kjm|\vec{J}\cdot\vec{V}|kjm\rangle = \langle \vec{J}\cdot\vec{V}\rangle_{kj} = \alpha(k,j)\,j(j+1)\hbar^2$$

$$\Rightarrow \boxed{\alpha(k,j) = \frac{\langle \vec{J}\cdot\vec{V}\rangle_{kj}}{j(j+1)\hbar^2}} \quad — (68)$$

$$\langle \vec{J}\cdot\vec{V}\rangle_{kj} = \langle \psi_{kj}|\vec{J}\cdot\vec{V}|\psi_{kj}\rangle = \alpha(k,j)\,j(j+1)\hbar^2$$

$\downarrow$

as long as $|\psi_{kj}\rangle \in \mathcal{E}_{kj}$ subspace

It is independent of m, depends only on j

$\therefore$ Over the subspace $\mathcal{E}_{kj}$ we will have

$$\boxed{\vec{V} = \frac{\langle \vec{J}\cdot\vec{V}\rangle_{kj}}{j(j+1)\hbar^2}\vec{J}} \quad — (69)$$

~~For another operator~~ V.

For any other vector operator $\vec{W}$

$$\boxed{\vec{W} = \frac{\langle \vec{J}\cdot\vec{W}\rangle_{kj}\ \vec{J}}{j(j+1)\hbar^2}} \quad \text{— (TO)}$$

$$\therefore \boxed{\vec{W} = \frac{\langle \vec{J}\cdot\vec{W}\rangle_{kj}}{\langle \vec{J}\cdot\vec{V}\rangle_{kj}}\cdot\vec{V} \quad \text{OR} \quad \vec{V} = \frac{\langle \vec{J}\cdot\vec{V}\rangle_{kj}}{\langle \vec{J}\cdot\vec{W}\rangle_{kj}}\ \vec{W}}$$

But $\langle \vec{J}\cdot\vec{W}\rangle_{kj}$, $\langle \vec{J}\cdot\vec{V}\rangle_{kj}$ are independent of m and decided only by j

$\therefore$ Over the subspace $\mathcal{E}_{kj}$ any two vector operators are proportional to each other

~~Before~~ All this was a result of the commutation relations between $[V_x, J_\pm]$ etc. Before generalising to a tensor operator of higher rank let us first show ~~the~~ a use of this theorem to calculate Lande g-factor involved in calculation of the splitting of an energy level in a magnetic field.

Consider $\vec{B}$ $\parallel^{ed}$ to z axis.

~~Consider, Let $[H_0, \vec{J}] = 0$~~ Consider $H_0 \ni [H_0, \vec{J}] = 0$

Consider ~~the~~ state space $\mathcal{E}_{kj}$ spanned by $|E_0, l, s, j, m\rangle$.

$\vec{J} = \vec{L} + \vec{S}$ $\qquad |E_0, l, s, j, m\rangle$, $-j \leq m \leq j$

are all degenerate with energy E_0

$$J_{\pm} |E_0, l, s, j, m\rangle = \hbar \sqrt{j(j+1) - m(m\pm1)}\; |E_0, l, s, j, m\pm1\rangle$$

But $[J_{\pm}, H_0] = 0 \Rightarrow (2j+1)$ states in $\mathcal{E}_{kj}$ are all degenerate with Evalue E_0.

Let $\vec{B} = B\hat{k}$

$H = H_0 + H_{pert} = H_0 + \vec{\mu}\cdot\vec{B}$

$$\boxed{H = H_0 + \mu_z B}$$

What is $\vec{\mu} = ?$

$$\vec{\mu}_L = -\frac{\beta_0}{\hbar}\vec{L}\ , \quad \vec{\mu}_S = -\frac{\beta_0}{\hbar}\cdot 2\vec{S}$$

$$\therefore \vec{\mu} = -\frac{\beta_0}{\hbar}\left[\vec{L} + 2\vec{S}\right] = -\frac{e}{2m_e c}\left[g_L\vec{L} + g_S\vec{S}\right] \qquad (71)$$

$$g_L = 1, \quad g_S = 2$$

$\vec{L}, \vec{S}$: Both vector operators. $\therefore \vec{\mu}$ too is a vector op.

Matrix elements of $\vec{\mu}$ are proportional to $\vec{J}$. We must determine constant of proportionality which can depend on E_0 & j.

$$H^{pert} = -\frac{e}{2m_e c}\left[L_z + 2S_z\right]B = -\frac{\beta_0}{\hbar}\left[L_z + 2S_z\right]B.$$

If B is not too large the effect of B on energy levels can be computed by calculating $\langle E_0, l, s\, j\, m | H^{pert} | E_0, l, s, j, m\rangle$

$$\vec{L} = \frac{\langle \vec{L}\cdot\vec{J}\rangle_{E_0 j}\ \vec{J}}{j(j+1)\hbar^2}, \quad \vec{S} = \frac{\langle \vec{L}\cdot\vec{S}\rangle_{E_0, j,}\ \vec{J}}{j(j+1)\hbar^2}$$

$\langle \vec{L}\cdot\vec{J}\rangle_{E_0, l, s, j, m}$ = depends only ~~only~~ on l, j, s. Not on m.

$$\vec{L}\cdot\vec{J} = \vec{L}\cdot(\vec{L}+\vec{S}) = L^2 + \vec{L}\cdot\vec{S}$$
$$= L^2 + \frac{1}{2}\left[J^2 - L^2 - S^2\right]$$

$|E_0, l, s, j, m\rangle$ is Estate of L^2, S^2, J^2

~~$\langle \vec{L}\cdot\vec{J}\rangle_{E_0, l, s, j, m}$~~

(72.1)
$$\boxed{\begin{aligned}\langle \vec{L}\cdot\vec{J}\rangle_{E_0, l, s, j, m} &= \left[l(l+1) + \tfrac{1}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)\right]\hbar^2 \\ &= \hbar^2\left[l(l+1) + j(j+1) - s(s+1)\right]\tfrac{1}{2}\end{aligned}}$$

~~$\langle \vec{S}\cdot\vec{J}\rangle_{E_0, l, s, j, m} = \frac{\hbar^2}{2}\left[\ldots\right]$~~

(72.2)
$$\boxed{\langle \vec{S}\cdot\vec{J}\rangle_{E_0, l, s, j m} = \frac{\hbar^2}{2}\left[s(s+1) + j(j+1) - l(l+1)\right]}$$

$$H^{pert} = -\frac{\beta_0 B}{\hbar}\left[\frac{\langle \vec{L}\cdot\vec{J}\rangle_{E_0,l,s,j,m}}{j(j+1)\,\hbar^2} J_z + 2 J_z \frac{\langle \vec{S}\cdot\vec{J}\rangle_{E_0,l,s,j,m}}{j(j+1)\,\hbar^2}\right]$$

$$H^{pert} = -\frac{\beta_0}{\hbar}\cdot B\left[J_z\right]\frac{1}{j(j+1)}\left[\langle \vec{L}\cdot\vec{J}\rangle + 2\langle \vec{S}\cdot\vec{J}\rangle\right]\frac{1}{\hbar^2}$$

$$H^{pert} = -\frac{\beta_0}{\hbar}\cdot B\left[\frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)}\right] J_z$$

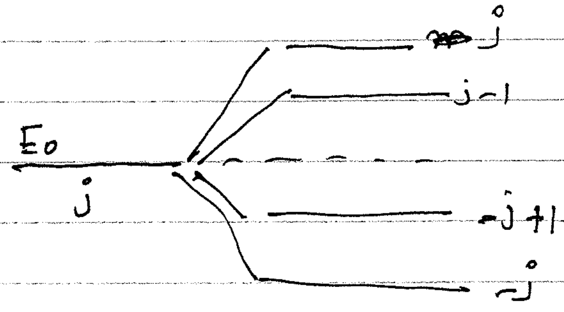
$$\boxed{H^{pert} = -\frac{\beta_0}{\hbar}\cdot B\, g_J J_z} \qquad \boxed{g_J = \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)}} \quad (73)$$

$$\boxed{\langle \,|H^{pert}|\,\rangle_{E_0,l s j m} = -\frac{\beta_0}{\hbar} B g_J \cdot m}$$

~~Ener~~ $2j+1$ Energy levels are split & have energy

$$(74) - \boxed{E_0 - \frac{\beta_0}{\hbar} B g_J m} \qquad -j \le m \le j$$

$$\beta_0 = \frac{-e}{2m_e c} \qquad \boxed{e < 0 \text{ for electron}}$$



$$\boxed{\text{The spacing is } \frac{e}{2m_e c}\cdot B\cdot g_J}$$

$\Rightarrow$ We have calulated expressions fo Lande-g factor.

General statement of the Wigner Eckart Theorem

To write this statement we need to give a formal definition of ~~th~~ an irreducible, spherical tensor of rank K.

This is defined as a set of $2K+1$ operators T_K^q, with $q = -K, \dots, K$ which transform under rotation given by $D^{(K)}_{q'q}$

$$\boxed{\left(T_K^q\right)' = U_R T_K^q U_R^{+} = \sum_{q'=-K}^{K} T_K^{q'} D^{(K)}_{q'q}(R)}$$

→ 75

Using definition of $U_R = \exp\left(-i\frac{\vec{J}\cdot\hat{n}\theta}{\hbar}\right)$ in infintesimal form one can see that this means

$$\boxed{\begin{aligned} [J_z, T_K^q] &= \hbar q T_K^q \\ [J_+ \; T_K^q] &= \hbar\sqrt{K(K+1) - q(q+1)}\; T_K^{q+1} \\ [J_- \; T_K^q] &= \hbar\sqrt{K(K+1) - q(q-1)}\; T_K^{q-1} \end{aligned}}$$

→ 76

Recall that these are similar to what one derived for $\vec{V}$.

Using (75) and (76) one can show,

$$\boxed{\langle k'j'm' | T_K^q | kjm \rangle = \langle jm; kq | j'm' \rangle \cdot \langle k'j' \| T_K \| kj \rangle} \quad (77)$$

small k indicating additional conserved quantum #s

~~counterpart~~ reduced matrix element

capital K

Recall $$\boxed{\langle k'j'm' | \vec{V} | kjm \rangle = \frac{\langle \vec{V} \cdot \vec{J} \rangle_{kj}}{j(j+1)\hbar^2} \langle k'j'm' | \vec{J} | kjm \rangle}$$

depends on j alone

see similarity.

$$\boxed{\langle k'j' \| T_K \| kj \rangle \ : \text{counterpart of } \alpha(k, j)}$$

Looks a little difft. as our derivation of vector operator is ~~a bit~~ in terms of V_x, V_y, V_z and not in terms of $V_\pm, V_z$ which are components of a spherical tensor of rank 1.

Vector operator : $\equiv$ irreducible spherical tensor of rank 1.

$T_1^{-1}, T_1^{1}, T_1^{0}$: Three components of a irreducible spherical tensor of rank 1.

Check ~~that~~ using commutation relations (63.1) – (63.5)

that

$$\boxed{T_1^{1} = -\frac{V_+}{\sqrt{2}}, \quad T_1^{0} = V_z, \quad T_1^{-1} = \frac{V_-}{\sqrt{2}}} \quad (77)$$

satisfy Eqs. (76)

Since $\vec{x}$ is a vector operator

$$\boxed{\begin{array}{ccc} T_1^{1} = -\frac{x+iy}{\sqrt{2}}, & T_1^{0} = z, & T_1^{-1} = \frac{x-iy}{\sqrt{2}} \\ \propto Y_1^{1} & \propto Y_1^{0} & \propto Y_1^{-1} \end{array}} \longrightarrow (78)$$

$\therefore$ $\boxed{Y_1^{m} \text{ are the three components of an irreducible spherical tensor of rank 1}}$

Steps to be taken to prove the theorem

Definition 75 is similar to Eqs. 61', 59, 60. Using these we can then derive 76 similar to derivation of 61.

Using 75 one can show that $\langle k'j'm' | T_K^q | kjm \rangle$ satisfy an equation with same structure as the C.G. series

$$\Rightarrow \quad \langle k'j'm' | T_K^q | kjm \rangle \propto C^{j_1 j_2 j_3}_{m_1 m_2 m_3}$$

with $j_1 = j$, $j_2 = K$, $j_3 = j'$
$m_1 = m$, $m_2 = q$, $m_3 = m'$

i.e. $C^{jKj'}_{mqm'}$.

$$\therefore \underbrace{\boxed{\langle k'j'm' | T_K^q | kjm \rangle \propto C^{jKj'}_{mqm'}}}$$

leads to statement of the thm in Eqn. 77.

How does it follow?

One can prove using C.G. series that if D matrices are

I] known C.G. coeffs. can be determined upto a constant factor.

If the D matrices are known, $\langle k'j'm' | T_K^q | kjm \rangle$ can

II] also be determined upto a constant factor.

III] Eqns. satisfied by C.G. coeffs. and $\langle k'j'm' | T_K^q | kjm \rangle$ are the same.

IV] $\langle k'j'm' | T_K^q | kjm \rangle$ proportional to $C^{jKj'}_{mqm'}$

Follow Merzbacher Chapter 16 for this
Note: notation slightly different!!

[Not done in class]

Matrix element of a vector operator from the general formulation of W-E thm. for irreducible spherical tensor.

Statement

$$\langle k'j'm' | T_K^q | kjm \rangle = \langle jm\, kq | j'm' \rangle \langle k'j' \| T_K \| kj \rangle$$

A vector operator V_x, V_y, V_z

$T_1^0 = V_z$. $T_1^1, T_1^{-1} \propto V_+, V_-$ respectively

~~$\langle k'jj | J_z | kjj \rangle = j\hbar \delta_{kk'} = 1$~~

For two different vector operators $\vec{V}$, $\vec{W}$ then one will have

$$\boxed{\frac{\langle k'j'm' | T_1^q | kjm \rangle}{\langle k'j' \| T_1^q \| kj \rangle} = \frac{\langle k'j'm' | T_1'^q | kjm \rangle}{\langle k'j' \| T_1'^q \| kj \rangle} = \langle jm\, kq | jk\, j'm' \rangle}$$ (79)

C.G. coeff.

Use $T_1'^0 = J_z$, $T_1^1, T_1^{-1} \propto J_\pm$ as defined in eqs. (77') & (78).

From 79 we have for any vector operator $\vec{A}$

$$\boxed{\langle k'j'm' | A^\alpha | kjm \rangle = \frac{\langle k'j' \| \vec{A} \| kj \rangle}{\langle k'j' \| \vec{J} | kj \rangle} \langle k'j'm' | J^\alpha | kjm \rangle} \quad (80)$$

We should then have an expression for $\langle k'j' \| \vec{J} | kj \rangle$

(This has to be indep. of which component of $\vec{A}$, $\vec{J}$ we are taking)

Consider therefore

$$\langle k'jj | J_z | kjj \rangle = \langle jj ; 10 | 1j ; jj \rangle \langle k'j \| \vec{J} \| kj \rangle$$

$$\therefore \hbar j \delta_{kk'} = \langle jj ; 10 | 1j ; jj \rangle \langle k'j \| \vec{J} \| kj \rangle$$

But $\langle jj ; 10 | 1j ; jj \rangle = \sqrt{\dfrac{j}{j+1}}$

$$\therefore \boxed{\hbar \sqrt{j(j+1)} \, \delta_{kk'} \, \delta_{jj'} = \langle k'j' \| \vec{J} \| kj \rangle} \quad (81)$$

For any scalar operator for $j' = j$

$$\boxed{\langle k'jm' | \vec{J} \cdot \vec{A} | kjm \rangle = c \langle k'j \| \vec{A} | kj \rangle} \quad (82)$$

Put $\vec{A} = \vec{J}$

$$\boxed{\langle k'jm' | \vec{J}^2 | kjm \rangle = \delta_{mm'} \delta_{kk'} \, j(j+1) \hbar^2} \quad (83)$$

'c' in Eq. 82 should be independent of $\vec{A}$.

$$c \langle k'j \| \vec{J} \| kj \rangle = j(j+1)\hbar^2$$

But $\boxed{c \langle k'j \| \vec{J} \| kj \rangle = \hbar\sqrt{j(j+1)}\; c}$ → from Eq. 81

$$\Rightarrow \quad c = \sqrt{j(j+1)}\,\hbar$$

Now Eq. 82 then gives

$$\boxed{\langle k'jm' | \vec{J}\cdot\vec{A} | kjm \rangle = \sqrt{j(j+1)}\,\hbar\, \langle k'j \| \vec{A} \| kj \rangle} \quad (84)$$

Combining 84 with 80 and 81, we get

$$(85) \quad \boxed{\langle k'jm' | A^{\alpha} | kjm \rangle = \frac{\langle k'jm | \vec{J}\cdot\vec{A} | kjm \rangle}{j(j+1)\hbar^2} \langle jm' \| J^q \| jm \rangle}$$

C-T derives this more rigorously using ~~C-T 11~~ projection theorem.