Wigner-Eckart Theorem

CTDL, pages 999 - 1085, esp. 1048-1053

Final lecture on $1e^-$ Angular Part
Next: 2 lectures are on $1e^-$ radial part
Many-e^- problems − 8 lectures!

Previous Lecture: $|JLSM_J\rangle$ coupled vs. $|LM_LSM_S\rangle$ uncoupled

Transformation between these basis sets is general and tabulated

Vector Coupling Coefficients
Clebsch-Gordan Coefficients
3-j Coefficients

Same information, increasingly convenient formats.

Correlation Diagrams between limiting cases

* <u>non-crossing rule</u> for states with the same value of rigorously good quantum numbers (zero calculation approach)

* non-degenerate perturbation theory
  sequence of steps for inclusion of information about the opposite limit: $E^{(0)}$, $E^{(0)} + E^{(1)}$, $E^{(0)} + E^{(1)} + E^{(2)}$

* exact diagonalization

How does the pattern of energy levels for one limiting case morph into that for the other limiting case?

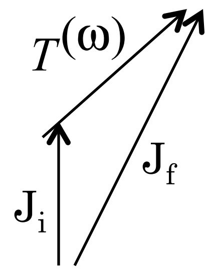
Note that $\mathbf{J}_i$, $\mathbf{L}_i$, $\mathbf{S}_i$ operators cannot cause off-diagonal matrix elements in $|JM_J\rangle$, $|LM_L\rangle$ or $|SM_S\rangle$ basis sets, respectively.

However $\mathbf{L}_z$ and $\mathbf{S}_z$ can cause $\Delta J = \pm 1$ matrix elements in the $|JM_J\rangle$ basis set.

Why? Because **L** and **S** are vectors with respect to **J**.

Triangle Rule: $|L - S| \leq J \leq L + S$

Maybe it is better to think about classification of operators as "like" an angular momentum $\rightarrow T_{\mu}^{(\omega)}$! Spherical tensor operators behave like angular momenta.



$$T_{\mu}^{(\omega)}\left|J_i M_i\right\rangle \text{ gives } J+\omega, J+\omega-1, \ldots |J-\omega|$$

This works! We construct operators classified by what they do to members of the $|JM_J\rangle$ basis set.

How? Commutation Rule definitions of the $T_{\mu}^{(\omega)}$ operators:

$$\left[\mathbf{J}_{\pm}, T_{\mu}^{(\omega)}\right] = \hbar\left[\omega(\omega+1) - \mu(\mu \pm 1)\right]^{1/2} T_{\mu\pm1}^{(\omega)}$$

$$\left[\mathbf{J}_{z}, T_{\mu}^{(\omega)}\right] = \hbar\mu T_{\mu}^{(\omega)}$$

All matrix elements $T_{\mu}^{(\omega)}$ in the $|JM_J\rangle$ basis set are derivable (and inter-related) from these commutation rules.

Do the above commutation rules look familiar? We see the same thing from $J_{\pm}|JM\rangle$ and $J_z|JM\rangle$.

This is a mixture of intuition plus rigor based on tabulated coupling constants.

The Wigner-Eckart Theorem gives us everything we need. The derivation of the W-E theorem from commutation rules is extremely tedious. The Herschbach handout illustrates some of the derivation. [Supplement #1]

Scalar, Vector, and Tensor Operators

Selection Rules

Scalar	S	$T_0^{(0)}$	matrix elements are $\Delta J = 0$, $\Delta M = 0$	M-independent
Vector	V	$T_\mu^{(1)}$	matrix elements are $\Delta J = 0, \pm 1$, $\Delta M = 0, \pm 1$	explicitly M-dependent
Tensor	$T_\mu^{(\omega)}$		ω = rank, μ = component	

We seldom see Tensors with $\omega > 2$.

Construct and classify operators via Commutation Rules

		Rank: ω	"Like"	components: μ
Scalar	1 component	0	J = 0	$\mu = 0$
Vector	3 components	1	J = 1	$\mu = 0 \leftrightarrow z$ $+1 \longrightarrow -(2)^{1/2}(x + iy)$ $-1 \longrightarrow +(2)^{1/2}(x - iy)$ (not quite like $\mathbf{J}_\pm$)
Tensor	$2\omega + 1$ components	ω	J = ω	+2, +1, 0, –1, –2, (for $\omega = 2$)

Example: **J** – **L** + **S**

1. $[\vec{\mathbf{L}},\vec{\mathbf{S}}] = 0$. **L** and **S** act as scalar operators with respect to each other (because they operate on different coordinates)

2. $\vec{\mathbf{L}}$ and $\vec{\mathbf{S}}$ act as vector operators with respect to $\vec{J}$

3. $\vec{\mathbf{L}} \cdot \vec{\mathbf{S}}$ acts like a scalar operator with respect to $\vec{J}$

4. $\vec{\mathbf{L}} \times \vec{\mathbf{S}}$ gives 3 components of a vector operator with respect to $\vec{J}$

We can use commutation rules to project out of any operator the part that acts like a $T_\mu^{(\omega)}$ or we can construct such $T_\mu^{(\omega)}$ operators explicitly!

Wigner-Eckart Theorem

$$\left\langle N'J'M'_J \middle| T_\mu^{(\omega)} \middle| NJM_J \right\rangle = A_{M\mu M'}^{J\omega J'} \delta_{M' M+\mu} \left\langle N'J' \middle\| T^{(\omega)} \middle\| NJ \right\rangle$$

N' and N are radial quantum numbers (i.e. everything that is not a specified angular momentum)

$A_{M\mu M'}^{J\omega J'}$ is a tabulated vector coupling coefficient (or Clebsch-Gordan or 3-j)

$\left\langle N'J' \middle\| T^{(\omega)} \middle\| NJ \right\rangle$ is a "reduced matrix element"

It is reduced in the sense that M', μ, and M are removed.

Often the reduced matrix elements of $T_\mu^{(\omega)}$ can be evaluated by looking at matrix elements of "stretched staes": $\vec{\boldsymbol{J}} = \vec{\boldsymbol{J}} + \vec{\boldsymbol{J}}_2$, $J = J_1 + J_2$ and $\mu = \omega$.

Recall that *extreme members* of coupled and uncoupled basis sets are equal.

$$\left| J = L+S, L, S, M_J = L+S \right\rangle = \left| LM_L = L, SM_S = S \right\rangle$$

Major simplifications result for stretched states.

How to build specified $T_\mu^{(\omega)}$ operators out of components of specific angular momenta [denoted in square brackets].

$$T_{\pm 1}^{(\omega)}[L] = \mp 2^{-1.2}[L_x \pm iL_y]$$

$$T_0^{(1)}[L] = L_z$$

What about $T_{\pm 2}^{(2)}[L]? \rightarrow (L_\pm)^2$, but what about $T_{\pm 1}^{(2)}$ and $T_{\pm 1}^{(1)}$?

Suppose we want tensor operators constructed from two vector operators.

$$T_0^{(0)}\left[A,B\right] = \sum_{k=-\omega}^{\omega} (-1)^k T_k^{(\omega)}[A] T_{-k}^{(\omega)}[B]$$

$$T_2^{(2)}\left[A,B\right] = T_1^{(1)}[A] T_1^{(1)}[B] \to A_+ B_+$$

$$T_1^{(2)}\left[A,B\right] = T_1^{(1)}[A] T_0^{(1)}[B] + T_0^{(1)}[A] T_1^{(1)}[B] \to A_+ B_0 + A_0 B_+$$

Display this scheme more clearly and compactly:

μ	$T_\mu^{(2)}\left[A,B\right]$	$T_\mu^{(1)}\left[A,B\right]$	$T_0^{(0)}\left[A,B\right]$
2	(+ +)		
1	(+ 0) + (0 +)	(+ 0) – (0 +)	
0	(+ –) + (– +)	(+ –) – (– +)	(0 0)
–1	(0 –) + (– 0)	(0 –) – (– 0)	
–2	(– –)		

Notice how we get $T^{(2)}$, $T^{(1)}$, and $T^{(0)}$ as orthogonal combinations of $A_i + B_i$.

Vector Coupling Coefficient

$$\underset{\text{coupled}}{\left|J,J_1,J_2,M\right\rangle} = \sum_{\substack{M_2=M-M_1 \\ M_2=-J_2}}^{J_2} \underbrace{\left|J_1,M_1,J_2,M_2\right\rangle \left\langle J_1,M_1,J_2,M_2\right|}_{\text{completeness}} \overbrace{\left\langle J_1,M_1,J_2,M_2 \middle| J,J_1,J_2,M\right\rangle}^{\text{vector coupling coefficient}}$$

$$\underset{3-j}{\begin{pmatrix} J_1 & J_2 & J \\ M_1 & M_2 & -M \end{pmatrix}} = (-1)^{J_1-J_2-M}(2J+1)^{-1/2} \quad \underset{\text{Clebsch-Gordan}}{\left\langle J_1,M_1,J_2,M_2 \middle| J_1,J_2,J-M\right\rangle}$$

constraint $M_1 + M_2 - M = 0$

Vector Coupling:	no symmetry, no explicit constraints
Clebsch-Gordan	some symmetry, explicit constraint $M_1 + M_2 - M = 0$
3 – j:	maximum symmetry, maximum constraints (rules for permutation of columns)

Examples of Use of Commutation Rules to Reveal the Properties of Scalar Operators

Scalar Operator: $[\mathbf{J}_i, \mathbf{S}] = 0$ all i

1. **ΔJ = 0** selection rule from $[\mathbf{J}^2, \mathbf{S}] = 0$

$0 = [\mathbf{J}^2, \mathbf{S}]$ $\quad 0 = \langle J' M' | \mathbf{J}^2\mathbf{S} - \mathbf{S}\mathbf{J}^2 | JM \rangle = \hbar[J'(J'+1) - J(J+1)]\langle J' M' | \mathbf{S} | JM \rangle$

either J = J′ or $\langle J' M' | \mathrm{S} | JM \rangle = 0$

ΔJ = 0 selection rule

2. **ΔM = 0** selection rule from $[\mathbf{J}_z, \mathbf{S}] = 0$

$$0 = \langle JM' | J_z S - S J_z | JM \rangle = \hbar(M' - M)\langle JM' | S | JM \rangle$$

either M′ = M or $\langle JM' | \mathrm{S} | JM \rangle = 0$

ΔM = 0 selection rule

3. **M independence of $\langle JM | \mathrm{S} | JM \rangle$ from $[\mathbf{J}_\pm, \mathbf{S}] = 0$**

$$0 = \langle JM' | \mathrm{J}_\pm \mathrm{S} - \mathrm{S}\mathrm{J}_\pm | JM \rangle = S_{JM}\langle JM' | \mathrm{J}_\pm | JM \rangle - S_{JM'}\langle JM' | \mathrm{J}_\pm | JM \rangle$$
$$= (S_{JM} - S_{JM'})\langle JM' | \mathrm{J}_\pm | JM \rangle$$

$\langle JM' | \mathbf{J}_\pm | JM \rangle \neq 0$ when $M' = M \pm 1$

Thus $S_{JM} = S_{JM\pm1}$, which means that S_{JM} is independent of M.

What is so great about Wigner-Eckart Theorem?

Massive reduction in number of independent matrix elements.

For example, J = 10, $\omega = 1$

$$\langle J'M' | T_\mu^{(1)} | JM \rangle$$

J′ limited to J ± 1 by triangle rule

J′	# of matrix elements			# of reduced matrix elements
9	(2·9 + 1)(2·10 + 1)	399	1	$c_{-}(10) = \langle 9 \Vert T_{\mu}^{(1)} \Vert 10 \rangle$
10	(2·10 + 1)(2·10 + 1)	441	1	$c_{0}(10) = \langle 10 \Vert T_{\mu}^{(1)} \Vert 10 \rangle$
11	(2·11 + 1)(2·10 + 1)	483	1	$c_{+}(10) = \langle 11 \Vert T_{\mu}^{(1)} \Vert 10 \rangle$
	total	1323	3	only 3

(one might argue that 1323 is a factor of 7 too large)

$\frac{1323}{7} \leftrightarrow 3$ is a huge reduction of what we need to know!

Special case for $\Delta J = 0$ Matrix Elements of $\vec{\mathbf{V}}$!! Memorable!

$$\langle JM' | \vec{\mathbf{V}} | JM \rangle = \frac{\langle J \Vert \mathbf{J} \cdot \mathbf{V} \Vert J \rangle}{\hbar^2 J(J+1)} \langle JM' | \vec{\mathbf{J}} | JM \rangle = c_0(J) \langle JM' | \vec{\mathbf{J}} | JM \rangle$$

We can replace a $\Delta J = 0$ matrix element of $\vec{\mathbf{V}}$ by the corresponding matrix element of $\vec{\boldsymbol{J}}$.

An extremely convenient (practical) operator replacement. Derive effective **H** by replacing $\vec{\mathbf{V}}$ by $\vec{\boldsymbol{J}}$.

$c_0(J)$ can also be evaluated by reference to the easily derived matrix elements of stretched states.

Also can derive similar relationships via Commutation Rules

$$\left\langle J+1, M\left|V_z\right|JM\right\rangle = c_+(J)\left[(J+M+1)(J-M+1)\right]^{1/2}$$
$$\left\langle J+1, M\pm1\left|V_\pm\right|JM\right\rangle = c_+(J)\left[(J\pm M+2)(J\pm M+1)\right]^{1/2}$$
$$\left\langle JM\left|V_z\right|JM\right\rangle = c_0(J)M$$

$$\left\langle JM\pm1\left|V_z\right|JM\right\rangle = c_0(J)\left[J(J+1)-M(M\pm1)\right]^{1/2}$$
$$\left\langle J-1, M\left|V_z\right|JM\right\rangle = c_-(J)\left[(J-M)(J+M)\right]^{1/2}$$
$$\left\langle J-1, M\pm1\left|V_z\right|JM\right\rangle = \pm c_-(J)\left[(J\mp M)(J\pm M+1)\right]^{1/2}$$

This has been just a taste of the power of spherical tensor algebra for problems with exact or approximate spherical symmetry.

3-j, 6-j, 9-j algebra too burdensome to learn and remember unless you are going to use it immediately.