Last lecture on 1e⁻ Angular Part
Next: 2 lectures on 1e⁻ radial part
Many-e⁻ problems

What do we know about 1 particle angular momentum?

1. |JM⟩ Basis set
   \[ [J_i, J_j] = i\hbar \sum_k \varepsilon_{ijk} J_k \]
   definition → all matrix elements in |JM⟩ basis set.

2. \( J = J_1 + J_2 \) Coupling of 2 angular momenta
   coupled ↔ uncoupled basis sets
   transformation via \( J_z = L_z + S_z \) plus orthogonality. Also more general methods.

   \( H^{SO} + H^{Zeeman} \) example
   * easy vs. hard basis sets
   * limiting cases, correlation diagram
   * pert. theory – patterns at both limits plus distortion

TODAY:
2. Statement of the Wigner-Eckart Theorem
3. Derive some matrix elements from Commutation Rules

Scalar \( S \)
\[ \Delta J = \Delta M = 0, M \text{ independent} \]

Vector \( V \)
\[ \Delta J = 0, \pm 1, \Delta M = 0, \pm 1, \text{ explicit } M \text{ dependences of} \]
matrix elements

These commutation rule derivations of matrix elements are tedious. There is a more direct but abstract derivation via rotation matrices. The goal here is to learn how to use 3-j coefficients.
Classification of Operators via Commutation Rules with CLASSIFYING ANGULAR MOMENTUM

<table>
<thead>
<tr>
<th>Type</th>
<th>Components</th>
<th>Like Components</th>
<th>Components(µ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>scalar</td>
<td>&quot;constant&quot;</td>
<td>0 J = 0</td>
<td>µ = 0</td>
</tr>
<tr>
<td>vector</td>
<td>3 components</td>
<td>1 J = 1</td>
<td>µ = 0 ↔ z</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>+1 ↔ −2¹/²(x + iy)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>−1 ↔ +2⁻¹/²(x − iy)</td>
</tr>
<tr>
<td>tensor</td>
<td>(2ω + 1) components</td>
<td>2² 2</td>
<td>+2, ..., −2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3rd 3</td>
<td></td>
</tr>
</tbody>
</table>

Spherical Tensor Components [CTDL, page 1089 #8] ...

Definition: 
\[
\begin{align*}
\tilde{J}_z, T^{(µ)}_ω &= \hbar[(ω(ω + 1) − µ(µ ± 1)]^{1/2} T^{(µ)}_{µ ± 1} \\
\tilde{J}_z, T^{(µ)}_ω &= \hbar µ T^{(µ)}_ω
\end{align*}
\]

This classification is useful for matrix elements of \(T^{(µ)}_ω\) in \(|JM\rangle\) basis set.

Example: \(J = L + S\)

1. \([\tilde{L}, \tilde{S}] = 0 \implies L & S\ act as scalar operators with respect to each other.
2. \(\tilde{L}\) and \(\tilde{S}\) act as vectors wrt \(J\)
3. \(\tilde{L} \cdot \tilde{S}\) acts as scalar wrt \(J\)
4. \(\tilde{L} \times \tilde{S}\) gives components of a vector wrt \(J\).

[Because \(L \times S\) is composed of products of components of two vectors, it could act as a second rank tensor. But it does not!]

[Nonlecture: given 1 and 2, prove 3]

Once operators are classified (classifications of same operator are different wrt different angular momenta), Wigner-Eckart Theorem provides angular factor of all matrix elements in any basis set!

\[
\langle N'J'M'|T^{(µ)}_ω|NJM\rangle = A^{J\omega J}_{Mµ}[M'] \delta_{M',M+µ} \langle N'J'|T^{(µ)}_ω|NJ\rangle
\]

specifies everything else

redundant—usually omitted

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* triangle rule $|l - o| \leq j' \leq j + o$: selection rule for $T_\mu^{(\omega)}$, $\Delta j = \pm \omega, \pm (\omega - 1), \ldots 0$.

* reduced matrix element contains all radial dependence – when there is no radial factor in the operator, then the $J', J$ dependence can often be evaluated as well.


Nonlecture: $L$ & $S$ act as vectors wrt $J$ but scalars wrt each other

• $[L, S] = 0$ scalars wrt each other

• $[J, L] = [L + S, L] = [L, L]$ :: vector wrt. $J$ if $L$ is an angular momentum components of $L$ satisfy the $T_\mu^{(1)}$ definition

\[
[T_1^{(1)}] = -2^{-1/2}[L_\chi + iL_\gamma]
\]

• $[J, -2^{-1/2}[L_\chi + iL_\gamma]] = -2^{-1/2}i\hbar[L_\gamma - iL_\chi] = -2^{-1/2}i\hbar[L_\chi + iL_\gamma]$

\[
[J, T_1^{(1)}[L]] = \hbar (1) T_1^{(1)}[L]
\]

• $[J, S] = [S, S]$ :: $S$ is vector wrt $J$

$I = L + S$

etc.

• Show that $L \cdot S$ acts as scalar wrt $J$

\[
[J_x, L \cdot S] = [J_x, L_x S_x + L_y S_y + L_z S_z] \pm i [J_y, L_x S_x + L_y S_y + L_z S_z]
\]

\[
= \text{four terms}
\]

\[
[J_x, L \cdot S] = [L_x, L \cdot S] + [L_y, L \cdot S] + [L_z, L \cdot S]
\]

\[
\pm [L_x, L \cdot S] \pm [L_y, L \cdot S] \pm [L_z, L \cdot S]
\]

\[
= [i\hbar (L_y S_z - L_z S_y) + i\hbar (L_z S_y - L_y S_z)]
\]

\[
\pm i\hbar (-L_z S_x + L_x S_z) \pm i\hbar (-L_z S_x + L_x S_z)
\]

\[
= 0
\]

\[
[J_z, L \cdot S] = [L_z, L \cdot S] + [S_z, L \cdot S]
\]

\[
= i\hbar (L_y S_z - L_z S_y) + i\hbar (L_z S_y - L_y S_z)
\]

\[
= 0
\]

\[
\therefore L \cdot S \text{ acts as } T_0^{(0)}
\]

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

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What is so great about W-E Theorem?

vast reduction of independent matrix elements

e.g. \( J = 10, \omega = 1 \) (vector operator)

possible values of \( J' \) limited to 9, 10, 11 by triangle rule

W-E Theorem is an extension of V-C idea because we think of operators as “like angular momenta” and we couple them to angular momenta to make new angular momentum eigenstates.

What is so great about W-E Theorem?

All serve same function

Vector Coupling Coefficients

Clebsch - Gordan Coefficients

3-J coefficients

all related to what you already know how to obtain by ladders and orthogonality for

\[
\begin{align*}
|JJ,J_M,M_J\rangle &= \sum_{M_{J_1}=-J_1}^{+J_1} |J_{M_1},J_{M_2},J_{M_3}\rangle \langle J_{M_1},J_{M_2},J_{M_3}|JJ,J_M,M_J\rangle \\
&= (-1)^{J_1-J_2-J_3} (2J_3+1)^{-\frac{1}{2}} \langle J_{M_1}J_{M_2}J_{M_3}|J_{J_1}J_{J_2}J_{J_3}-M_3\rangle
\end{align*}
\]

Constraint: \( M_1 + M_2 + M_3 = 0 \) This constraint is imposed in \( | \) notation but not in \( \langle \rangle \) notation.

p. 46 Edmonds (1974) general formula

3-J: \( \begin{pmatrix} J_1 & J_2 & J_3 \\ M_1 & M_2 & M_3 \end{pmatrix} = (\begin{pmatrix} J_1-J_2-M_1 \\ J_2 \end{pmatrix})^{-1}(2J_3+1)^{-\frac{1}{2}} \langle J_{M_1}J_{M_2}J_{M_3}|J_{J_1}J_{J_2}J_{J_3}-M_3\rangle \]

vector coupling (v.c.) coefficients

completeness

Constraint: \( M_1 + M_2 + M_3 = 0 \) This constraint is imposed in \( | \) notation but not in \( \langle \rangle \) notation.
Outline proof of various parts of W-E Theorem

Scalar Operators $S$

$[J_i, S] = 0$  \[\text{Definition (for all i)}\]

1. $\Delta J = 0$ selection rule from $[J^2, S] = 0$
2. $\Delta M = 0$ selection rule from $[J_z, S] = 0$
3. M - independence from $[J_z, S] = 0$

1. show $\Delta J = 0$: $\langle J'M|S|JM \rangle = 0$ if $J' \neq J$

\[ [J^2, S] = 0 \]
\[ 0 = \left\langle J'M \right| \left( J^2S - SJ^2 \right) |JM \rangle = \hbar^2 \left( J'(J' + 1) - J(J + 1) \right) \left\langle J'M \right| S |JM \rangle \]

\[ \text{direction of operation by } J^2 \]

either $J' = J$ or $\langle J'M|S|JM \rangle = 0$

(only $\Delta J = 0$ matrix elements of $S$ can be nonzero)

2. show $\Delta M = 0$: $\langle J'M|S|JM \rangle = 0$ if $M' \neq M$

\[ [J_z, S] = 0 \]
\[ 0 = \left\langle JM \right| \left( J_zS - SJ_z \right) |JM \rangle = \hbar \langle M' - M \rangle \left\langle J'M \right| S |JM \rangle \]

\[ \text{either } M' = M \text{ or } \langle J'M|S|JM \rangle = 0 \]

3. show M - Independence of matrix elements

\[ [J_z, S] = 0 \]
\[ 0 = \left\langle JM \right| \left( J_zS - SJ_z \right) |JM \rangle = s_{JM} \left\langle JM \right| J_z |JM \rangle - s_{JM'} \left\langle JM \right| J_z |JM \rangle \]
\[ = (s_{JM} - s_{JM'}) \left\langle JM \right| J_z |JM \rangle \]

uses $\Delta J = \Delta M = 0$ for $S$

\[ \text{direction of operation by } S \]

we already know that $S$ is diagonal in $M$.

[Should skip pages 27-6, 7, 8 and go directly to recursion relationship on page 27-10.]
Thus either \( s_{JM} = s_{JM'} \) or \( \langle JM' \mid J_\pm \mid JM \rangle = 0 \)

Thus \( s_{JM} \) is independent of \( M \)

Putting all results for \( S \) together
\[
\langle J'M' \mid S \mid JM \rangle = \delta_{JJ'} \delta_{MM'} \langle J \parallel S \parallel J' \rangle
\]

Vector Operators \( \mathbf{V} \)
\[
[J_j, V_j] = i\hbar \sum_k \varepsilon_{ijk} V_k
\]

1. \( M \) selection rules from \([J_z, \mathbf{V}]\)
2. \( J \) selection rules from \([J^2, [J^2, \mathbf{V}]]\)
3. \( M \) - dependence of matrix elements of \( \mathbf{V} \) from double commutator

1. \( M \) selection rules
   a. \( [J_z, V_z] = 0 \)
   \[
   0 = \langle J'M' \mid (J_z V_z - V_z J_z) \mid JM \rangle = \hbar(M' - M) \langle J'M' \mid V_z \mid JM \rangle
   \]
   either \( M = M' \) or \( ME = 0 \)

   b. \( [J_z, V_\pm] = [J_z, V_\pm] \pm i [J_z, V_j] = i\hbar (V_j \pm i(-V_j)) = \pm \hbar V_\pm \)
   \[
   \langle J'M' \mid (J_z V_\pm - V_\pm J_z) \mid JM \rangle = \pm \hbar \langle J'M' \mid V_\pm \mid JM \rangle
   \]
   \[
   \hbar(M' - M) \langle J'M' \mid V_\pm \mid JM \rangle = \pm \hbar \langle J'M' \mid V_\pm \mid JM \rangle
   \]
   \[
   \hbar(M' - M \mp 1) \langle J'M' \mid V_\pm \mid JM \rangle = 0
   \]
   \( M' = M \pm 1 \) or \( ME = 0 \)
2. M selection rules

need to use a result that requires lengthy derivation

\[ [J^2, [J^2, V]] = 2\hbar^2 [J^2V - 2(J \cdot V)J + VJ^2] \]

see proof in Condon and Shortley, pages 59-60

Take \( \langle J'M' | JM \rangle \) Matrix elements of both sides of above Eq.

\[
\begin{align*}
\text{LHS} &= \langle J'M' | J^2(J^2V) - J^2VJ^2 - J^2VJ^2 + VJ^2J^2 | JM \rangle \\
&= \hbar^4 \left[ (J'(J' + 1))^2 - 2J(J + 1)J'(J' + 1) + J^2(J + 1)^2 \right] \langle J'M' | V | JM \rangle \\
\text{RHS} &= 2\hbar^4 \left[ J'(J' + 1) + J(J + 1) \right] \langle J'M' | V | JM \rangle - 4\hbar^4 \langle J'M' | (J \cdot V)J | JM \rangle \\
&= \text{scalar}
\end{align*}
\]

\[
\begin{align*}
\langle J'M' | (J \cdot V)J | JM \rangle &= \sum_{J''M''} \langle J'M' | (J \cdot V)J''M'' | J''M'' \rangle \langle J''M'' | J | JM \rangle \\
&= \langle J''M'' | J | JM \rangle \langle J | J''M'' | J'M' | J | JM \rangle \\
&= \langle J | J''M'' | J'M' | JM \rangle \delta_{J,J''}
\end{align*}
\]

two cases for overall matrix element

A. \( J' \neq J \)
B. \( J' = J \)
A. \( J' \neq J \)

\[ \text{RHS} = 2\hbar^4 \left[ J'(J'+1) + J(J+1) \right] \langle J'M' | \vec{V} | JM \rangle \]

\[ \text{LHS} = \hbar^4 \left[ J'^2(J'+1)^2 - 2J(J+1)J'(J'+1) + J^2(J+1)^2 \right] \langle J'M' | \vec{V} | JM \rangle \]

\[ 0 = \text{LHS} - \text{RHS} = \text{algebra} = \hbar^4 \langle J'M' | \vec{V} | JM \rangle \left[ (J' - J)^2 - 1 \right] \left[ (J' + J + 1)^2 - 1 \right] \]

\[ \text{ME} = 0 \text{ unless } J' = J \pm 1 \text{ or } J' = -J \]

(J' = -J is impossible except for J' = -J = 0, but this violates J' \neq J assumption)

\[ \therefore \Delta J = \pm 1 \text{ selection rule for } \vec{V} \]

B. \( J' = J \)

\[ \text{LHS} = 0 \]

\[ 0 = \text{RHS} = 4\hbar^2 \left[ \hbar^2 J(J+1) \langle JM' | \vec{V} | JM \rangle - \langle J | J \cdot \vec{V} | J \rangle \langle JM' | J | JM \rangle \right] \]

\[ \langle JM' | \vec{V} | JM \rangle = \frac{\langle J | J \cdot \vec{V} | J \rangle}{\hbar^2 J(J+1)} \frac{\langle JM' | J | JM \rangle}{C_0(J)} \]

A WONDERFUL AND MEMORABLE RESULT. It says that all \( \Delta J = 0 \) matrix elements of \( \vec{V} \) are \( \propto \) corresponding matrix element of \( \vec{J} \). A simplified form of W - E Theorem for vector operators.
Lots of (NONLECTURE) algebra needed to generate all $\Delta J = \pm 1$ matrix elements of $\tilde{V}$.

SUMMARY OF C.R. RESULTS: Wigner-Eckart Theorem for Vector Operator

\[ \Delta J = 0 \quad \langle JM\mid V_+\mid JM \rangle = C_o(J)M \]
\[ \langle JM \pm l\mid V_\pm \mid JM \rangle = C_o(J) \left[ J(J + 1) - M(M + 1) \right]^{1/2} \]

special case: These are exactly the same form as corresponding matrix element of $J_z$.

\[ \Delta J = 1 \quad \langle J + 1M \pm l\mid V_\pm \mid JM \rangle = \mp C_+(J) \left[ (J \pm M + 2)(J \pm M + 1) \right]^{1/2} \]
\[ \langle J + 1M\mid V_+\mid JM \rangle = + C_+(J) \left[ (J + M + 1)(J - M + 1) \right]^{1/2} \]

\[ \Delta J = -1 \quad \langle J - 1M \pm l\mid V_\pm \mid JM \rangle = \pm C_-(J) \left[ (J \mp M)(J \pm M + 1) \right]^{1/2} \]
\[ \langle J - 1M\mid V_+\mid JM \rangle = + C_-(J) \left[ (J - M)(J + M) \right]^{1/2} \]

only $C_o(J)$, $C_+(J)$, $C_-(J)$ : 3 unknown $J$-dependent constants for each $J$.

NONLECTURE (to end of notes). Example of how recursion relationships (reduced matrix elements) are derived for each possible $\Delta J$.

$\Delta J = \pm 1$ matrix elements of $\tilde{V}$

$\Delta M = +1$ using $[J_+, V_+] = 0$

$\Delta M$ selection rule for $V_+$ is $\Delta M = +1$

$\Delta M$ selection rule for $J_+, V_+$ is $\Delta M = +2$

\[ \langle CR \rangle = 0 = \left( J + 1M + 1 \right) \left( J_+ V_+ - V_+ J_+ \right) \langle JM - 1 \rangle \]
\[ 0 = \langle J + 1M + 1\mid J_+ V_+ - V_+ J_+ \mid JM - 1 \rangle \]
\[ - \langle J + 1M + 1\mid V_+ J_+ \mid JM - 1 \rangle \] expand using completeness

(arrow denotes $J_+$ operates to right)

($J_+$ operates to left)

The matrix elements in the denominator are to be replaced by their values, and a common factor is cancelled.

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multiply both sides by \((J + M + 1)^{1/2}\) to display symmetry
\[
\frac{\langle J + 1M|V_+|JM - 1 \rangle}{(J + M)^{1/2}(J + M + 1)^{1/2}} = -\frac{\langle J + 1M + 1|V_+|JM \rangle}{(J + M + 1)^{1/2}(J + M + 2)^{1/2}} \equiv -C_+(J)
\]

\(M \rightarrow M + 1\) recursion relationship

sign chosen so that \(V_z\) matrix elements will be +

\[
\text{ratio is independent of } M
\]
\[
C_+(J) \equiv \langle \alpha'J + 1\|V\|\alpha J \rangle
\]
\[
\langle J + 1M + 1|V_+|JM \rangle = -C_+[(J + M + 1)(J + M + 2)]^{1/2}
\]

Remaining to do for \(\Delta J = \pm 1\) matrix elements

A. \([J_-, V_z] = -2hV_z\) gives \(V_z\) matrix element when we take \(\Delta M = 0\)

matrix element of both sides

B. \([J_-, V_z] = hV_\) gives \(V_\) matrix element when we take \(\Delta M = -1\)

matrix element of both sides

A. \([J_-, V_z] = -2hV_z\) \(\Delta M = 0\) selection rule for both sides

\[
\text{RHS} = -2h\langle J + 1M|V_z|JM \rangle
\]
\[
\text{LHS} = \langle J + 1M(J^-V_+ - V_+J^-)|JM \rangle
\]
\[
= \langle J + 1M|J^-J + 1M + 1\rangle\langle J + 1M + 1|V_+|JM \rangle
\]
\[
-\langle J + 1M|V_+JM - 1\rangle\langle JM - 1|J^-JM \rangle
\]
\[
= h[(J + 1)(J + 2) - M(M + 1)]^{1/2}\langle J + 1M + 1|V_+|JM \rangle
\]
\[
- h[J(J + 1) - M(M - 1)]^{1/2}\langle J + 1M|V_+|JM - 1 \rangle
\]

rearrange this and use \(V_+\) recursion rule from above

\[
\text{LHS} = hC_+(J)[(J + M + 1)(J - M + 1)]^{1/2}[(J + M) - (J + M + 2)]
\]
\[
= -2hC_+(J)[(J + M + 1)(J - M + 1)]^{1/2}
\]
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RHS = LHS

\[ \langle J + 1M | V_z | JM \rangle = C_+ (J) \left( (J + M + 1)(J - M + 1) \right)^{1/2} \]

B. \[ [J_-, V_z] = \hbar V_- \]

\[ \text{take } \langle J + 1M - 1 | \cdots | JM \rangle \]

RHS = \hbar \langle J + 1M - 1 | V_- | JM \rangle

LHS = \langle J + 1M - 1 | J_- | J + 1M \rangle \langle J + 1M | V_z | JM \rangle

- \langle J + 1M - 1 | V_z | JM - 1 \rangle \langle JM - 1 | J_- | JM \rangle

= \hbar C_+ (J) \left( (J - M + 2)(J - M + 1) \right)^{1/2}

\[ \langle J + 1M - 1 | V_- | JM \rangle = + C_+ (J) \left( (J - M + 2)(J - M + 1) \right)^{1/2} \]

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VERY COMPLICATED AND TEDIOUS ALGEBRA