Wigner-Eckart Theorem

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Wigner-Eckart Theorem (Statement)

Consider an irreducible tensor operator T_q^k, the matrix element

$$\langle \gamma' j' m' | T_q^k | \gamma j m \rangle = \langle \gamma' j' \| T^k \| \gamma j \rangle \langle j' m' | j k m q \rangle$$

Where $\langle \gamma' j' \| T^k \| \gamma j \rangle$ is the reduced matrix element, $\langle j' m' | j k m q \rangle$ is the Clebsch-Gordan coefficients .

Main focus

1. How do we define irreducible tensor operator?
2. Proof of Wigner-Eckart theorem
3. Applications of Wigner-Eckart theorem

Spherical Basis

Consider a rotation about z-axis

In Cartesian coordinate:

$$x \longrightarrow x\cos\phi + y\sin\phi$$

$$y \longrightarrow -x\sin\phi + y\cos\phi$$

$$z \longrightarrow z$$

Mixing up x and y !

In spherical basis:

$$x \pm iy \longrightarrow (x\cos\phi + y\sin\phi) \pm i(-x\sin\phi + y\cos\phi) = e^{-i\phi}(x \pm iy)$$

$$z \longrightarrow z$$

Define

$$\widehat{e_1} = \frac{x+iy}{\sqrt{2}} \qquad \widehat{e_0} = \hat{z} \qquad \widehat{e_{-1}} = \frac{x-iy}{\sqrt{2}}$$

Spherical basis as $j = 1$ representation

Using spherical basis to expand a vector $x_q = \boldsymbol{X} \cdot \widehat{\boldsymbol{e_q}}$

The wave function : $\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell m}(\Omega)$

To find the matrix element of electric dipole moment operator between two states, we must evaluate $\langle n\ell m|\boldsymbol{X}|n'\ell' m'\rangle$

$$\begin{cases} rY_{11}(\theta,\phi) = -r\sqrt{\dfrac{3}{8\pi}}\sin\theta\, e^{i\phi} = \sqrt{\dfrac{3}{4\pi}}\left(-\dfrac{x+iy}{\sqrt{2}}\right), \\ rY_{10}(\theta,\phi) = r\sqrt{\dfrac{3}{4\pi}}\cos\theta = \sqrt{\dfrac{3}{4\pi}}\ z, \\ rY_{1,-1}(\theta,\phi) = r\sqrt{\dfrac{3}{8\pi}}\sin\theta\, e^{-i\phi} = \sqrt{\dfrac{3}{4\pi}}\left(\dfrac{x-iy}{\sqrt{2}}\right). \end{cases} \quad \Longrightarrow Y_{1q}\,(\theta,\phi) = \sqrt{\dfrac{3}{4\pi}}\ x_q$$

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$$\Longrightarrow Y_{1q}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\, x_q$$

The spherical components of position operator are naturally connected to Y_{1q}

Spherical basis as $j = 1$ representation

The generators of rotation operators are angular momentum operator ($\hbar \equiv 1$)

$$J_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad J_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \qquad J_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$J_+ = J_1 + iJ_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -i \\ 1 & i & 0 \end{pmatrix} \qquad J_- = J_1 - iJ_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & -i \\ -1 & i & 0 \end{pmatrix}$$

Spherical basis satisfies

$J_3 \widehat{e_q} = q \widehat{e_q}$ and $J_\pm \widehat{e_q} = \sqrt{(1 \mp q)(1 \pm q + 1)}\, \widehat{e_{q\pm1}}, q = -1, 0, 1$

Completely analogous to

$J_z |jm\rangle = \hbar m |jm\rangle$ and $J_\pm |jm\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}\, |j, m \pm 1\rangle$.

Irreducible tensor operator

A rotation operator: $U(R) = e^{-\frac{i}{\hbar}\theta \hat{\mathbf{n}}\cdot\mathbf{J}}$.

<u>Rotation in ket space:</u>

$$U|\gamma jm\rangle = \sum_{m'} |\gamma jm'\rangle D^{j}_{m'm}$$

In previous page, I have showed that the position operator transform like a $j = 1$ object

Can we find a set of "operators" that transform like $|\gamma jm\rangle$?

Irreducible tensor operator

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Rotation in operator space:

Rotation of operator A is defined as $A \mapsto UAU^{\dagger}$

Irreducible tensor operator of rank-k T^k_q :
Operators that transform like $|kq\rangle$ under rotations, where $q = -k, -k+1, \dots, k-1, k$

And T^k_q satisfies

$$U(R) T^k_q U^{\dagger}(R) = \sum_{q'} T^k_{q'} D^k_{q'q}(R)$$

Vector operators can be written as rank-1 irreducible tensor

Wigner-Eckart Theorem (Statement)

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Where $\langle \gamma' j' \| T^k \| \gamma j \rangle$ is the reduced matrix element, $\langle j' m' | j k m q \rangle$ is the Clebsch-Gordan Coefficients

Proof of Wigner-Eckart Theorem

First, we need to evaluate $\left[\mathbf{J}, T_q^k\right]$

Let's start from

$$U(R)T_q^k U^\dagger(R) = \sum_{q'} T_{q'}^k D_{q'q}^k(R)$$

Consider an infinitesimal rotation

Left-hand side

$$U(R)T_q^k U^\dagger(R) = \left(1 - \frac{i}{\hbar}\theta\hat{n}\cdot\mathbf{J}\right) T_q^k \left(1 + \frac{i}{\hbar}\theta\hat{n}\cdot\mathbf{J}\right)$$

To the first order θ

$$U(R)T_q^k U^\dagger(R) \approx T_q^{(k)} - \frac{i}{\hbar}\theta\left[(\hat{n}\cdot\mathbf{J}), T_q^{(k)}\right]$$

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Let's start from

$$U(R)T_q^k U^\dagger(R) = \sum_{q'} T_{q'}^k D_{q'q}^k(R)$$

Consider an infinitesimal rotation

Right-hand side

Because T_q^k transform like $|kq\rangle$

$$D_{q'q}^{(k)}(R) = \left\langle kq' \left| \left(1 - \frac{i}{\hbar}\theta\hat{n}\cdot\mathbf{J}\right) \right| kq \right\rangle = \delta_{q'q} - \frac{i}{\hbar}\theta\langle kq'|\hat{n}\cdot\mathbf{J}|kq\rangle$$

$$\sum_{q'} T_{q'}^{(k)}\left[\delta_{q'q} - \frac{i}{\hbar}\theta\langle kq'|\hat{n}\cdot\mathbf{J}|kq\rangle\right] = T_q^{(k)} - \frac{i}{\hbar}\theta\sum_{q'} T_{q'}^{(k)}\langle kq'|\hat{n}\cdot\mathbf{J}|kq\rangle$$

Proof of Wigner-Eckart Theorem

Equating LHS and RHS

$$T_q^{(k)} - \frac{i}{\hbar}\theta\left[(\hat{n}\cdot\mathbf{J}), T_q^{(k)}\right] = T_q^{(k)} - \frac{i}{\hbar}\theta\sum_{q'} T_{q'}^{(k)}\langle kq'|\hat{n}\cdot\mathbf{J}|kq\rangle$$

$$\Rightarrow \left[\mathbf{J}, T_q^{(k)}\right] = \sum_{q'} T_{q'}^{(k)}\langle kq'|\mathbf{J}|kq\rangle\,.$$

Now, we will calculate $\left[J_z, T_q^k\right]$, $\left[J_+, T_q^k\right]$, $\left[J_-, T_q^k\right]$

$$\left[J_z, T_q^k\right] = \sum_{q'} T_{q'}^k\langle kq'|J_z|kq\rangle = \sum_{q'} T_{q'}^k \hbar q\,\delta_{q'q} = \hbar q T_q^k$$

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

Proof of Wigner-Eckart Theorem

We obtain the selection rule by

$$\langle\gamma' j' m'|[J_z, T_q^k]|\gamma j m\rangle = \langle\gamma' j' m'|J_z T_q^k|\gamma j m\rangle - \langle\gamma' j' m'|T_q^k J_z|\gamma j m\rangle$$
$$= \hbar m'\langle\gamma' j' m'|T_q^k|\gamma j m\rangle - \hbar m\langle\gamma' j' m'|T_q^k|\gamma j m\rangle$$
$$= \hbar q\langle\gamma' j' m'|T_q^k|\gamma j m\rangle$$

The matrix element $\langle\gamma' j' m'|T_q^k|\gamma j m\rangle = 0$ unless $m' - m = q$

We obtain the recursion relation by

$$\langle\gamma' j' m'|[J_\pm, T_q^k]|\gamma j m\rangle = \langle\gamma' j' m'|J_\pm T_q^k|\gamma j m\rangle - \langle\gamma' j' m'|T_q^k J_\pm|\gamma j m\rangle$$
$$= \hbar\sqrt{(j' \pm m')(j' \mp m' + 1)}\,\langle\gamma' j', m' \mp 1|T_q^k|\gamma j m\rangle$$
$$-\hbar\sqrt{(j \mp m)(j \pm m + 1)}\,\langle\gamma' j' m'|T_q^k|\gamma j, m \pm 1\rangle$$
$$= \hbar\sqrt{(k \mp q)(k \pm q + 1)}\,\langle\gamma' j' m'|T_{q\pm 1}^k|\gamma j m\rangle$$

Proof of Wigner-Eckart Theorem

Compare with the CG coefficients

Selection rule

$$\langle j'm'|jkmq\rangle = 0 \quad \text{unless} \quad m' = m + q \quad \text{and} \quad |j-k| \le j' \le j+k.$$

Recursion relation

Since T_q^k transform like $|kq\rangle$ $\quad |jm\rangle \otimes |kq\rangle = |jkmq\rangle$

$$\sqrt{(j' \pm m')(j' \mp m' + 1)}\,\langle \gamma' j', m' \mp 1|T_q^k|\gamma j m\rangle$$
$$- \sqrt{(j \mp m)(j \pm m + 1)}\,\langle \gamma' j' m'|T_q^k|\gamma j, m \pm 1\rangle$$
$$= \sqrt{(k \mp q)(k \pm q + 1)}\,\langle \gamma' j' m'|T_{q\pm1}^k|\gamma j m\rangle$$

Proof of Wigner-Eckart Theorem

Recursion relation

Since T_q^k transform like $|kq\rangle$ $\quad |jm\rangle \otimes |kq\rangle = |jkmq\rangle$

$$\sqrt{(j' \pm m')(j' \mp m' + 1)}\,\langle \gamma' j', m' \mp 1 | T_q^k | \gamma j m\rangle$$
$$- \sqrt{(j \mp m)(j \pm m + 1)}\,\langle \gamma' j' m' | T_q^k | \gamma j, m \pm 1\rangle$$
$$= \sqrt{(k \mp q)(k \pm q + 1)}\,\langle \gamma' j' m' | T_{q\pm 1}^k | \gamma j m\rangle$$

Can be written as

$$\sqrt{(j' \pm m')(j' \mp m' + 1)}\,\langle j', m' \mp 1 | jkmq\rangle - \sqrt{(j \mp m)(j \pm m + 1)}\,\langle j' m' | jk, m \pm 1, q\rangle$$
$$= \sqrt{(k \mp q)(k \pm q + 1)}\,\langle j' m' | jkm, q \pm 1\rangle$$

The selection rule and recursion relation are the same

Proof of Wigner-Eckart Theorem

The selection rule and recursion relation are the same between the matrix elements and CG coefficients, so

$$\langle \gamma' j' m' | T_q^k | \gamma j m \rangle = c \langle j' m' | j k m q \rangle.$$

And c cannot depend on m, m', q, since they are already determined by the recursion relation, so $c \equiv \langle \gamma' j' \| T^k \| \gamma j \rangle$

$$\Longrightarrow \langle \gamma' j' m' | T_q^k | \gamma j m \rangle = \langle \gamma' j' \| T^k \| \gamma j \rangle \langle j' m' | j k m q \rangle$$

Q.E.D.

Application 1 — Selection Rule

Electron dipole transition

Interaction Hamiltonian $H'_{int} = -\boldsymbol{d} \cdot \boldsymbol{E},\ \boldsymbol{d} = -e\boldsymbol{r}$

$\boldsymbol{d}$ is a vector operator $\Longrightarrow T_q^k$ with $k = 1$, so we consider $\langle \gamma' j' m' | T_q^1 | \gamma j m \rangle$

Applying Wigner-Eckart theorem, we have

$$\langle \gamma' j' m' | T_q^1 | \gamma j m \rangle = \langle \gamma' j' \| T^1 \| \gamma j \rangle \langle j' m' | j, 1, m q \rangle$$

Selection rule is given by $\langle j' m' | j, 1, m q \rangle$

$$\langle j' m' | j k m q \rangle = 0 \quad \text{unless} \quad m' = m + q \quad \text{and} \quad |j - k| \leq j' \leq j + k.$$

Plugging in $k = 1$, we have

$$\Delta j \equiv j' - j = 0, \pm 1, \quad j = 0 \nleftrightarrow j' = 0, \quad \text{and} \quad \Delta m \equiv m' - m = 0, \pm 1$$

Application 2 — Zeeman Effect

Weak-Field Zeeman Effect

The first order energy correction: $E_Z^1 = \langle n\ell j m_j | H_Z' | n\ell j m_j \rangle = \frac{e}{2m} B_{\text{ext}} \hat{z} \cdot \langle \mathbf{L} + 2\mathbf{S} \rangle$

By Wigner-Eckart theorem, since $\boldsymbol{L} + 2\boldsymbol{S}$ is a vector operator, we have

$$\langle n\ell j m_j | L_z + 2S_z | n\ell j m_j \rangle = \alpha \langle n\ell j m_j | J_z | n\ell j m_j \rangle.$$

α is actually the Lande g-factor g_J (can be proved), thus

$$\langle n\ell j m_j | L_z + 2S_z | n\ell j m_j \rangle = g_J m_j \hbar$$

$$\Longrightarrow E_Z^1 = \mu_B B_{\text{ext}} g_J m_j, \text{ where } \mu_B = \frac{e\hbar}{2m}$$

Reference

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Thank you!