

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:

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

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

$$z \rightarrow z$$

Mixing up x and y !

In spherical basis:

$$x \pm iy$$

$$\rightarrow (x \cos \phi + y \sin \phi)$$

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

$$z \rightarrow z$$

Define

$$\hat{e}_1 = \frac{x + iy}{\sqrt{2}} \quad \hat{e}_0 = \hat{z} \quad \hat{e}_{-1} = \frac{x - iy}{\sqrt{2}}$$

Spherical basis as $j = 1$ representation

Using spherical basis to expand a vector $x_q = \mathbf{X} \cdot \widehat{\mathbf{e}}_q$

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 $\langle n\ell m | \mathbf{X} | n'\ell' m' \rangle$

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

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

$$\left(rY_{1,-1}(\theta, \phi) = r \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi} = \sqrt{\frac{3}{4\pi}} \left(\frac{x - iy}{\sqrt{2}} \right) \right).$$

Spherical basis as $j = 1$ representation

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

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

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

Spherical basis satisfies

$$J_3 \widehat{e}_q = q \widehat{e}_q \text{ and } J_{\pm} \widehat{e}_q = \sqrt{(1 \mp q)(1 \pm q + 1)} \widehat{e}_{q \pm 1}, q = -1, 0, 1$$

Completely analogous to

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

Irreducible tensor operator

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

Rotation in ket space:

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

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 ket space:

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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_q^k :

Operators that transform like $|kq\rangle$ under rotations, where $q = -k, -k + 1, \dots, k - 1, k$

And T_q^k satisfies

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

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 $[\mathbf{J}, T_q^k]$

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

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

Proof of Wigner-Eckart Theorem

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Let's start from

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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

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

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

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

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

Proof of Wigner-Eckart Theorem

We obtain the selection rule by

$$\begin{aligned}\langle \gamma' j' m' | [J_z, T_q^k] | \gamma j m \rangle &= \langle \gamma' j' m' | J_z T_q^k | \gamma j m \rangle - \langle \gamma' j' m' | T_q^k J_z | \gamma j m \rangle \\ &= \hbar m' \langle \gamma' j' m' | T_q^k | \gamma j m \rangle - \hbar m \langle \gamma' j' m' | T_q^k | \gamma j m \rangle \\ &= \hbar q \langle \gamma' j' m' | T_q^k | \gamma j m \rangle\end{aligned}$$

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

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

Proof of Wigner-Eckart Theorem

Recursion relation

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

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

Can be written as

$$\begin{aligned} & \sqrt{(j' \pm m')(j' \mp m' + 1)} \langle j', m' \mp 1 | j k m q \rangle - \sqrt{(j \mp m)(j \pm m + 1)} \langle j' m' | j k, m \pm 1, q \rangle \\ & = \sqrt{(k \mp q)(k \pm q + 1)} \langle j' m' | j k m, q \pm 1 \rangle \end{aligned}$$

Same recursion relation as the CG coefficient $\langle j' m' | j k m q \rangle$

Proof of Wigner-Eckart Theorem

The recursion relations 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 $c \equiv \langle \gamma' j' || T^k || \gamma j \rangle$

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

Q.E.D.

Application 1 — Selection Rule

Since $\langle \gamma' j' m' | T_q^k | \gamma j m \rangle = \langle \gamma' j' || T^k || \gamma j \rangle \langle j' m' | j k m q \rangle$, the selection rule is given by $\langle j' m' | j k m q \rangle$ (CG coefficient).

I have showed that the matrix element $\langle \gamma' j' m' | T_q^k | \gamma j m \rangle = 0$ unless $m' - m = q$.

Since T_q^k transform like $|k q\rangle \quad |j m\rangle \otimes |k q\rangle = |j k m q\rangle$

$$j \otimes k = (j + k) \oplus (j + k - 1) \oplus \dots \oplus |j - k|$$

$$\Rightarrow j' = j + k, j + k - 1, j + k - 2, \dots, |j - k|$$

$$\Rightarrow |j - k| \leq j' \leq j + k.$$

Selection rule for T_q^k : $m' - m = q$ and $|j - k| \leq j' \leq j + k$.

Application 1 — Selection Rule

Electron dipole transition

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

\mathbf{d} is a vector operator $\Rightarrow T_q^k$ with $k = 1$, so we consider $\langle n' l' m' | T_q^1 | n l m \rangle$

Applying Wigner-Eckart theorem, we have

$$\langle n' l' m' | T_q^1 | n l m \rangle = \langle n' l' || T^1 || n l \rangle \langle l' m' | l, 1, m q \rangle$$

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

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

Plugging in $k = 1$, we have

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

Application 2 — Simplification of Calculation

Electron dipole transition

The goal is to calculate $\langle n'l'm' | r_q | nlm \rangle$, using Wigner-Eckart theorem and replacing T_q^1 with r_q

$$\langle n'l'm' | r_q | nlm \rangle = \langle n'l' || r || nl \rangle \langle l'm' | l, 1, mq \rangle$$

We can simply choose $q = 0$ to calculate $\langle n'l' || r || nl \rangle$, since $r_0 = z = r \cos \theta$

After calculation, divide the integral by the CG coefficient (but we have to make sure that the CG coefficient is not 0)

Application 2 — Simplification of Calculation

Electron dipole transition

For example, we want to calculate $\langle 32m' | r_q | 21m \rangle$ (2p to 3d transition)

We can start from $\langle 320 | z | 210 \rangle$:

$$\begin{aligned} \langle 320 | z | 210 \rangle &= \int \psi_{320}(\mathbf{r}) r \cos \theta \psi_{210}(\mathbf{r}) d^3 \mathbf{r} \\ &= \int R_{32}^*(r) r R_{21}(r) r^2 dr \int Y_2^0(\theta, \phi)^* \cos \theta Y_1^0(\theta, \phi) d\Omega = \frac{2^{12} 3^3 \sqrt{3}}{5^7} a \\ &= \langle 32 || r || 21 \rangle \langle 20 | 1, 1, 00 \rangle = \sqrt{\frac{2}{3}} \langle 32 || r || 21 \rangle \end{aligned}$$

Application 2 — Simplification of Calculation

Therefore

$$\langle 32||V||21\rangle = \frac{2^{12}3^4}{5^7\sqrt{2}} a$$

Now, we can obtain other matrix elements easily.

For example,

$$\langle 321|z|211\rangle = \langle 21|1110\rangle\langle 32||r||21\rangle = \frac{1}{\sqrt{2}}\langle 32||r||21\rangle$$

$$\langle 322|r_1|211\rangle = \langle 22|1111\rangle\langle 32||r||21\rangle = \langle 32||r||21\rangle$$

Note that

$$r_1 = -\frac{x + iy}{\sqrt{2}} \quad r_{-1} = \frac{x - iy}{\sqrt{2}} \quad r_0 = z$$

Application 3 — Zeeman Effect

Weak-Field Zeeman Effect

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

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

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

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

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

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

Reference

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Thank you!