Lect 7: Wigner - Eckart theorem, direct product Rep and, C-G coefficient, projection operator, etc

Definition: Consider an irreducible representation $D^j(G)$ for a group G. If there exists a set of wavefunctions $\psi^j_{\mu r}$ which transform under operation $g \in G$ as

$$g \psi^j_{\mu r} = \sum_\nu \psi^j_{\nu r} D^j_{\nu\mu}(g),$$

then we say $\psi^j_{\mu r}$ belonging to the μ-th basis of representation D^j. r is an index to distinguish different sets of basis belonging to the same representation.

Theorem (Wigner-Eckart) Consider two wavefunctions $\psi^j_{\mu r}$ and $\phi^k_{\rho r'}$ belonging to the μ-th basis of D^j and ρ-th basis of D^k, respectively.

Then $\langle \phi^k_{\rho r} | \psi^j_{\mu r'} \rangle = \delta_{kj} \delta_{\rho\mu} \langle kr || jr' \rangle$

where $\langle kr || jr' \rangle$ is a number only depending on representations but not on the basis index ρ and μ.

Proof: we define $\langle \phi^k_{\rho r} | \psi^j_{\mu r'} \rangle = X^{kj}_{\rho\mu}$ and treat it as a matrix with row and column indices $\rho\mu$. We prove $X^{kj} D^j(g) = D^k(g) X^{kj}$ for $\forall g \in G$, then we can arrive at the conclusion via Schur's lemma.

$$\langle \phi^k_{\rho r} | g \psi^j_{\mu r'} \rangle = \sum_\nu \langle \phi^k_{\rho r} | \psi^j_{\nu r'} \rangle D^j_{\nu\mu}(g) = \sum_\nu X^{kj}_{\rho\nu} D^j_{\nu\mu}$$

$$\|$$

$$\langle g^{-1} \phi^k_{\rho r} | \psi^j_{\mu r'} \rangle = \sum_\lambda \left(D^k_{\lambda\rho}(g^{-1}) \right)^* \langle \phi^k_{\lambda r} | \psi^j_{\mu r'} \rangle = \sum_\lambda D^k_{\rho\lambda}(g) \langle \phi^k_{\lambda r} | \phi^j_{\mu r'} \rangle$$

$$= \sum_\lambda D^k_{\rho\lambda} X^{kj}_{\lambda\mu}$$

hence $X^{kj} D^j(g) = D^k(g) X^{kj}$ for $\forall g \in G$

According to Schur's theorem, we have $X^{kj} = 0$ if $k \neq j$.

If $k = j$, then X^{kj} is a constant matrix, i.e $X^{kj}_{\rho\mu} = \delta_{\rho\mu} \delta_{kj} \langle kr \| jr' \rangle$.

☆ representations by using operators

We have discussed extensively how to make representation by using wavefunctions. If there exist a set of opearators $\hat{O}^j_\mu$ transform under $g \in G$ as

$$g \hat{O}^j_\mu g^{-1} = \sum_\nu \hat{O}^j_\nu D^j_{\nu\mu}(g),$$

then we say $\hat{O}^j_\mu$ belonging to the μ-th basis of the rep D^j.

Example: irreducible (spherical) tensor operators in QM.

For example $r_1 = -\frac{1}{\sqrt{2}}(x+iy)$ $r_0 = z$ $r_{-1} = \frac{1}{\sqrt{2}}(x-iy)$

$$g \rightarrow e^{-i\vec{L}\cdot\hat{n}\theta}$$

$$\Rightarrow \boxed{g\, r_m\, g^{-1} = \sum_{m'} r_{m'} D^{j=1}_{m'm}(g)}$$

⊛ Decomposition of direct product of representations

Consider two coupled systems ⟶ one big system, say a 2-particle system.

$$H = H_1(\vec{r}) + H_2(\vec{r}\,') + H_{12}(\vec{r}, \vec{r}\,')$$

say $H_1(\vec{r})$, $H_2(\vec{r}\,')$ has rotation symmetry with respect to r, r', respectively.

and $H_{12}(\vec{r}, \vec{r}\,') \propto \vec{r} \cdot \vec{r}\,'$ is only invariant under the simultaneous rotation of $\vec{r}$ and $\vec{r}\,'$. The rotation group for the combined system $g_i = g_{1i} \cdot g_{2i}$. Please note that the "$i$" means the same operation for systems 1 and 2. Suppose $\varphi^i_\mu(r)$ and $\psi^j_\nu(r')$ belong to representations D^i and D^j for systems 1 and 2, seperately.

Then $\boxed{\Psi^{i\times j}_{\mu\nu} = \varphi^i_\mu(r)\, \psi^j_\nu(r')}$ is also a representation of $G = \{g_i = g_{1i} \cdot g_{2i}\}$. G is isomorphic to G_1 and G_2.

This representation $\boxed{D^{i\times j}_{\mu\nu,\mu'\nu'}(g_i) = D^i_{\mu\mu'}(g_{1i})\, D^i_{\nu\nu'}(g_{2i})}$

↗ **Direct product representation, its character**

$$\chi^{i\times j}(g_i) = \chi^i(g_{1i}) \cdot \chi^j(g_{2i})$$

We can use the character table to decompose $D^{i\times j}$.

Since $\{g_i\}$ is isomorphic to $\{g_{1i}\}$ and $\{g_{2i}\}$, we do not view them as different groups. For example, $\{g_i\}$ is associated with the total angular momentum, while $\{g_{1i}\}$ and $\{g_{2i}\}$ are for subsystems 1 and 2

$$X^{-1} D^{i}(g) \otimes D^{j}(g) X = \bigoplus_J a_J D^J(g)$$

§ Clebash – Gorden coefficient for D_3 group

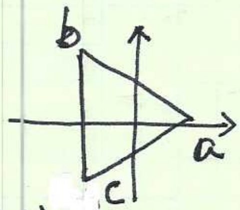
D_3 has A_1, A_2 and E-representations. We have

$$\begin{cases} A_1 \otimes A_1 = A_1 \\ A_1 \otimes A_2 = A_2 \\ A_1 \otimes E = E \\ A_2 \otimes E = E \end{cases}$$

we can focus on $E \otimes E$.

	E	$2C_3$	$3C_2'$
$\chi(E\otimes E)$	4	1	0

Hence $E \otimes E \sim A_1 \oplus A_2 \oplus E$



If we use the basis $|\psi^E_+\rangle = \frac{1}{\sqrt{3}} (|a\rangle + \omega |b\rangle + \omega^2 |c\rangle)$

$$|\psi^E_-\rangle = \frac{1}{\sqrt{3}} (|a\rangle + \omega^2 |b\rangle + \omega |c\rangle)$$

In which $E: \begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$, $R_z(\frac{2\pi}{3}): \begin{pmatrix} e^{-i\frac{2}{3}\pi} & 0 \\ 0 & e^{i\frac{2}{3}\pi} \end{pmatrix}$, $R_x(\pi) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, etc.

we can use the angular momentum around the z-axis to guide the decomposition

$|\psi^E_+(1)\rangle \otimes |\psi^E_-(2)\rangle$ and $|\psi^E_-(1)\rangle \otimes |\psi^E_+(2)\rangle$ both have $L_z \equiv 0 \pmod 3$

Hence, they belong to A-representations, Now perform $R_x(\pi)$.

Then $R_x(\pi) [\psi^E_+(1) \otimes |\psi^E_-(2)\rangle] = |\psi^E_-(1)\rangle \otimes |\psi^E_+(2)\rangle$

and $R_x(\pi) [|\psi^E_-(1)\rangle \otimes |\psi^E_+(2)\rangle] = |\psi^E_+(1)\rangle \otimes |\psi^E_-(2)\rangle$

$\Rightarrow$ for A_1-rep, which is even under $R_x(\pi)$, we have

$$|\psi^{A_1}\rangle = \frac{1}{\sqrt{2}} [|\psi^E_+(1)\rangle \otimes |\psi^E_-(2)\rangle + |\psi^E_-(1)\rangle \otimes |\psi^E_+(2)\rangle]$$

for A_2-rep, which is odd $\Rightarrow |\psi^{A_2}\rangle = \frac{1}{\sqrt{2}} [|\psi^E_+(1)\rangle \otimes |\psi^E_-(2)\rangle - |\psi^E_-(1)\rangle \otimes |\psi^E_+(2)\rangle]$

As for E-rep: we have: $|\psi_-^E(1)\rangle \otimes |\psi_-^E(2)\rangle$, it $L_z = -2 \equiv 1 \pmod 3$

$|\psi_+^E(1)\rangle \otimes |\psi_+^E(2)\rangle$ $\quad L_z = 2 \equiv -1 \pmod 3$

$$\Rightarrow \boxed{\begin{aligned} |\psi_+^E\rangle &= |\psi_-^E(1)\rangle \otimes |\psi_-^E(2)\rangle \\ |\psi_-^E\rangle &= |\psi_+^E(1)\rangle \otimes |\psi_+^E(2)\rangle \end{aligned}}$$

For the general case of direct product of D_N's representations, we leave it for exercises.

§: direct product representation and its decomposition for T group

T has A, E, E' → three 1d representations.

$A \otimes E = E$, $A \otimes E' = E'$, $A \otimes T = T$

$E \otimes E' = A$, $E \otimes T = T$, $E' \otimes T = T$

Check $T \otimes T$:

	E	$3T^2$	$4R$	$4R^2$
$\chi(T\otimes T)$:	9	1	0	0

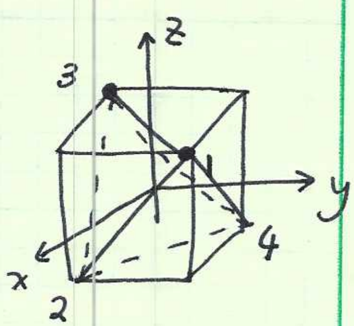
then we have $T \otimes T \sim A \oplus E \oplus E' \oplus T \oplus T$

Remember for T-rep

$|\psi_x\rangle = \frac{1}{2}[|1\rangle + |2\rangle - |3\rangle - |4\rangle] \to x$

$|\psi_y\rangle = \frac{1}{2}[|1\rangle - |2\rangle - |3\rangle + |4\rangle] \to y$

$|\psi_z\rangle = \frac{1}{2}[|1\rangle - |2\rangle + |3\rangle - |4\rangle] \to z$



under this basis

$E: \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$, $T_z^2 \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$ $R_1: \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

Now consider two electrons filling in T-orbit, we have 9 possible basis.

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0 A: $x^2+y^2+z^2$. $\frac{1}{\sqrt{3}}\{|\psi_x(1)\rangle\otimes|\psi_x(2)\rangle+|\psi_y(1)\rangle\otimes|\psi_y(2)\rangle+|\psi_z(1)\rangle\otimes|\psi_z(2)\rangle\}$

1 T: $|\psi_z\rangle = \frac{1}{\sqrt{2}}[|\psi_x(1)\rangle\otimes|\psi_y(2)\rangle - |\psi_y(1)\rangle\otimes|\psi_x(2)\rangle]$

$|\psi_x\rangle = \frac{1}{\sqrt{2}}(|\psi_y(1)\rangle\otimes|\psi_z(2)\rangle - |\psi_z(1)\rangle\otimes|\psi_y(2)\rangle]$

$|\psi_y\rangle = \frac{1}{\sqrt{2}}[|\psi_z(1)\rangle\otimes|\psi_x(2)\rangle - |\psi_x(1)\rangle\otimes|\psi_z(2)\rangle]$

2 T $|\psi'_z\rangle = \frac{1}{\sqrt{2}}[|\psi_x(1)\rangle\otimes|\psi_y(2)\rangle + |\psi_y(1)\rangle\otimes|\psi_x(2)\rangle] \to xy$

$|\psi'_x\rangle = \frac{1}{\sqrt{2}}[|\psi_y(1)\rangle\otimes|\psi_z(2)\rangle + |\psi_z(1)\rangle\otimes|\psi_y(2)\rangle]$ yz

$|\psi'_y\rangle = \frac{1}{\sqrt{2}}[|\psi_z(1)\rangle\otimes|\psi_x(2)\rangle + |\psi_x(1)\rangle\otimes|\psi_z(2)\rangle]$ zx

E: . $\frac{1}{\sqrt{3}}[|\psi_z(1)\rangle\otimes|\psi_z(2)\rangle + \omega^2|\psi_x(1)\rangle\otimes|\psi_x(2)\rangle + \omega|\psi_y(1)\rangle\otimes|\psi_y(2)\rangle$

E': $\frac{1}{\sqrt{3}}[|\psi_z(1)\rangle\otimes|\psi_z(2)\rangle + \omega|\psi_x(1)\rangle\otimes|\psi_x(2)\rangle + \omega^2|\psi_y(1)\rangle\otimes|\psi_y(2)\rangle]$

complex time-reversal symmetry breaking states

superposition of x^2-y^2, $x^2+y^2-2z^2$

§ <u>direct product of the representations of the O group</u>

O group has a D_2 invariant subgroup, and $O/D_2 \sim D_3$.

The A_1, A_2 and E representations of O, can also be viewed as the Rep. of D_3 group, hence their direct product can be decomposed according to the D_3's representation.

$A_1 \otimes T_1 = T_1$, $A_1 \otimes T_2 = T_2$, $A_2 \otimes T_1 = T_2$, $A_2 \otimes T_2 = T_1$

check $E \otimes T_1$:

	E	$3C_4^2$	$8C_3'$	$6C_4$	$6C_2''$
$\chi(E\otimes T_1)$	6	-2	0	0	0
$\chi(E\otimes T_2)$	6	-2	0	0	0

$\rightarrow E \otimes T_1 = T_1 \oplus T_2$

$E \otimes T_2 \simeq T_2 \oplus T_1$

$T_1 \otimes T_1 \simeq T_2 \otimes T_2 \simeq A_1 \oplus E \oplus T_1 \oplus T_2$

$T_1 \otimes T_2 \simeq A_2 \oplus E \oplus T_1 \oplus T_2$

	E	$3C_4^2$	$8C_3'$	$6C_4$	$6C_2''$
$\chi(T_1\otimes T_1)$, $\chi(T_2\otimes T_2)$	9	1	0	1	1
$\chi(T_1\otimes T_2)$	9	1	0	-1	-1

⊗ Projection operaters

Let us begin with $g\psi^j_{\nu'} = \sum_{\mu'} \psi^j_{\mu'} D^j_{\mu'\nu'}(g)$.

$$[D^i(g)^{-1}]_{\nu\mu}\, g\psi^j_{\nu'} = \sum_{\mu'} \psi^j_{\mu'} D^j_{\mu'\nu'}(g)\, [D^i(g^{-1})]_{\nu\mu}$$

$$\sum_g D^{i,*}_{\mu\nu}(g)\, g\psi^j_{\nu'} = \sum_{\mu'} \psi^j_{\mu'} \underbrace{\sum_g D^{i,*}_{\mu\nu}(g) D^j_{\mu'\nu'}(g)}_{\nwarrow\ \frac{|G|}{m_i}}$$

$$= \sum_{\mu'} \psi^j_{\mu'} \delta_{ij} \delta_{\mu\mu'} \delta_{\nu\nu'} \frac{|G|}{m_i}$$

$$= \psi^j_\mu \delta_{ij} \delta_{\nu\nu'} |G|/m_i$$

$$\Rightarrow \left[\frac{m_i}{|G|} \sum_g D^{i,*}_{\mu\nu}(g)\cdot g\right] \psi^j_{\nu'} = \psi^i_\mu \delta_{ij} \delta_{\nu\nu'}$$

defin $P^i_{\mu\nu} = \frac{m_i}{|G|} \sum_g D^{i,*}_{\mu\nu}(g)\cdot g \Rightarrow P^i_{\mu\nu} \psi^j_{\nu'} = \delta_{ij} \delta_{\nu\nu'} \psi^i_\mu$

If we begin with a general state $\psi = \sum_{j\nu'} C^j_{\nu'} \psi^j_{\nu'}$

then $P^i_{\mu\mu}\psi = \sum_{j\nu'} C^j_{\nu'} P^i_{\mu\mu}\psi^j_{\nu'} = \sum_{j\nu'} C^j_{\nu'} \delta_{ij}\delta_{\mu\nu'}\psi^i_{\mu}$

$= C^i_\mu \psi^i_\mu \leftarrow$ $P^i_{\mu\mu}$: projector operator

$P^i_{\mu\nu}\psi = \sum_{j\nu'} C^j_{\nu'} P^i_{\mu\nu}\psi^j_{\nu'} = \sum_{j\nu'} C^j_{\nu'} \delta_{ij}\delta_{\nu\nu'}\psi^i_\mu = C^i_\nu \psi^i_\mu$

↑ transfer operator

we have
$$P_{nm}P_{\ell k} = \delta_{m\ell}P_{nk}.$$
$$P_{nn}P_{mm} = \delta_{mn}P_{nn}.$$

we can also define the projection operator to a subspace.

$$P^i = \sum_\mu P^i_{\mu\mu} = \frac{m_i}{|G|}\sum_g \chi^i(g)^* g$$

we can start with any function ψ that is not orthogonal to the representation

$$\varphi^i_\mu = P^i_{\mu\nu}\psi$$ ← transform according to $D^i_{\mu\nu}(g)$

If only the character table is known, we apply $P^i\psi$, then we produce some function in the irreducible space i. We can choose another function ψ' and do $P^i\psi'$, and repeat this process until we have enough number of linearly independent basis.

Suppose we already have a set of basis functions $|\psi^i_\mu\rangle$, we can form another set of basis functions $|\varphi^i_\mu\rangle$ with the same transformation property starting from an arbitary function $|\psi\rangle$.

$$\frac{m_i}{|G|}\sum_g g\left(|\psi\rangle\langle\psi^i_\mu|\right) = \sum_\mu |\phi^i_\mu\rangle\langle\psi^i_\mu|, \text{ where } |\phi^j_\mu\rangle = P^i_{\mu\nu}|\psi\rangle$$

Proof $\quad g(|\psi\rangle\langle\psi^j_\mu|) = (g|\psi\rangle)(g|\psi^j_\nu\rangle)^\dagger$

$$g|\psi^j_\nu\rangle = \sum_\mu |\psi^j_\mu\rangle D^j_{\mu\nu}(g) \Rightarrow (g|\psi^j_\nu\rangle)^\dagger = \sum_\mu D^{*,j}_{\mu\nu}(g)\langle\psi^j_\mu|$$

$$\Rightarrow g(|\psi\rangle\langle\psi^j_\mu|) = \sum_\mu D^{*,j}_{\mu\nu}(g)\, g\,|\psi\rangle\langle\psi^j_\mu|$$

$$\Rightarrow \frac{m_i}{|G|}\sum_g g\left(|\psi\rangle\langle\psi^i_\mu|\right) = \sum_\mu \underbrace{\frac{m_i}{|G|}\sum D^{*,j}_{\mu\nu}(g)\, g}_{P^j_{\mu\nu}}\,|\psi\rangle\langle\psi^i_\mu|$$

$$= \sum_\mu \underbrace{P^j_{\mu\nu}|\psi\rangle}\langle\psi^i_\mu|$$

$$= \sum_\mu \underbrace{|\phi^j_\mu\rangle}\langle\psi^i_\mu|$$

we can arrive at $|\phi^j_\mu\rangle$ as the coefficent of $\langle\psi^i_\mu|$

with $|\phi^j_\mu\rangle = P^j_{\mu\nu}|\psi\rangle$.

★ Crystal harmonics (under cubic group)

C_4^2: $x \to -x$, $y \to -y$, $z \to z$

C_3^1 $x \to y$, $y \to z$, $z \to x$

C_4: $x \to y$, $y \to -x$, $z \to z$

C_2'' $x \to y$, $y \to x$, $z \to -z$

$l=0$ $\quad 1 \quad A_1$

$l=1$ $\quad x, y, z \quad T_1$

$l=2$ $\quad \underbrace{xy,\ yz,\ zx}_{T_2} \quad \underbrace{\frac{3z^2-r^2}{2\sqrt{3}},\ \frac{x^2-y^2}{2}}_{E}$

$l=3$ $\quad \underbrace{xyz}_{A_2}, \quad \underbrace{\frac{z(5z^2-3r^2)}{2\sqrt{15}},\ \frac{x(5x^2-3r^2)}{2\sqrt{15}},\ \frac{y(5y^2-3r^2)}{2\sqrt{15}}}_{T_1}$

$$\underbrace{\frac{z(x^2-y^2)}{2},\ \frac{x(y^2-z^2)}{2},\ \frac{y(z^2-x^2)}{2}}_{T_2}$$

$l=4$

A_1 # $5(x^4+y^4+z^4)-6r^4$

T_1: $xy(x^2-y^2)$, $yz(y^2-z^2)$, $zx(z^2-x^2)$

T_2: $\frac{xy(7z^2-r^2)}{\sqrt{7}}$ $\frac{yz(7x^2-r^2)}{\sqrt{7}}$ $\frac{zx(7y^2-r^2)}{\sqrt{7}}$

E: $\underbrace{\frac{(x^2-y^2)(7z^2-r^2)}{2\sqrt{7}},\ \frac{(y^2-z^2)(7x^2-r^2)}{2\sqrt{7}},\ \frac{(z^2-x^2)(7y^2-r^2)}{2\sqrt{7}}}_{\text{only 2 are independent}}$

example: C_{3v} : $\{E, C_3^1, C_3^2, \sigma, C_3\sigma, C_3^2\sigma\}$ → σ: reflection with respect to y

The polar vector Rep $\Gamma_1^- = (x, y, z)$ is decomposed to $E = (x, y)$ and $A_1 = z$

If we want to use quadratic polynomials to form the E-representation

Let's choose $|\psi\rangle = 2xy$, then

$$\frac{m_E}{|G|} \sum_g g\,|\psi\rangle\langle X| = \frac{2}{6}(E + C_3^1 + C_3^2 + \sigma + C_3\sigma + C_3^2\sigma)\,|2xy\rangle\langle X|$$

Since $\sigma x = -x$, $\sigma y = y$ $\Rightarrow$ $\frac{2}{6} \times 2 \times 2\,(E + C_3 + C_3^2)\,|xy\rangle\langle X|$

$$= \frac{4}{3}\Big\{|xy\rangle\langle X| + \Big|\Big(-\frac{x}{2} - \frac{\sqrt{3}}{2}y\Big)\Big(\frac{\sqrt{3}}{2}x - \frac{1}{2}y\Big)\Big\rangle\Big\langle -\frac{X}{2} - \frac{\sqrt{3}}{2}Y\Big|$$

$$+ \Big|\Big(-\frac{x}{2} + \frac{\sqrt{3}}{2}y\Big)\Big(-\frac{\sqrt{3}}{2}x - \frac{1}{2}y\Big)\Big\rangle\Big\langle -\frac{X}{2} + \frac{\sqrt{3}}{2}Y\Big|\Big\}$$

$$= |2xy\rangle\langle X| + |x^2 - y^2\rangle\langle Y|$$

hence $[2xy, x^2 - y^2]$ transform the same as (x, y) under the E-representation.

⊙ or we use $(E \otimes E) = A_1 \oplus A_2 + E$, and A_1 and E are symmetric

since $E = (x, y)$, $E \otimes E \sim (x^2, xy, y^2)$. obviously $x^2 + y^2 \sim A_1$

hence we have $[2xy, a(x^2 - y^2)]$, in which a is a coefficient to be determined.

$$C_3(2xy) = 2\Big(-\frac{x}{2} - \frac{\sqrt{3}}{2}y\Big)\Big(\frac{\sqrt{3}x}{2} - \frac{y}{2}\Big) = -\frac{\sqrt{3}}{2}x^2 + \frac{\sqrt{3}}{2}y^2 - xy$$

$$= -\frac{1}{2}(2xy) - \frac{\sqrt{3}}{2}a(x^2 - y^2) \Rightarrow a = 1$$