Theorem of orthonormal basis

$D_i : G \to L(\mathcal{H})$

$D_j : G \to L(\mathcal{H})$

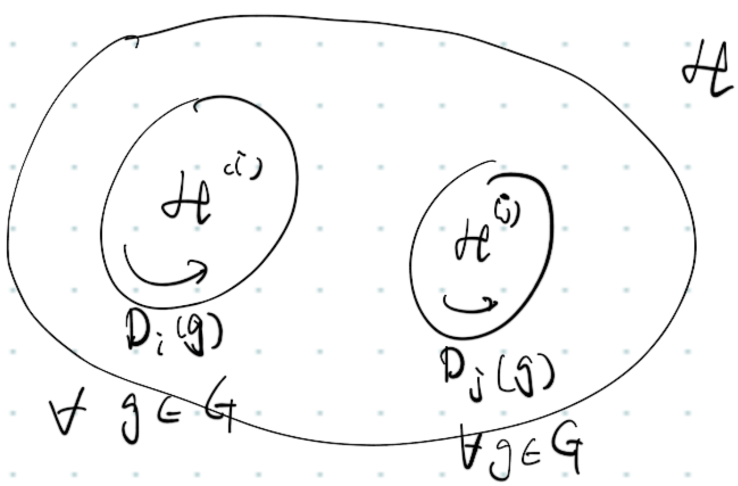
D_i, D_j are unitary irrep

if D_i, D_j are inequivalent

$\Rightarrow \ \exists \ \mathcal{H}^{(i)} \subset \mathcal{H} \quad D_i : G \to L(\mathcal{H}^{(i)})$

$\qquad \mathcal{H}^{(j)} \subset \mathcal{H} \quad D_j : G \to L(\mathcal{H}^{(j)})$

and $\underline{\underline{\mathcal{H}^{(i)} \perp \mathcal{H}^{(j)}}}$



inequivalent unitary irreps are carried by mutually orthogonal subspaces in $\mathcal{H}$

Theorem (orthogonality of matrix elements)

Let's assume G to be a finite group, i.e., G has only a finite number of elements

$$\left.\begin{aligned} D^{(i)} &: G \to L(\mathcal{H}^{(i)}) \\ D^{(j)} &: G \to L(\mathcal{H}^{(j)}) \end{aligned}\right\} \text{unitary irrep.}$$

$f^{(i)}_{\alpha = 1 \cdots \dim(\mathcal{H}^{(i)})}$ orthogonal basis in $\mathcal{H}^{(i)}$

$f^{(j)}_{\beta = 1 \cdots \dim(\mathcal{H}^{j})}$ orthogonal basis in $\mathcal{H}^{(j)}$

$$\langle f^{(i)}_\alpha | f^{(j)}_\beta \rangle = \delta^{ij} \delta_{\alpha\beta} \, r$$

constant.

matrix elements of rep.

functions on G (rep. functions)
$$\begin{cases} D^{(i)}_{\alpha\beta}(g) = \langle f^{(i)}_\alpha | D^{(i)}(g) | f^{(i)}_\beta \rangle \\ D^{(j)}_{\alpha\beta}(g) = \langle f^{(j)}_\alpha | D^{(j)}(g) | f^{(j)}_\beta \rangle \end{cases}$$

orthogonality of rep. functions

$$\sum_{g \in G} D^{(i)}_{\alpha\delta}(g)^{*} D^{(j)}_{\beta\gamma}(g) = \delta_{ij}\delta_{\alpha\beta}\delta_{\delta\gamma} \frac{h}{\dim(\mathcal{H}^{(i)})}$$

rank of the group

Lie group (infinite group)

$$\sum_{g \in G} \to \int_G dg$$

<u>Character</u> : group G, rep D : $G \to L(\mathcal{H})$

$$g \mapsto D(g) \in L(\mathcal{H})$$

character : $\chi(g) = \mathrm{tr}(D(g))$

$$= \sum_{\alpha} D_{\alpha\alpha}(g)$$

properties : (1) conjugacy class : group conjugate :

$|$ $\quad g \mapsto hgh^{-1} \quad \forall\, g, h \in G$

obit of group conjugate

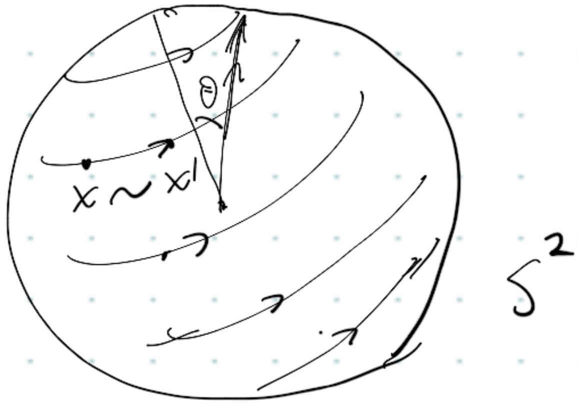
$g \to$ obit of hgh^{-1}

$\{hgh^{-1} \mid \forall h \in G\}$

$$\chi(g) \to \chi(hgh^{-1}) = \mathrm{tr}(D(hgh^{-1}))$$
$$= \mathrm{tr}(D(h)D(g)D(h^{-1}))$$
$$= \mathrm{tr}(\underline{D(h)}D(g)\underline{D(h)^{-1}})$$
$$= \mathrm{tr}(D(g)) = \chi(g)$$

i.e. $\chi(g)$ inv. under conjugate

χ is function of conjugacy classes in G



an orbit = a circle with const. θ

= one class.

$\{\text{classes}\} = \{\text{orbits}\}$

$= [0, \pi]$

$f(\theta, \varphi)$

$\underline{\underline{\cos\theta}}$ is a function of $\theta \in [0,\pi]$

is a function of classes (orbits)

2) unitary reps D' is equivalent to D

$$\forall g \in G, \ D'(g) = U D(g) U^{-1} \qquad U: \mathcal{H} \to \mathcal{H} \text{ unitary}$$

$$\chi'(g) = \operatorname{tr} D'(g) = \operatorname{tr}\left(U D(g) U^{-1}\right)$$

$$= \operatorname{tr} D(g) = \chi(g)$$

equivalent reps have the same charater.

3) reducible rep. $D = D_1 \oplus D_2 \oplus \cdots$

$$\forall g \in G \quad \chi(g) = \mathrm{tr}\, D(g) = \sum_i \mathrm{tr}\, D_i(g) = \sum_i \chi_i(g)$$

$$D(g) = \begin{pmatrix} \boxed{D_1(g)} & & 0 \\ & \boxed{D_2(g)} & \\ 0 & & \ddots \end{pmatrix}$$

charater of reducible rep = sum of characters of irreps.

<u>Theorem (orthogonality of χ)</u>

(1) G finite group, $D^{(i)}$, $D^{(j)}$ irrep, then

$$\underbrace{\sum_{g \in G} \chi^{(i)}(g)^* \chi^{(j)}(g)}_{\parallel} = h\, \delta^{ij}$$

↑ rank of the group.

$$\sum_{C \in \binom{\text{conjugacy}}{\text{classes}}} h_C\, \chi^{(i)}(C)^* \chi^{(j)}(C)$$

h_C = # of elements in conjugacy class C.

(2) $D^{(i)}$ irrep of G (finite group)

$i \in I \leftarrow$ set of all irreps of G.

$$\sum_{i \in I} \chi^{(i)}(C_l)^* \chi^{(i)}(C_m) = \frac{h}{h_l} \delta_{lm}$$

lth conjugacy class

h_l : # of elements in C_l

<u>symmetries of Schrödinger eqn</u>

Let G be the symmetry group of the system

i.e. $\forall g \in G$, $D(g)$: unitary transf. on $\mathcal{H}$

(D ; unitary rep G, carried by $\mathcal{H}$)

s.t. $\underline{D(g)\hat{H}D(g)^{-1} = \hat{H}}$ $\quad \forall g \in G$

eigen-eqn of $\hat{H}$ $\quad \hat{H}|\psi_{ni}\rangle = E_n|\psi_{ni}\rangle$

$i = 1 \cdots d(n)$

$d(n)$: degeneracy of energy level E_n

$\{\psi_{ni}\}_{i=1\cdots d(n)}$ span the $\underbrace{\text{eigen space}}_{\mathcal{H}^{(n)}}$ of $\hat{H}$ at the eigenvalue E_n

$$|\psi_{ni}\rangle \rightarrow D(g)|\psi_{ni}\rangle \equiv |\psi'_{ni}\rangle \quad \forall g \in G$$

$$\underline{\hat{H} D(g)|\psi_{ni}\rangle} = D(g)\hat{H}|\psi_{ni}\rangle = \underline{E_n D(g)|\psi_{ni}\rangle}$$

$D(g)|\psi_{ni}\rangle$ belongs to the eigenspace $\mathcal{H}^{(n)}$

($D(g)$ leaves $\mathcal{H}^{(n)}$ inv) $\forall g \in G$

$\{|\psi_{ni}\rangle\}_{i=1\cdots d(n)}$ basis in $\mathcal{H}^{(n)}$

$$D(g)|\psi_{ni}\rangle = \sum_j |\psi_{nj}\rangle D^{(n)}_{ji}(g)$$

rep matrix.

Any eigenspace $\mathcal{H}^{(n)}$ of $\hat{H}$ is a rep space of the

Symmetry group

$$\mathcal{H} = \bigoplus_{n=1}^{\infty} \mathcal{H}^{(n)}$$

$$D = \bigoplus_{n=1}^{\infty} D^{(n)}$$

$(\mathcal{H}, D)$ is a reducible rep of G.

<u>Example</u> (1) central potential $\hat{H} = \frac{\hat{p}^2}{2m} + \underline{V(r)}$

rotational inv.

$$\boxed{G = SO(3)}$$

group of 3d rotations.

on the hand, $\hat{H}\psi_{nlm}(r,\theta,\varphi) = E_{nl}\,\psi_{nlm}(r,\theta,\varphi)$

$$\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)\,Y_{lm}(\theta,\varphi)$$

spherical harmonics

$l = 0, 1, 2 \ldots$

$m = -l, -l+1 \ldots l$

eigenspace $\underline{\underline{\mathcal{H}^{(n,l)}}}$ is spanned by $\{Y_{lm}\}_{m=-l \dots l}$

$$\underline{\dim \mathcal{H}^{(n,l)} = 2l+1}$$

$\underline{\underline{\mathcal{H}^{(n,l)}}}$ are irrep. of $G = SO(3)$

all irreps of $SO(3)$ are $(\mathcal{H}_l, D_l)$

s.t. $\dim \mathcal{H}_l = 2l+1$

$\{ |l, m\rangle \}_{m=-l,\dots,l}$ spans $\mathcal{H}_l$ carrier space of irrep of $SO(3)$

(2) hydrogen atom : $\hat{H} = \frac{\hat{p}^2}{2m} - \frac{e^2}{r}$

$$\hat{H} \psi_{nlm}(r,\theta,\varphi) = E_{\underline{\underline{n}}} \psi_{n\underline{\underline{lm}}}(r,\theta,\varphi)$$

$$\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r) \overline{Y_{lm}(\theta,\varphi)}$$

eigenspace $\mathcal{H}^{(n)}$ is spanned by $\{ R_{nl}(r) Y_{lm}(\theta,\varphi) \}$

$l = 0, 1 \dots n-1$

$m = -l \dots l$

$$\dim \mathcal{H}^{(n)} = \sum_{l=0}^{n-1} (2l+1) = n^2$$

$$\rightarrow \mathcal{H}^{(n)} = \bigoplus_{l=0}^{n-1} \mathcal{H}^{(n,l)} \qquad \dim(\mathcal{H}^{(n,l)}) = 2l+1$$

$\mathcal{H}^{(n)}$: reducible rep of $SO(3)$

$\mathcal{H}^{(n,l)}$: irrep of $SO(3)$

for any system, for any eigenspace $\mathcal{H}^{(n)}$ of the hamiltonian, there exists a symmetry group G, s.t. $\mathcal{H}^{(n)}$ is an irrep of G

for hydrogen atom, $G \neq SO(3)$

we expect there is a larger group $G \supset SO(3)$

$H \subset G$, H is a subgroup.

any irrep D of G is also a rep. D' of H

D' may be a reducible rep of H.

$$SO(4) \quad \text{is local}$$

hydrogen atom has a larger symmetry group $G \simeq Spin(4) \supset SO(3)$

(dynamical symmetrie)

there exists hidden symmetry of $\hat{H}$,

reverse procedure, reduce the symmetry $\cancel{G} \to G_{small}$

by adding perturbations to $\hat{H}$

$\mathcal{H}^{(n)}$ irrep of $G \supset G_{small}$

$$\mathcal{H}^{(n)} = \mathcal{H}_1^{(n)} \oplus \mathcal{H}_2^{(n)} \oplus \cdots$$

$\mathcal{H}^{(n)}$: reducible rep of G_{small}

$\mathcal{H}_1^{(n)}$: irrep of G_{small}

$$\hat{H} \to \hat{H}_{new} = \hat{H}_0 + \hat{H}'$$

G

$\hat{H}'$: perturbation

$$E_n \to E_n + \Delta E_{ni}$$

ΔE_{ni}: different values at $\mathcal{H}_i^{(n)}$

$$\hat{H}_{new} |\psi_{ni}\rangle = (E_n + \Delta E_{ni}) |\psi_{ni}\rangle$$

$$|\psi_{ni}\rangle \in \mathcal{H}_i^{(n)}$$

---

the total Hilbert space $\mathcal{H}$, $\hat{H}_0$, E_n,

degeneracy at E_n : $d(n)$,

symmetry of $\hat{H}_0$: G, i.e $\forall g \in G$

$$\underline{\underline{D(g)}} \hat{H}_0 D(g)^{-1} = \hat{H}_0$$

let's assume eigenspace $\mathcal{H}^{(n)}$ of E_n is an irrep of G

add perturbation : $\hat{H} = \hat{H}_0 + \hat{H}'$

- if $\hat{H}'$ doesn't break the symmetry, i.e. $\forall g \in G$,

  $D(g) \hat{H}' D(g')^{-1} = \hat{H}' \Rightarrow D(g) \hat{H} D(g)^{-1} = \hat{H}$

  energy level $E_n \to E_n + \Delta E_n$

  but degeneracy $d(n)$ must unchange,

because the eigenspace $\mathcal{H}^{(n)}$ must still be the irrep of G

$\rightarrow \dim(\mathcal{H}^{(n)})$ is fixed

- more generally, $\hat{H}'$ may break some symmetry

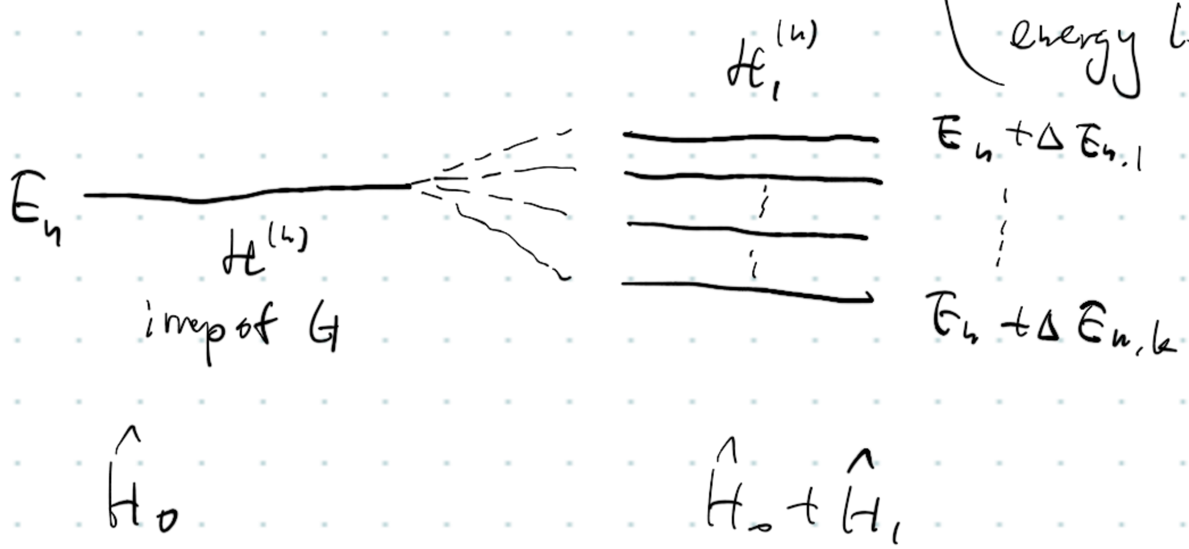
i.e., $\exists g \in G$, s.t. $D(g)\hat{H}' D(g)^{-1} \neq \hat{H}'$

G is broken into subgroup $G_{new} < G$

irrep of G : $\underset{\substack{\uparrow \\ \text{eigenspace of } \hat{H}_0}}{\mathcal{H}^{(n)}} = \bigoplus_{i=1}^{k_n} \underset{\substack{\uparrow \\ \text{irreps of } G_{new}}}{\underline{\mathcal{H}_i^{(n)}}}$

irreps of G_{new} = eigenspace of $\hat{H} = \hat{H}_0 + \hat{H}'$

(correspond to different energy levels)



splitting of energy levels predicted by group theory.

splitting of the energy level,

each new energy level has smaller degeneracy

Example : an atom in a crystal.

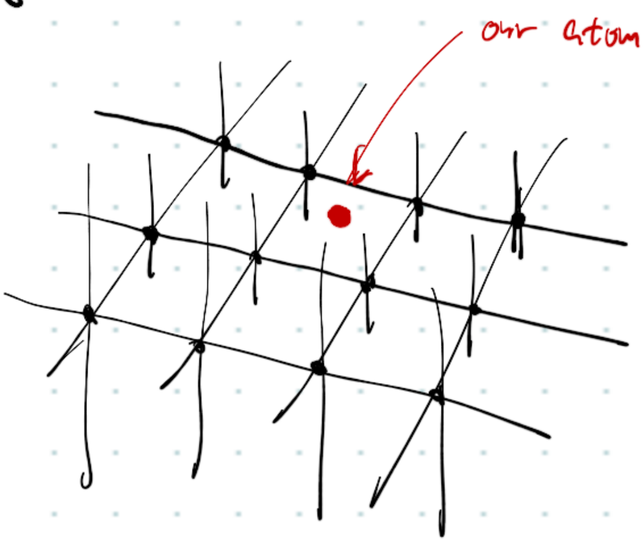
$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + V(r) \qquad \hat{H}_0 \psi_{nlm} = \underline{\underline{E_{nl}}} \psi_{nlm}$$

Symmetry group $SO(3)$ eigenspace of E_{nl} : $\mathcal{H}^{(n,l)}$

irrep of $SO(3)$

$\dim \mathcal{H}^{(n,l)} = 2l+1$

crystal : cubic lattice



$$\hat{H} = \hat{H}_0 + V_{lattice}(\vec{r})$$

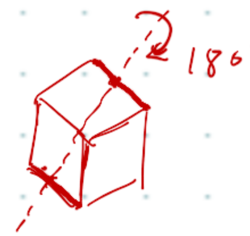
break $SO(3)$ symmetry down to $O \subset SO(3)$

O group: Symmetry group of cubic lattice (finite group)

O group has 24 elements (5 conjugacy classes)

- identity E
- $8C_3$

- $6C_2$



- $3C_2$

- $6C_4$

irrep of $SO(3)$

irreps of O

E_{nl} $2l+1$

$E_{nl}^{(i)}$ $d_{nl}^{(i)}$

$$\sum_i d_{nl}^{(i)} = d(n,l) = 2l+1$$

H_0

$$\mathcal{H}^{(\cancel{n},l)} = \bigoplus_i \mathcal{H}_i^{(\cancel{n},l)}$$

irrep of SO(3)   irrep of O

$$\chi(E) = \mathrm{tr}\, D(E) = \mathrm{tr}\, \mathbb{1} = \dim(D)$$

$$\underbrace{D^{(\cancel{n},l)} = \bigoplus_i D_i^{(\cancel{n},l)}}_{\text{character of O group}}$$

value of $\chi(g)$	E	$8C_3$	$6C_2$	$3C_2$	$6C_4$
T_1	1	1	1	1	1
T_2	1	1	-1	1	-1
T_3	2	-1	0	2	0
T_4	3	0	-1	-1	1
T_5	3	0	1	-1	-1

irreps of O

$$\chi_l(g) = \sum_i \chi_i^{(l)}(g) \quad \forall g \in O$$

value of characters of SO(3) for elements in $O \subset SO(3)$

$\chi_l(g)$	E	$8C_3$	$6C_2$	$3C_2$	$6C_4$
$l=0$, s-state	1	1	1	1	1
$l=1$, p	3	0	-1	-1	1
$l=2$, d	5	-1	1	1	-1
$l=3$, f	7	1	-1	-1	1
$l=4$ g	9	0	1	1	1
$\vdots$	$\vdots$				

- $l=0$ $\quad D^{(l=0)} = T_1 \qquad \chi_{l=0}(g) = \chi_{T_1}(g)$

$E^{(n,0)}$ ——— ---- ——— $E^{(n,0)}_{new}$

no split for s-state.

- $l=1$ $\quad D^{(l=1)} = T_4 \qquad \chi_{l=1}(g) = \chi_{T_4}(g) \quad \forall g \in O$

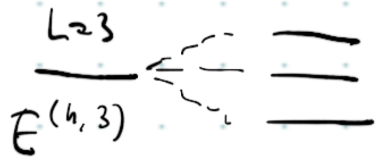
$E^{(n,1)}$ $\underline{l=1}$ ---- $\underline{T_4}$ $E^{(n,1)}_{new}$

• $l=2$: $D^{(l=2)} = T_3 \oplus T_5$

$(d=5)$ $\quad$ $(d=2)$ $\quad$ $(d=3)$

• $l=3$: $D^{(l=3)} = T_2 \oplus T_4 \oplus T_5$

$(d=7)$ $\quad$ $d=1$ $\quad$ $d=3$ $\quad$ $d=3$



• $L=4$ $\quad$ $D^{(l=3)} = T_1 \oplus T_3 \oplus T_4 \oplus T_5$

$(d=9)$ $\quad$ $d=1$ $\quad$ $d=2$ $\quad$ $d=3$ $\quad$ $d=3$

....

HW check the splitting at $l=2, 3, 4$.

We obtain energy level splitting & degeneracy just by symmetry & group theory, no need to solve Schrödinger eqn

Dynamical symmetry

$2l+1$

hydrogen atom : $\hat{H} = \frac{\hat{p}^2}{2m} - \frac{e^2}{r}$ $SO(3)$ symm.

E_n degeneracy $d(n) = n^2$

$\mathcal{H}^{(n)}$ is reducible rep of $SO(3)$

there should be a larger symmetry group

$G \supset SO(3)$

classical mechanics $V(r) \sim \frac{1}{r}$ Kepler problem

Conserved quantities : energy, angular momentum,

$\hat{\vec{L}} \times \hat{\vec{L}} = i\hbar \hat{\vec{L}}$

$[\hat{L}_i, \hat{L}_j] = i\hbar \varepsilon_{ijk} \hat{L}_k$

Runge-Lenz vector.

$$\vec{M} = \frac{1}{me^2} \vec{p} \times \vec{L} - \frac{\vec{r}}{r}$$

quantization : $\hat{\vec{M}} = \frac{1}{2me^2} \left(\hat{\vec{P}} \times \hat{\vec{L}} - \hat{\vec{L}} \times \hat{\vec{P}} \right) - \hat{\vec{N}}$

$$\hat{\vec{N}} = \frac{\hat{\vec{R}}}{\hat{R}}$$ orientation operator

(1) $[\hat{\vec{M}}, \hat{H}] = 0$

(2) $\hat{\vec{M}} \times \hat{\vec{M}} = -i\hbar \frac{2}{me^4} \hat{\vec{L}} \hat{H}$

(3) $\hat{M}^2 = \frac{2}{me^4} \hat{H} (\hat{L}^2 + \hbar^2) + 1$

<u>HW</u> show (1), (2), (3)

(submit HW before 17th Feb)

Given a energy Level, E_n ($E_n < 0$), eigenspace $\mathcal{H}^{(n)}$

$$\hat{H} \psi_n = E_n \psi_n \quad \forall \psi_n \in \mathcal{H}^{(n)}$$

define $\hat{\vec{K}} = \sqrt{\frac{me^4}{2(-\hat{H})}} \hat{\vec{M}}$

on $\mathcal{H}^{(n)}$, $\hat{\vec{K}} = \sqrt{\frac{me^4}{2(-E_n)}} \hat{\vec{M}}$

(2) $\rightarrow$ $\hat{\vec{M}} \times \hat{\vec{M}} = -i\hbar \frac{2}{me^4} \hat{\vec{L}} E_n$

$$\hat{\vec{K}} \times \hat{\vec{K}} = i\hbar \hat{\vec{L}}$$

i.e., $[\hat{K}_i \ \hat{K}_j] = i\hbar \varepsilon_{ijk} \hat{L}_k$

HW check: $[\hat{L}_i \ \hat{K}_j] = i\hbar \varepsilon_{ijk} \hat{K}_k$

we know that (1) $[H, \hat{\vec{K}}] = 0$

(2) $[H, \hat{\vec{L}}] = 0$

both $\hat{\vec{K}}$, $\hat{\vec{L}}$ leaves $\mathcal{H}^{(n)}$ inv.

we obtain operators $\hat{K}_{i=1,2,3}$, $\hat{L}_{i=1,2,3}$ with closed commutator algebra

$$[L_i \ L_j] = i\hbar \varepsilon_{ijk} L_k \quad \leftarrow$$

$$[L_i \ K_j] = i\hbar \varepsilon_{ijk} K_k$$

$$[K_i \ K_j] = i\hbar \varepsilon_{ijk} L_k$$

$$\hat{L}_i \rightarrow D(\varphi, \vec{n}) = e^{-\frac{i}{\hbar}\varphi \vec{n} \cdot \hat{\vec{L}}}, \quad \varphi, \vec{n}$$

3 parameters

unitary rep of $SO(3) \underset{\text{local}}{\simeq} SU(2)$

$$\begin{pmatrix} \alpha & -\bar{\beta} \\ \beta & \bar{\alpha} \end{pmatrix} \quad \alpha, \beta \in \mathbb{C}$$

$$\det = 1$$

$$\hat{L}_i, \hat{k}_i \rightarrow D(\varphi, \vec{n}, \vec{\theta}) = e^{-\frac{i}{\hbar}\varphi \vec{n}\cdot\hat{\vec{L}}} \cdot e^{-\frac{i}{\hbar}\vec{\theta}\cdot\hat{\vec{k}}}$$

$$3 + 3 = 6$$

parameters

we obtain a larger group rep. on $\mathcal{H}^{(4)}$

Let's determine this larger group.

linear combination of $\vec{k}$ and $\vec{L}$

$$\hat{\vec{J}}^{(+)} = \frac{1}{2}(\hat{\vec{L}} + \hat{\vec{k}})$$

$$\hat{\vec{J}}^{(-)} = \frac{1}{2}(\hat{\vec{L}} - \hat{\vec{k}})$$

$$\Rightarrow \begin{cases} [\hat{\vec{J}}^{(+)}, \hat{\vec{J}}^{(-)}] = 0 \\ [J_i^{(+)}, J_j^{(+)}] = i\hbar\, \varepsilon_{ijk} J_k^{(+)} \\ [J_i^{(-)}, J_j^{(-)}] = i\hbar\, \varepsilon_{ijk} J_k^{(-)} \end{cases}$$

(to check this.)

$$D(\vec{\theta}^{(+)}, \vec{\theta}^{(-)}) = \underbrace{e^{-\frac{i}{\hbar}\vec{\theta}^{(+)}\cdot\hat{\vec{J}}^{(+)}}}_{\text{uni. rep. of } SU(2)} \underbrace{e^{-\frac{i}{\hbar}\vec{\theta}^{(-)}\cdot\hat{\vec{J}}^{(-)}}}_{\text{uni. rep. of } SU(2)}$$

6 parameters

is unitary rep. of $\underline{SU(2) \times SU(2)} \simeq Spin(4)$

is local

$SO(4)$

4×4 matrices Λ

$\Lambda^T \Lambda = 1_{4\times4}$

$\det \Lambda = 1$

explain degeneracy of $\mathcal{H}^{(n)}$

$$\mathcal{H}^{(n)} \text{ is irrep of } SU(2)\times SU(2) \ni (\underset{\substack{\cup\\ SU(2)}}{g_1}, \underset{\substack{\cup\\ SU(2)}}{g_2})$$

irrep. $D_{j_1 j_2}(g) = D_{j_1}(g_1) \otimes D_{j_2}(g_2)$

$$\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2}$$

$$\dim(\mathcal{H}_j) = 2j+1$$

$$\dim(j_1, j_2) = (2j_1+1)(2j_2+1)$$

$$\begin{array}{c} \| \\ \dim(\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2}) \end{array}$$