Theorem of orthonormal basis

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

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

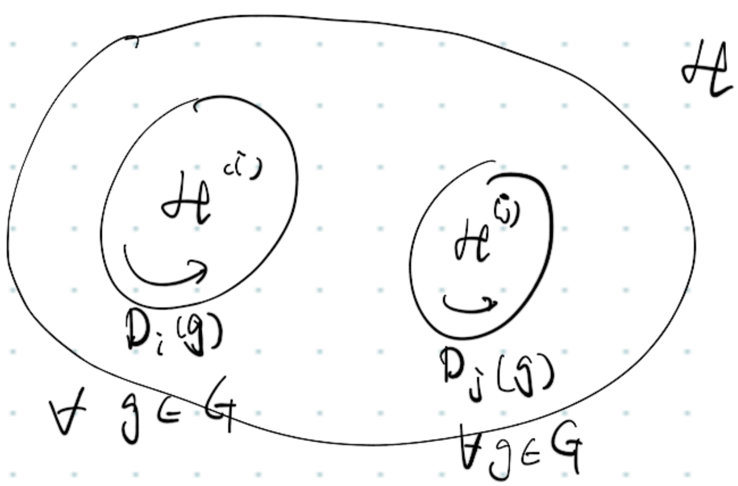
D_i, D_j are unitary irrep

if D_i, D_j are inequivalent

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

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

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

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

$f^{(i)}_{\alpha=1 \cdots \dim(\mathcal{H}^{(i)})}$ 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)
$$\left\{ \begin{array}{l} D^{(i)}_{\alpha\beta}(g) = \langle f^{(i)}_\alpha | D^{(i)}(g) | f^{(i)}_\beta \rangle \\ D^{(j)}_{\alpha\beta}(g) = \langle f^{(j)}_\alpha | D^{(j)}(g) | f^{(j)}_\beta \rangle \end{array}\right.$$

orthogonality of rep. functions

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

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 : $\chi(g) = tr(D(g))$

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

properties : (1) conjugacy class : group conjugate :

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

obit of group conjugate

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

$$\simeq \qquad \qquad \shortparallel$$

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

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

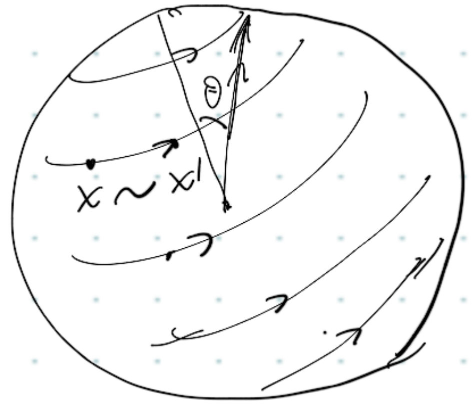
$$= tr(D(h)\, D(g)\, D(h^{-1}))$$

$$= tr(\underline{D(h)}\, D(g)\, \underline{D(h)^{-1}})$$

$$= tr(D(g)) = \chi(g)$$

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

χ is function of conjugacy classes in G



S^2

an orbit = a circle with const. θ

$\Updownarrow$ 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.

Theorem (orthogonality of χ)

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

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

rank of the group.

$$\underbrace{\sum_{g \in G} \chi^{(i)}(g)^* \chi^{(j)}(g)}_{=\ \sum_{C \in (\text{conjugacy classes})} h_C\, \chi^{(i)}(C)^* \chi^{(j)}(C)}$$

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

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

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 eigen $\underbrace{\text{space}}_{\mathcal{H}^{(n)}}$ of $\hat{H}$ at the eigenvalue E_n

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

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

$D(g)|\psi_{ni}\rangle$ 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 $\hat{H} = \dfrac{\hat{p}^2}{2m} + \underline{V(r)}$

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 $\{Y_{lm}\}_{m=-l..l}$

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

$\underline{\underline{\mathcal{H}}}^{(n,l)}$ 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 $\{ R_{nl}(r) Y_{lm}(\theta,\varphi) \}$

$$l = 0, 1 \ldots n-1$$
$$m = -l \ldots l$$

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

$$\rightarrow \underbrace{\mathcal{H}^{(n)}}_{\text{reducible rep of } SO(3)} = \bigoplus_{l=0}^{n-1} \underbrace{\mathcal{H}^{(n,l)}}_{\text{irrep of } SO(3)} \qquad \dim(\mathcal{H}^{(n,l)}) = 2l+1$$

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.

$$\begin{matrix} SO(4) \\ |\text{S local} \end{matrix}$$

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

$$\begin{matrix} \cup \\ SO(3) \end{matrix}$$

(dynamical symmetrie)

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

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

by adding perturbations to $\hat{H}$

$H^{(n)}$ irrep of G $\quad \mathcal{H}^{(n)} = \underline{\mathcal{H}_1^{(n)} \oplus \mathcal{H}_2^{(n)} \oplus \cdots}$

$\cup$

G_{small}

reducible rep of G_{small}

irrep of G_{small}

$$\hat{H} \to \hat{H}_{new} = \hat{H}_0 + \hat{H}' \qquad E_n \to E_n + \Delta E_{ni}$$

G

perturbation

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

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

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

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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. $D(g)\hat{H}'D(g)^{-1} \neq \hat{H}'$

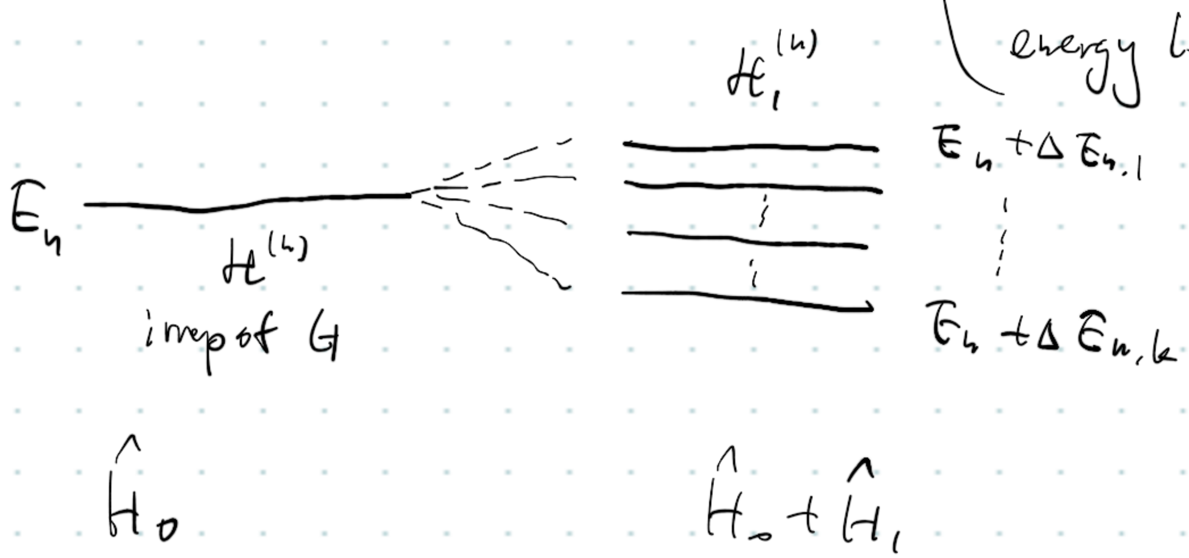
G is broken into subgroup $G_{new} < G$

irrep of G : $\mathcal{H}^{(n)} = \bigoplus_{i=1}^{k_n} \mathcal{H}_i^{(n)}$

eigenspace of $\hat{H}_0$

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.

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + V(r)$$

$$\hat{H}_0 \psi_{nlm} = E_{nl} \psi_{nlm}$$

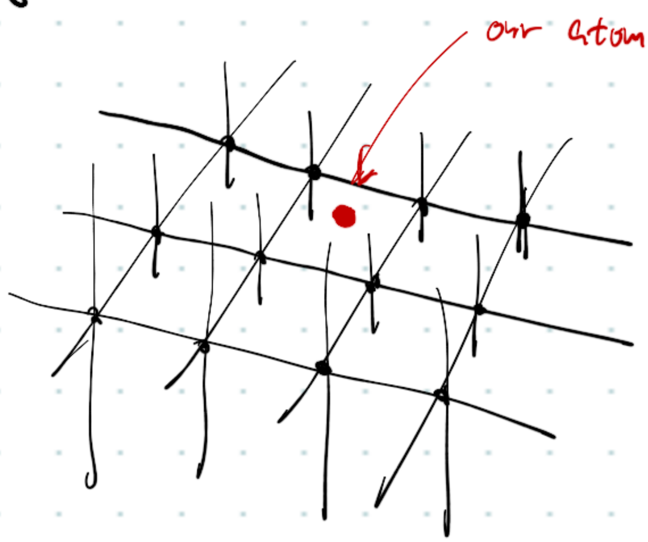
Symmetry group $SO(3)$

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)