lecture 2023-11-22

last lecture group basics and subgroups H < G -> factor group G/H
splitting in smaller groups

$H \subset G$

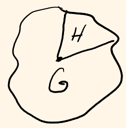
$H \triangleleft G$

example euclidian group E(d) " geometrical motions"
translations T(d) < E(d)

$T(d) \triangleleft E(d)$

$\frac{E(d)}{T(d)} \simeq K(d)$ rotations

only shore 4 matrix



inverse operation:
direct product $\underset{g_1}{G_1}, \underset{g_2}{G_2}$ $\quad G_1 \otimes G_2 \ni (g_1, g_2)$

$(g_1 g_2)(h_1, h_2) = (g_1 h_1, g_2 h_2)$

neutral element e_1, e_2

E(d) semidirect product

$(\underset{\text{rotation}}{R_1}, \underset{\text{translation}}{b_1})(R_2, b_2) = (R_1 R_2, b_1 + R_1 b_2)$

G acting on Hilbert space $\mathcal{H}_1$ and G_1 on $\mathcal{H}_2$

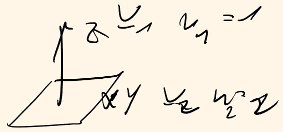
$g_1 \otimes g_2 \,|u_1 \otimes u_2\rangle = g_1|u_1\rangle \otimes g_2|u_2\rangle$

for a representation M, concept of "decompose" it via subscpaces V_1 V_2 $\subset V$ vectorspace

if $M(g)$ $n \times n$ matrix orthogonal spaces

"split into blocks"

$M(g) = \left(\begin{array}{c|c} M_1(g) & 0 \\ \hline 0 & M_2(g) \end{array}\right) = M_1 \oplus M_2$



M_1, M_2 choose basis vectors $\quad \underset{S}{\exists} \underset{g}{\forall} M(g) = S^{-1}(M_1(g) \oplus M_2(g)) S$

M is "reducible" if this block form applies for all $g \in G$ $\quad \underset{v_1, v_2}{\exists} \underset{\substack{u_1 \in v_1 \\ u_2 \in v_2}}{\forall} M(g)|u_1\rangle$

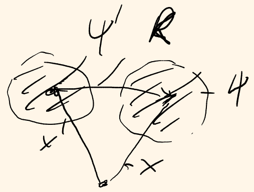
remember $M(gg') = \overbrace{M(g) M(g')}$ maybe a phase number (projective representation)

D dim of V is much larger than G

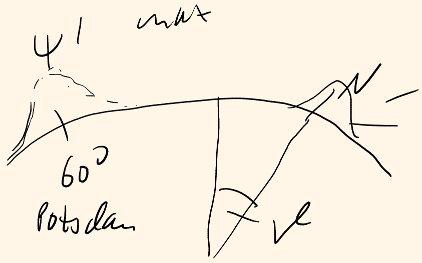
wave functions $\psi \in \underline{V}$

rotation R (3x3 Matrix) $\quad \psi(x) \to \psi'(x') = \psi(x)$

with $x' = Rx$



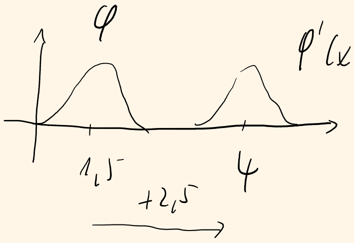
equivalent form



$\psi'(x) = \psi(R^{-1}x)$ or $\psi' = \psi \circ R^{-1}$

$\vartheta(\text{Potsdam}) = R\vartheta(N) \quad (-38^\circ)$

$\underset{P}{\psi_{ice}(\vartheta)} = \underset{N}{\psi_{ice}}(\vartheta + 38^\circ)$



$\varphi'(x) = \varphi(x - 2{,}5)$

"inverse" map inside argument of ψ, φ ...

$R_1: \psi' = \psi \circ R_1^{-1} \xmapsto{R_2} \psi'' = (\psi \circ R_1^{-1}) \circ R_2^{-1} = \psi \circ R_1^{-1} R_2^{-1}$

$= \psi \circ (R_2 R_1)^{-1}$

image of ψ under $R_2 R_1$

$\alpha \psi + \beta \chi$

1D subscpace of representation spanned by $\psi(\vec{x}) = \varphi_{1s}(|\vec{x}|) = \varphi_{1s}(\vec{r})$

"invariant" $\varphi'_{1s} = \varphi_{1s}$

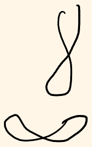
$= \mathbb{1}_1 \varphi_{1s}$

1x1 block $\quad M_{1s} = \mathbb{1}_1 = (1)$

p-states form a 3D subspace $\{|p_x\rangle, |p_y\rangle, |p_z\rangle\}$ states the same quantum numbers

rotate p_x $\Rightarrow$ get linear combinations of p_x, p_y, p_z

$$\left.\begin{aligned} \langle \vartheta, \varphi | p_z \rangle &= \cos\vartheta \\ \langle \vartheta, \varphi | p_x \rangle &= \sin\vartheta \sin\varphi \\ \langle \vartheta, \varphi | p_y \rangle &= \sin\vartheta \cos\varphi \end{aligned}\right\} = \hat{r}$$



p_z orbital

p_x orbital $\quad \varphi'_p = R\varphi_p$

$M_p = R$

in chem lit basis

real vectors

d-states 5 states "stay among them self"

closed under rotation

"reduction of ∞ dim represent. in 1, 3, 5 dim spaces

$$M(R) = \begin{pmatrix} 1 & & & \\ & \underset{3\times 3}{R^{[1]}} & & \\ & & \underset{5\times5}{D^{[2]}(R)} & \\ & & & \ddots \end{pmatrix}$$

d: $\ell = 2$

subspace

irreducible (no split of $M_1 \oplus M_2$)

with 1 t matrix

2 possibilities dim subspace $= 0$

dim subspace $=$ the full space

take $\operatorname{tr} M(g) = \operatorname{tr}[S^{-1} M_1 \oplus M_2 S] = \operatorname{tr}[\underbrace{S S^{-1}}_{=1} M_1 \oplus M_2]$

trace of matrix

$= \operatorname{tr} M_1 + \operatorname{tr} M_2$

for rotation $\operatorname{tr} R^{[1]} = 1 + 2\cos\alpha$ α - rot angle

in d-states $\operatorname{tr} D^{[2]}(R) = \ldots \cos\alpha, \sin\alpha$

Fourier components (analysis)

in physics: "elementary" particles "multiple" irreducible representation of a symmetry group

(Wigner-Weyl) like color change

next week continous trafos