The Character of a Representation ①

* matrix reps. which are related to each other via unitary transformations are equivalent → different representations have a large degree of arbitrariness

⇓ ⇓

try to find way to characterize them which are invariant under unitary transformations

↳ trace of a matrix is invariant

⇒ <u>character of a representation</u>

$\chi^{(j)}(E), \chi^{(j)}(A_2), \ldots, \chi^{(j)}(A_n)$

$$\chi^{(j)}(A_e) = \sum_{\mu} \Gamma^{(j)}_{\mu\mu}(A_e)$$

$\chi^{(i)}(A_e)$ is the trace of matrix which represents group element A_e

* since classes consist of elements related to each other via unitary transformations

⇓

all elements in the same class have the same character

→ character of a rep.: specify only one from each class: $\chi^{(j)}(E), \chi^{(j)}(C_n) \ldots$

recall : great orthogonality theorem

$$\sum_R \Gamma^{(i)}_{\mu\nu}(R)^* \Gamma^{(j)}_{\alpha\beta}(R) = \frac{h}{l_i}\delta_{ij}\delta_{\mu\alpha}\delta_{\nu\beta}$$

can be converted to an expression in terms of ~~classes~~ (characters)

$$\sum_{\mu\alpha}\sum_R \Gamma^{(i)}_{\mu\mu}(R)^* \Gamma^{(j)}_{\alpha\alpha}(R) = \frac{h}{l_i}\delta_{ij}\sum\delta_{\mu\alpha}\delta_{\mu\alpha}$$

$$\sum_R \chi^{(i)}(R)^* \chi^{(j)}(R) = h\,\delta_{ij}$$

or in terms of classes

$$\sum_k N_k\, \chi^{(i)}(C_k)^* \chi^{(j)}(C_k) = h\,\delta_{ij}$$

N_k - number of elements in class k

$\Downarrow$ $\Downarrow$ $\Downarrow$

number of classes defines dimensionality of vector space in which vectors $\chi^{(i)}(C_k)$ are orthogonal if representations are different

$\Downarrow$

number of classes $\geq$ number of representations (irreps)

In fact they are equal

number of classes $=$ number of representations (irreps) example: group of order 6

③

$E, C_{\frac{2\pi}{3}}, C_{-\frac{2\pi}{3}}, \sigma_A, \sigma_B, \sigma_C$

3 classes, order 6

dimensionalities must obey $\sum_{i=1}^{3} l_i^2 = h$ $\underbrace{h=6}$

$1+1+4 = 6$

$1+1+2^2 = 6$

usually this eq'n. has one solution

<u>character tables.</u>

	$E,$	$3C_2$	$2C_3$
$\Gamma^{(1)}$	1	1	1
$\Gamma^{(2)}$	1	−1	1
$\Gamma^{(3)}$	2	0	−1

obey: 1.) $\sum_k N_k \chi^{(i)}(C_k)\chi^{(j)}(C_k) = h\delta_{ij}$

(rows orthogonal)

2.) $\sum_i \chi^{(i)}(C_k)\chi^{(i)}(C_l) = \frac{h}{N_k}\delta_{kl}$

(columns orthogonal)

<u>second orthogonality relation for characters.</u>

construct matrix:

$$\bar{Q} = \begin{pmatrix} \chi^{(1)}(C_1) & \chi^{(1)}(C_2) & \dots \\ \chi^{(2)}(C_1) & \chi^{(2)}(C_2) & \dots \\ \vdots & & \end{pmatrix}$$

$$\bar{Q}' = \begin{pmatrix} \frac{N_1 \chi^{(1)*}(C_1)}{h} & \frac{N_1 \chi^{(2)*}(C_1)}{h} & \cdots \\ \frac{N_2 \chi^{(1)*}(C_2)}{h} & \frac{N_2 \chi^{(1)*}(C_2)}{h} & \cdots \\ \vdots & & \end{pmatrix}$$

product: $\bar{Q}\,\bar{\bar{Q}}' = \delta_{ij} = \sum_k \frac{N_k \chi^{(i)}(C_k)\chi^{(j)}(C_k)}{h}$

any matrix commutes with its inverse

$$\bar{\bar{Q}}'\vec{Q} = \delta_{ij}$$

$$\sum_i \chi^{(i)}(C_k)\chi^{(j)}(C_l) = \frac{h\,\delta_{kl}}{N_k}$$

(contains no new info)

Construction of character tables

rules for constructing character tables

1.) number of irreps = number of classes
- obtain number of classes by inspection or by multiplying matrices

2.) dimensionalities of irreps: $\sum_i l_i^2 = h$

since $\chi^{(i)}(E) = l_i \Rightarrow$ first column is thereby determined

first row is all ones (trivial representation) $\chi^{(1)}(C_k) = 1$

3.) orthogonality relation

$$\sum_k N_k \chi^{(i)*}(C_k) \cdot \chi^{(j)}(C_k) = h\,\delta_{ij}$$

4.) orthogonality relation

$$\sum_i \chi^{(i)}(C_k)\,\chi^{(i)*}(C_l) = \frac{h}{N_k}\,\delta_{kl}$$

5.) elements in the same row determined by

$$N_k \chi^{(i)}(C_k)\, N_l \chi^{(i)}(C_l) = l_i \sum_m \underline{C_{klm}}\, N_m \chi^{(i)}(C_m)$$

coefficients C_{klm} are those of class multiplication

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detour: class multiplication

in this case two sets are equal if they contain the same number of elements the same number of times

consider:

$$X^{-1} C X = C$$

X - any element of group

C - complete class

Proof: any element produced on left side will appear on the right → conjugate elements → definition of class

must appear <u>once</u> only → uniqueness of group multiplication converse is also true

any C for which $X^{-1} C X = C$

must consist of complete classes

consider two classes

$$C_i C_j = X^{-1} C_i X X^{-1} C_j X$$

$$= X^{-1} C_i C_j X$$

$\Downarrow$

so $C_i C_j$ consists of complete classes too

$$\underline{C_i \cdot C_j = \sum_k c_{ijk} C_k}$$

for a given group coefficients c_{ijk} can be calculated

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back to original statement

$$N_k \chi^{(i)}(C_k) N_e \chi^{(i)}(C_e) = l_i \sum_m c_{kem} N_m \chi^{(i)}(C_m)$$

<u>Proof:</u> $C_i C_j = \sum_n c_{ijn} C_n$

consider matrix $C_i \Rightarrow$ sum of all class elements

$\underline{X^{-1} C_i X = C_i}$ holds (definition of class)

$\Downarrow$

$C_i X = X C_i \Rightarrow C_i$ commutes with all X

by Schur's lemma $\Rightarrow C_i$ is a constant matrix $\Rightarrow C_i = \eta_i E$

$$\Rightarrow M_i M_j = \sum_k c_{ijk} M_k$$

$$\mathrm{Tr}\, C_i = m_i l_i$$

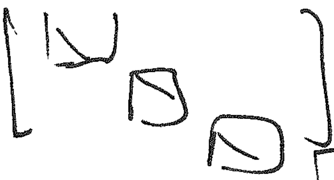
$$\mathrm{Tr}\, C_i = N_k \chi^{(j)}(C_k)$$

$$\Rightarrow M_k = \frac{N_k \chi^{(j)}(C_k)}{l_k}$$

$$\Rightarrow N_k \chi^{(i)}(C_k) N_l \chi^{(i)}(C_l) = l_i \sum_m c_{klm} N_m \chi^{(i)}(C_m)$$

Decomposition of Reducible Representations

character of a reducible rep must be sum of characters of irreps



$$\Rightarrow \chi(R) = \sum_j a_j \chi_j^{(j)}(R)$$

$$\boxed{\frac{1}{h} \sum_R \chi^{(i)}(R) \chi(R) = a_j}$$

from character tables one can find irreps

The regular representation.

given group: $E, A_2, \ldots$

$$
\begin{array}{c|cccccc}
 & E & A_2, & A_3 & \cdots & & \\
\hline
E & E & A_j & A_n & \cdots & & \\
A_2^{-1} & A_l & E & \cdots & & & \\
A_3^{-1} & \vdots & & E & & & \\
\vdots & \vdots & & & E & & \\
\vdots & & & & & E &
\end{array}
$$

form matrix from multiplication table

for element A_j → if element in table is not A_j ⇒ place zero in matrix

if element is A_j place 1

example: cyclic group of order 3

$$
\begin{array}{c|ccc}
 & E & A & A^2 \\
\hline
E & E & A & A^2 \\
A^2 & A^2 & E & A \\
A & A & A^2 & E
\end{array}
\Rightarrow E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad A^2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}
$$

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

characters: $\chi^{(reg)}(E) = h$ (order of group)

$\chi^{(reg)}(A_j) = 0$

does it form a representation?

$$\sum_j \Gamma_{A_i^{-1}A_j}(B)\,\Gamma_{A_j^{-1}A_n}(C) = ? = \Gamma_{A_i^{-1}A_n}(BC)$$

$$\Gamma_{A_i^{-1}A_j}(B) = \begin{cases} 1 & \text{if } A_i^{-1}A_j = B \\ 0 & \text{otherwise} \end{cases}$$

$$\Gamma_{A_j^{-1}A_n}(C) = \begin{cases} 1 & \text{if } A_j^{-1}A_n = C \\ 0 & \text{otherwise} \end{cases}$$

if $A_i^{-1}A_j \cancel{A_j^{-1}} = B$ and $A_j^{-1}A_n = C$

$$\Rightarrow A_i^{-1}A_n = BC$$

<u>Celebrated theorem</u>:

regular representation contains irreps as many times as is their dimensionality

$$\chi^{(reg)}(R) = \sum_j a_j \chi^{(j)}(R)$$

$$\sum_R \chi^{(i)}(R)\,\chi^{(reg)}(R) = h\,a_i$$

$$\chi^{(i)}(E)\,\chi^{(reg)}(E) = h\,a_i \Rightarrow a_i = l_i$$

$$\chi^{(reg)}(R) = \sum_j l_j \chi^{(j)}(R)$$

$$\chi^{(reg)}(E) = \sum_j l_j \chi^{(j)}(E) \Rightarrow \boxed{h = \sum_j l_j^2}$$

Application of Representation Theory (10)

in Quantum Mechanics

Transformation operators.

* group of interest: group of symmetry operators which leave the Hamiltonian invariant
* represent as matrix $\bar{\bar{R}}$

$$\bar{\bar{R}}\vec{x} = \vec{x}' \qquad x_i' = \sum_j R_{ij} x_j$$

R can represent rotation, reflection, inversion or any combination of these

$\Rightarrow$ $\bar{\bar{R}}$ - real orthogonal matrix

$$\bar{\bar{R}}^{-1} = \bar{\bar{R}}^{+} = \bar{\bar{R}}^{tr}$$

real orthogonal matrices form a group under matrix multiplication

$\rightarrow$ can also extend to other symmetry operations (coordinate permutation (exchange), translation)

* introduce a group isomorphic to group of matrices corresponding to symmetry operations

this group consist of transformation operators which operate on <u>functions</u> rather than coordinates define as: $$P_R f(\bar{\bar{R}}\vec{x}) = f(\vec{x})$$

$$P_R f(\vec{x}) = f(\bar{\bar{R}}^{-1}\vec{x})$$

P_R - changes the functional form of $f(\vec{x})$ in such a way ~~so~~ as to compensate for the change of $\bar{\bar{R}}$

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example:

$$\bar{\bar{R}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \qquad \bar{\bar{R}}^{-1} = \bar{\bar{R}}^{tr} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\bar{\bar{R}}^{-1}\vec{x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ -z \\ y \end{pmatrix}$$

in terms of $P_R \Rightarrow$

$$\underline{P_R f(x,y,z) = f(x,-z,y)}$$

p- functions $x\varphi(r)$, $y\varphi(r)$, $z\varphi(r)$

$$P_R(x\varphi(r)) = x\varphi(r)$$

$$P_R(y\varphi(r)) = -z\varphi(r)$$

$$P_R(z\varphi(r)) = y\varphi(r)$$

P_R - rotates contours of functions

$\bar{\bar{R}}$ - rotates coordinate axes

equivalent points of view

Operators P_R form a group

$$P_S P_R = P_{SR}$$

$$P_S \underbrace{P_R f(\vec{x})} = P_S g(\vec{x}) = g(S^{-1}\vec{x}) = f(R^{-1}S^{-1}x)$$

$$g(\vec{x}) = P_R f(\vec{x}) = f(R^{-1}\vec{x})$$

$$= f((SR)^{-1}\vec{x}) = P_{SR} f(\vec{x})$$

The group of the Schrödinger equation.

operators P_R which commute with the Hamiltonian operator H

example: $H = -\frac{\nabla^2}{2} + \frac{e^2}{(x^2+y^2+z^2)^{1/2}}$

any rotation/reflection leaves potential and kinetic energy unchanged

$\Downarrow$

$$P_R H = H P_R$$

set of all such operators is known as the group of the Schrödinger equation

$$P_R H \Psi_n = P_R E_n \Psi_n = E P_R \Psi_n = H P_R \Psi_n$$

$\Rightarrow$ Ψ_n eigenfunction with eigenvalue E_n

$P_R \Psi_n$ also an eigenfunction of H with eigenvalue E_n

application of symmetry operators generate
other states degenerate with the original
state

if this procedure yields all degenerate
eigenstates => normal degeneracy
distinct from accidental degeneracy
(no obvious origin in symmetry)

Representations.

assume: E_n is l_n-fold degenerate

$\Downarrow$ $\Downarrow$

we may chose a set of l_n orthonormal
eigenfunctions

P_R operating on ψ_n → generates another fn.
having the same energy

$\Downarrow$

l_n-degenerate eigenfunctions => basis vectors
in an l_n-dimensional vector space
space is an invariant subspace of the
Hilbert space

$\Downarrow$ $\Downarrow$ $\Downarrow$

P_R can be represented by a matrix
matrices can be worked out by applying
P_R on ψ_n's

$$P_R \Psi_\nu^{(n)} = \sum_\mu \Psi_\mu^{(n)} \Gamma_{\mu\nu}^{(n)}(R)$$

$\Gamma_{\mu\nu}^{(n)}(R)$ – l_n-dimensional matrices $\Rightarrow$

form an l_n-dimensional representation of the group of the Schrödinger equation

- representation is irreducible (smaller matrices can not express the most general transformation)

- form a group?

$$P_{SR} \Psi_\nu = P_S P_R \Psi_\nu = P_S \sum_\mu \Psi_\mu \Gamma_{\mu\nu}(R)$$

$$= \sum_\mu \sum_{\mu'} \Psi_{\mu'} \Gamma_{\mu'\mu}(S) \Gamma_{\mu\nu}(R)$$

$$= \sum_{\mu'} \Psi_{\mu'} \left[\Gamma(S)\Gamma(R)\right]_{\mu'\nu}$$

$$\Gamma(SR) = \Gamma(S)\Gamma(R)$$

l_n degenerate eigenfunctions $\Psi_\nu^{(n)}$ of energy E_n form basis functions for an l_n-dimensional irrep $\Gamma^{(n)}$ of the group of the Schrödinger equation representation is unitary: assume Ψ_κ is an orthonormal basis

$$\delta_{\kappa\nu} = (\Psi_\kappa, \Psi_\nu)$$

$$= (P_R \Psi_\kappa, P_R \Psi_\nu)$$

$$= \sum_{\lambda,\mu} (\Psi_\lambda \Gamma_{\lambda\kappa}(R), \Psi_\mu \Gamma_{\mu\nu}(R))$$

$$= \sum_{\lambda,\mu} (\Psi_\lambda, \Psi_\mu) \Gamma^*_{\lambda\kappa}(R) \Gamma_{\mu\nu}(R)$$

$$= \sum_{\lambda} \Gamma^*_{\lambda\kappa}(R) \Gamma_{\lambda\mu}(R)$$

$$= \sum_{\lambda} \Gamma^\dagger_{\kappa\lambda}(R) \Gamma_{\lambda\mu}(R)$$

$\Gamma^\dagger \Gamma = E$ - representation is unitary

Group theory and quantum numbers.

change of basis $\quad \Psi'_\mu = \sum_\nu \Psi_\nu \alpha_{\nu\mu}$

$$P_R \Psi'_\mu = P_R \sum_\nu \Psi_\nu \alpha_{\nu\mu} = \sum_\nu \sum_\lambda \Psi_\lambda \Gamma_{\lambda\nu}(R) \alpha_{\nu\mu}$$

$$= \sum_\nu \sum_\lambda \sum_{\lambda'} \Psi'_{\lambda'} \underbrace{[\alpha^{-1}]_{\lambda'\lambda} \Gamma_{\lambda\nu}(R) \alpha_{\nu\mu}}$$

$$\Downarrow$$

$$\Gamma' = \alpha^{-1} \Gamma \alpha$$

equivalent representations

row index of a representation ⇒ quantum number (good quantum number)

degeneracy → dimensionality of representation

working out irreps → determine degeneracies

perturbation will lift degeneracy if it reduces the symmetry group

↳ possible irreps change

if representation matrices worked out, they contain transformation properties of all eigenfns. under symmetry operators of the group