

Group Theory

①

Invertible linear transform $f: V \rightarrow V$, eg., basis transform, have these properties:

- a) can be undone: $f^{-1} f |V\rangle = |V\rangle$
- b) given f_1, f_2 : f_1, f_2 ~~also~~ also defines a transform.
- c) $f_1(f_2 f_3 |V\rangle) = (f_1 f_2) f_3 |V\rangle = f_1 f_2 f_3 |V\rangle$
- d) can define "no transform" I : $I |V\rangle = |V\rangle \forall |V\rangle \Rightarrow I f |V\rangle = f |V\rangle$
 $\forall f$ ~~not~~

Example: rot. on $\mathbb{R}^2$; reflection on $\mathbb{R}^2$

objects satisfying a) - d) are said to constitute a group.

Example of transforms that do not form group: projection operation.

Def. Group: G = a set of objects $\{a, b, c, \dots\}$ with a law of multiplication such that

$$\forall a, b \in G, ab \in G$$

$$\exists e \text{ s.t. } ea = a \forall a$$

$$\exists a^{-1} \forall a \text{ s.t. } a^{-1}a = e$$

$$\text{associativity: } (ab)c = a(bc)$$

Examples: i) Set of integers under addition. $e=0$, $a^{-1}=-a$. ' $ab=ab$ '
(Set of +ve integers: do not form group)

ii) Set of rational num (excl. 0) under multiplication $ab=ba$

iii) Set of rotations in 2d ~~about~~

iv) Set of rotations in 3d

v) Set $\{e, a, a^2\}$ with $a^3 = e$

If $ab = ba$, abelian group. Example: i-iii) and v) above. iv) non-abelian.

If # elements is finite, $\Rightarrow$ finite group. Only v) above is finite.

Order of a group = # of elements.

Some properties of inverse & identity:

① right inverse exists and is equal to left inverse:

$$\text{If } a^{-1}a = e, \quad aa^{-1} = (a^{-1})^{-1}a^{-1}aa^{-1} = (a^{-1})^{-1}a^{-1} = e$$

② If $ea = a$, $ae = a^{-1}a^{-1}a = ea = a$

③ If $ab = ac \Rightarrow b = c$

④ identity unique: if $ae = a$, $ae^{-1} = a \Rightarrow e = e^{-1}$

⑤ $(a^{-1})^{-1} = a$; $(ab)^{-1} = b^{-1}a^{-1}$.

For a finite group, any element a must have the property that $a^r = e$ for some integer r . [otherwise completion of group requires $e, a, a^2, a^3, \dots$ to be elements $\Rightarrow$ infinite group]

If $a^r = e$, and $a^s \neq e$ for $0 < s < r \Rightarrow$ ~~minimum~~ a is called an element of order r .

If order of an element = order of the group: group is $\{1, a, a^2, \dots, a^{r-1}\}$

Such a group is called cyclic group.

Group of order 1: $\{e\}$

2: $\{e, a\}, a^2 = e$

multiplication table:

	e	a
e	e	a
a	a	e

3: $\{e, a, b\}$ has to be cyclic: $b = a^2$

[multiplication table: each element appears once in each row/column. If $a^2 = e, ab = b \Rightarrow a = e$ (X)]

	e	a	b
e	e	a	b
a	a	b	e
b	b	e	a

4: $\{e, a, b, c\}$ one option: $\{e, a, a^2, a^3\}$ (call (4a))

another option: $a^2 = b^2 = c^2 = e, ab = c$ etc

$\Rightarrow$

	e	a	b	c
e	e	a	b	c
a	a	e	c	b
b	b	c	e	a
c	c	b	a	e

(4b)

If $H \subset G$ is a group under same multiplication law: Subgroup
for any G , $\{e\}$ and G are Subgroups. Any other Subgroup is
called a proper Subgroup.

eg. for (4a), $\{e, a^2\}$ proper Subgroup. (4b): $\{e, a\}$ proper Subgroup

Now say H is proper Subgroup of G . Take $g \in G, g \notin H$.

gH is disjoint from H : if $ghi = hj$, $g = hjhi^{-1} \in H$.

Take $g' \notin H, g'H$ Then $g'H$ disjoint from H, gH

This way: $G = H + gH + g'H + \dots$ So $n_G = m \cdot n_H$.

(4)

$\Rightarrow$ order of a subgroup H is a factor of order of the group.

The sets $H, gH, g'H, \dots$ are called left cosets of H in G .

Similarly we could construct right cosets, which are different in general.

Since in a group, $\{e, a, a^2, \dots, a^{r-1}\}$ always forms a subgroup

$\Rightarrow$ order of the group is a multiple of order of any element.

$\Rightarrow$ If order of group = prime number, the group is cyclic.

If $aH = Ha \quad \forall a \in G$, H called an invariant subgroup of G

$$ha = ah \Rightarrow ha = ah a^{-1} \quad \forall a \in G$$

If G has no invariant subgroup $\Rightarrow$ simple.

no abelian invariant subgroup $\Rightarrow$ semisimple.

If $gag^{-1} = b$, where $a, g, b \in G$, a is said to be conjugate to b .

all elements formed doing gag^{-1} are said to form a conjugacy class.

For abelian groups, $gag^{-1} = a \Rightarrow$ each element forms a conjugacy class.

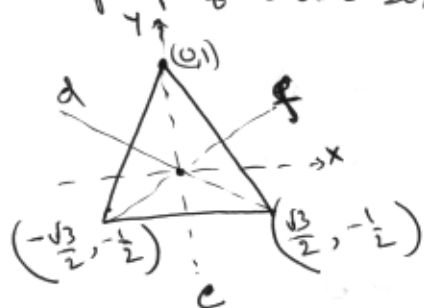
If H is an invariant subgroup of G , the cosets gH form a group with a multiplication law determined by that of G :

$$aH \cdot bH = abH \quad \text{Identity} = H.$$

This is called the quotient group G/H . order = $\frac{n_G}{n_H}$.

Ex: $G = \{e, a, a^2, a^3\}$, $H = \{e, a^2\}$ $G/H = \{E, A\} = \mathbb{Z}_2$

Ex: Group of order six: symmetries of an equilateral triangle



symmetries: along z-axis, rot by $\frac{2\pi}{3}, \frac{4\pi}{3}$
a b

reflections about the three axes: c, d, f

multiplication table:

	e	a	b	c	d	f
e	e	a	b	c	d	f
a	a	b	e	d	f	c
b	b	e	a	f	c	d
c	c	f	d	e	b	a
d	d	c	f	a	e	b
f	f	d	c	b	a	e

this is nonabelian (smallest non abelian group)
(This group is known as C_{3v}).

$H = \{e, a, b\}$: abelian invariant subgroup

quotient group: $\{H, A\}$ where $A = cH$.

Conjugacy classes: $\{e\}, \{a, b\}, \{c, d, f\}$.

Homomorphism If G, H are two groups, homomorphism $\phi: G \rightarrow H$ is a mapping that preserves the group multiplication structure: $\phi(g_1) \cdot \phi(g_2) = \phi(g_1 g_2)$.

Kernel of $\phi : \{g_i\}$ s.t. $\phi(g_i) = e_H$. Check $\text{Ker}(\phi)$ is ^{invariant} subgroup of G .
 image of ϕ : all elements $\phi(g_i)$. and $\text{Im}(\phi)$ subgroup of H .

If $\text{Im}(\phi) = H$, The mapping is onto.

If ϕ is one-one and onto, it is called isomorphism.

Check if mapping is isomorphism, $\text{Ker}(\phi) = \{e\}$.

Representation

Homomorphism ~~from G to H~~ $G \rightarrow H$

$G \rightarrow n \times n$ matrices $D(g)$. Called n -dim repr.

If g mapped to $D(g) \Rightarrow D(e) = I, D(g^{-1}) = D^{-1}(g),$

$$D(g_1 g_2) = D(g_1) \cdot D(g_2) \text{ etc.}$$

If mapping one-one, it is called a faithful repr.

Example For C_{3v} , from the coordinates, an obvious ^{2-dim} faithful repr.

$$e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, a = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, b = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix},$$

$$c = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, d = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, f = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

An unfaithful repr. : all elements $\rightarrow I$
 this is called the trivial repr.

Of course, by a change of basis, the repr. can be changed to
 $S^{-1} D(g) S \neq D(g)$. Reprs. connected like this are called equivalent repr.

Theorem

Any repr. of a finite group is equivalent to a unitary representation.

Proof : Say D not unitary $\Rightarrow \langle Dx | Dy \rangle \neq \langle x | y \rangle$

This means columns of D are not orthonormal (under normal inner product)
 $\langle x|y \rangle = \sum_i x_i^* y_i$

Define a new inner product: $\langle x|y \rangle = \frac{1}{n_G} \sum_{g \in G} \langle D(g)x | D(g)y \rangle$

check $\langle x|y \rangle$ is a valid inner product.

$\Rightarrow$ for any two vectors $|x\rangle, |y\rangle$: $\langle D(h)x | D(h)y \rangle = \langle x|y \rangle$

$\Rightarrow D$ unitary in this inner product

Now say $|e_i\rangle$ is orthonormal basis: $\langle e_i | e_j \rangle = \delta_{ij}$

and $|e'_i\rangle$ is orthonormal basis under the new inner product: $\langle e'_i | e'_j \rangle = \delta_{ij}$

Expand: $|e'_i\rangle = T_{ij} |e_j\rangle$. Form $\tilde{D}(g) = T^{-1} D(g) T$.

Then $\tilde{D}(g)$ is the required unitary repr.

$$\begin{aligned} \text{for, } \langle \tilde{D}(g)x | \tilde{D}(g)y \rangle &= \langle T^{-1} D(g) T x | T^{-1} D(g) T y \rangle \\ &= \langle D(g) T x | D(g) T y \rangle = \langle T x | T y \rangle = \langle x | y \rangle \end{aligned}$$

Reducible and irreducible repr.

If we have repr. of G on a n -dim vector space, but the ~~vector~~ ^{action of} elements of G ~~is such that~~ is such that a subspace of the vector space is invariant under G , we call it reducible repr.

If the repr. is reducible, ~~give a suitable choice~~ say W is m -dim subspace of n -dim V which is left invariant by G .
 Choosing a basis in V such that first m vectors span W : clearly all $D(g)$ are of the form $\begin{pmatrix} A_{m \times m} & B_{m \times (n-m)} \\ 0 & C_{(n-m) \times (n-m)} \end{pmatrix}$.

(8)

If $D(g)$ is unitary, the form becomes $\begin{pmatrix} A & 0 \\ 0 & C \end{pmatrix}$. ~~reduced~~

If a repr. is not reducible, it is called irreducible (or irrep).

Schur's lemma ① If $D(g)$ and $D'(g)$ two reprs, dim. n & n' with $n > n'$, $D(g)$ reducible if $\exists A$ such that $D(g)A = A D'(g)$.

Proof ~~If D is reducible~~ If D is repr. $\Rightarrow |V\rangle \rightarrow D|V\rangle$
 $v_i \rightarrow D_{ij} v_j$

If D reducible, $\exists$ a set $|V'\rangle = A|V\rangle$, $v'_i = A_{ij} v_j$

Such that $v'_i \rightarrow D'_{ij} v'_j = D'_{ij} A_{jk} v_k$

also $v'_i = A_{ij} v_j \rightarrow A_{ij} D'_{jk} v_k \Rightarrow D'_{ij} A_{jk} v_k = A_{ij} D_{jk} v_k$

Since this is true for all $|V\rangle$: $D'A = AD$.

Easy to see that the argument can be run back wards $\Rightarrow$ if $D'A = AD$ then D is reducible.

② If D, D' are irreps, with $AD = D'A$, then either $n = n'$ and A is invertible; or $A = 0$.

For, if $n > n'$, from the argument above, D is reducible. If $n' > n$, D' is obviously reducible.

If $n = n'$, if A is invertible then D & D' are equivalent.

If A not invertible, let $A = 0 \Rightarrow |V'\rangle = A|V\rangle$ span a lower dimensional space than that spanned by $|V\rangle$. Since this space is invariant under D , the n -dim repr. is reducible.

Schur's lemma ② If $AD(g) = D(g)A \quad \forall g \in G$ and $D(g)$ is irrep, then $A = \lambda I$.

Proof take $A|v\rangle = \lambda|v\rangle$

$$\text{Now } D(g)A|v\rangle = \lambda D(g)|v\rangle = A D(g)|v\rangle \Rightarrow D(g)|v\rangle \text{ is}$$

eigenvector with eigenvalue λ

Since it is irrep, all $D(g)|v\rangle$ span the space $\Rightarrow A = \lambda I$ in this space.

~~Example~~

Example Take the 2-dim irrep of C_{3v} .

Simpler to work in the basis such that a is diagonal:

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \quad S^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$$

$$\tilde{a} = S^{-1} a S = \begin{pmatrix} \omega & 0 \\ 0 & \omega^2 \end{pmatrix}, \quad \omega = e^{2\pi i/3} = -\frac{1}{2} + \frac{\sqrt{3}}{2}i, \quad \omega^2 = e^{4\pi i/3} = -\frac{1}{2} - \frac{\sqrt{3}}{2}i$$

$$\tilde{b} = S^{-1} b S = \begin{pmatrix} \omega^2 & 0 \\ 0 & \omega \end{pmatrix}, \quad \tilde{c} = S^{-1} c S = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \tilde{d} = S^{-1} d S = i \begin{pmatrix} 0 & \omega \\ \omega^2 & 0 \end{pmatrix}$$

$$\tilde{f} = S^{-1} f S = i \begin{pmatrix} 0 & \omega^2 \\ \omega & 0 \end{pmatrix}$$

Let $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ commute with all.

$$A\tilde{a} = \tilde{a}A \Rightarrow \begin{pmatrix} a\omega & b\omega^2 \\ c\omega & d\omega^2 \end{pmatrix} = \begin{pmatrix} a\omega & b\omega \\ c\omega^2 & d\omega^2 \end{pmatrix} \Rightarrow b=c=0 \Rightarrow \begin{pmatrix} a & 0 \\ 0 & d \end{pmatrix}$$

$$a\tilde{c} = \begin{pmatrix} 0 & a \\ -d & 0 \end{pmatrix} = \tilde{c}a = \begin{pmatrix} 0 & d \\ -a & 0 \end{pmatrix} \Rightarrow a=d \Rightarrow A = aI.$$

Corollary for abelian group, all irreps are 1-dim. Since if not,

since $D(h)$ commutes with all $D(g)$, $D(h) = a \cdot I \Rightarrow$ reducible.

Example $\{e, a, b\}$ is abelian in above example $\Rightarrow$ fully reducible.

Now take $A = \sum_g D(g) X D(g^{-1})$, X : $n_r \times n_r$ matrix and $D(g)$: n_r dim. irrep

$$\Rightarrow A D(g) = D(g) A \Rightarrow A = \lambda I$$

Take X : jk th element = 1, rest = 0

$$\Rightarrow \sum_g D(g)_{ij} D(g^{-1})_{kl} = \lambda \delta_{il}$$

Take $i=1$, sum $\Rightarrow \sum_g \sum_i D(g)_{ij} D(g^{-1})_{ki} = \sum_g \delta_{kj} = n_g \delta_{jk} = \lambda n_r$

$$\Rightarrow \lambda = \frac{n_g}{n_r} \delta_{jk}$$

$$\Rightarrow \sum_g D(g)_{ij} D(g^{-1})_{kl} = \frac{n_g}{n_r} \delta_{jk} \delta_{il}$$

If we take inequivalent irreps r, s : $A = 0$ So combining,

$$\sum_g D^r(g)_{ij} D^s(g^{-1})_{kl} = \frac{n_g}{n_r} \delta_{rs} \delta_{jk} \delta_{il}$$

If unitary repr. : $\sum_g D^r(g)_{ij} D^s(g)^*_{kl} = \frac{n_g}{n_r} \delta_{rs} \delta_{jk} \delta_{il}$

Think of $D^r(g)_{ij}$ as the j th component of a vector in an n_r -dim vector space $\Rightarrow$ The above reln. indicates $\sum_{\text{all irreps } r} n_r^2$ orthogonal vectors in this space. $\Rightarrow \sum_{\text{irreps } r} n_r^2 < n_g$.

Characters The explicit matrices $D(g)$ have superfluous information $\rightarrow$ eg. two equivalent irreps have different $D(g)$. We can, instead, work with $\text{tr } D(g)$, called character, $\chi(g)$. This does not have complete information : elements in same conjugacy class have same character (so better to talk of $\chi(c)$, character of a conjugacy class).

From the above orthogonality reln., $\sum_g \chi^r(g) \chi^s(g^{-1}) = n_g \delta_{rs}$

for unitary: $\sum_g \chi^r(g) \chi^s(g)^* = n_G \delta_{rs}$

if n_c : no. of elements in conjugacy class c ,

$$\Rightarrow \sum_c n_c \chi^r(c) \chi^s(c)^* = n_G \delta_{rs}$$

using similar arguments ($\sqrt{n_c} \chi^r(c)$ being c th component of a vector

$\Rightarrow$ n_{irrep} orthogonal vectors where n_{irrep} = total # of inequivalent irreps of G) $\Rightarrow$ no. of inequivalent irreps $\leq$ # of conjugacy classes

Now take a (possibly reducible) rep D in unitary rep, and use a basis

such that $D(g) = \bigoplus_r a_r D^r(g)$, The sum is over irreps and a_r is integer

$$\Rightarrow \chi_c = \sum_r a_r \chi_c^r$$

$$\Rightarrow \sum_c \chi_c^{s*} \chi_c n_c = \sum_r a_r \sum_c \chi_c^{s*} \chi_c^r n_c = n_G a_s$$

$$\Rightarrow a_r = \frac{1}{n_G} \sum_c \chi^r(c)^* \chi(c) n_c.$$

Using this, we can show that $\sum_{\text{irrep } r} n_r^2 = n_G$. For this,

we use a reducible $n_G \times n_G$ representation of G that follows directly from the

group multiplication table: if in the table, the row against a_i is

$a_{i1} \dots a_{in_G}$ (i.e. $a_i \cdot (a_1 \dots a_{n_G}) = a_{i1} \dots a_{in_G}$) then take

$$D(a_i)_{jk} = \delta_{k, j_i}$$

Example: from our multiplication table for C_{3v} , $D(e) = 1_G$,

$$D(a) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, D(b) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, D(c) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, D(d) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, D(f) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

In this repr., $D(e) = 1_{n_G}$ so $\chi(e) = n_G$, $\chi(g \neq e) = 0$

$$\text{Therefore } \sum_c \chi(c)^* \chi(c) n_c = n_G^2$$

Now if this repr. has irrep r with multiplicity a_r , etc,

$$\text{then } a_r = \frac{1}{n_G} \sum_c \chi^r(c)^* \chi(c) n_c = \frac{1}{n_G} \cdot n_r \cdot n_G = n_r$$

$$\begin{aligned} \text{also } \chi_c &= \sum_r a_r \chi^r(c) \Rightarrow n_G^2 = \sum_c \sum_r a_r \chi^r(c)^* \chi(c) n_c \\ &= \sum_r a_r \cdot n_G a_r = n_G \sum_r a_r^2 \end{aligned}$$

$$\Rightarrow n_G = \sum_r n_r^2$$

So, eg., C_{3v} has 1, 2-dim irrep and 2, 1-dim irreps.

We can construct a "character table" of the irreps.

	$C_1 = \{e\}$	$C_2 = \{a, b\}$	$C_3 = \{c, d, f\}$
$\chi^1_{(1\text{-dim})}$	1	1	1
$\chi^2_{(1\text{-dim})}$	1	1	-1
$\chi^3_{(2\text{-dim})}$	2	-1	0

Can be constructed by using: ① 1st row (trivial repr.) and 1st column (χ for identity) are obvious.

② use $\sum_c n_c \chi^r(c) \chi^s(c)^* = n_G \delta_{rs}$

③ C_3 : reflections. So $\chi^2_{(1\text{-dim})}(c_3) = \pm 1$. Similarly $\chi^3_{(2\text{-dim})}(c_2) = 1, e^{2\pi i/3}, e^{-2\pi i/3}$.

$\Rightarrow$ gives 2nd row.

Now for 3rd row, 2 orthogonality conditions $\Rightarrow$ determine the row.

Could also use restrictions like in ③ on 3rd row.

Of course, here we already knew the 2-d repr. So could write the third row straight.

Note that the columns ~~are~~ are orthogonal. This can be shown to be true in general: $\sum_p \chi^p(i) \chi^p(j)^* = \delta_{ij} \frac{n_G}{n_{C_i}}$

$\Rightarrow$ by similar arguments, # conjugacy classes $\leq$ # ineq. irreps

$\Rightarrow$ # conjugacy classes = # ineq. irreps.

Symmetry and quantum mechanics

One application of group theory is in finding the degeneracy of the energy eigenstates.

If ~~the system~~ ^{system} is invariant under a symmetry group R ,

take a unitary repn. $U_R : [U_R, H] = 0$

If $|\psi\rangle$ energy eigenstate: $H|\psi\rangle = E|\psi\rangle \Rightarrow H U_R |\psi\rangle = E U_R |\psi\rangle$

Take a d -dim irrep $D(U_R)$: d -fold degenerate eigenstate

$[H, D] = 0 \Rightarrow H = E \mathbb{1}$ in this subspace.

eg. take ~~a molecule~~ a molecule like BCl_3 , which has C_{3v} symmetry.

$\Rightarrow$ ground state, parity odd state, 2-dim irrep.

Continuous groups Take, eg., $GL(2, \mathbb{R})$: matrices $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, a, b, c, d real and $ad - bc \neq 0$

Non-abelian group with infinite elements $\Rightarrow$ the previous analyses not of much help.

Take an element close to unity: $A = \mathbb{1} + \delta a_i T_i$, where $T_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $T_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ etc.

This is example of a four-parameter continuous group. The T_i are called generators of this group.

The group composition law $M(a_1 \dots a_4) \cdot M(b_1 \dots b_4) = M(c_1 \dots c_4)$ give $c_i = \varphi_i(a, b)$. If φ_i differentiable $\Rightarrow$ Lie group. $GL(2, \mathbb{R})$ is a Lie group.

If we expand $[T_i, T_j] = f_{ijk} T_k \Rightarrow f_{ijk}$ are called structure constants. ~~Note: for abelian group~~ [only for nonabelian group]

Some examples ① $SO(3)$: 3-parameter group. Generators :

$$T_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, T_2, T_3 \text{ with } [T_i, T_j] = \epsilon_{ijk} T_k.$$

② $SU(N)$: $U^\dagger U = \mathbb{1}$, $\det U = 1$. $(N^2 - 1)$ parameter group.