Nuclear Theory Summer School

BRIDGING METHODS IN NUCLEAR THEORY (BMinNT)

Strasbourg - 26-30 June 2017

A SHORT INTRODUCTION TO GROUP THEORY

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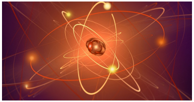

BMinNT: group theory is the perfect illustration of a Bridging Method in Nuclear Theory !

OUTLINE

- General considerations on group theory
- Some simple quantum mechanical applications
- Rotations in 2 and 3 dimensions
- Dynamical symmetries
- The unitary group U(n)

GENERAL CONSIDERATIONS ON GROUP THEORY

WHAT IS A GROUP ?

THIS IS A VERY NICE GROUP !

WHAT IS A GROUP ?

A group G is an ensemble of elements $G = \{E, A, B, C, D \ldots\}$ with an internal multiplication law $\circ$ such that:

- $\forall A, B \in G$, $A \circ B \in G$ and $B \circ A \in G$ (**closure relation**).
- $\forall A, B, C \in G$, $A \circ (B \circ C) = (A \circ B) \circ C$ (**associativity**).
- There exists an **identity** element E (from the german word Einheit) such that $\forall A \in G$, $A \circ E = E \circ A = A$.
- $\forall A \in G$, there exists an **inverse** $A^{-1} \in G$ such that $A \circ A^{-1} = A^{-1} \circ A = E$.

Remarks:

$\longrightarrow$ Often the symbol $\circ$ is omitted.

$\longrightarrow$ In general the commutation is NOT commutative.
If it is the case, the group is called **abelian**.

A FEW EXAMPLES...

- All integers under addition (infinite, discrete, abelian group).
- The n complex numbers $\exp(2\pi mi/n), m = 0, 1, \ldots, n-1$ under multiplication (cyclic group C_n, abelian).
- Two-dimensional rotation group R_2 (abelian).
- Three-dimensional rotation group R_3 (non-abelian !).
- Etc. etc. etc.

AN EXAMPLE OF A POINT GROUP

Symmetry group of the Eiffel Tower in Paris: C_{4v} (point-group)

$$C_{4v} = \{E, C_4, C_4^2, C_4^3, \sigma_v^{(1)}, \sigma_v^{(2)}, \sigma_v^{(3)}, \sigma_v^{(4)}\}$$

<u>EXERCISE</u>: explain what are the elements of the group C_{4v} !

SOME USEFUL DEFINITIONS

- The number of elements of a group $g \equiv |G|$ is the **order of the group**. If g is (in)finite, the groupe is called (in)finite.
- For a given element A, the different powers A^2, A^3 etc. belong to the group ! Therefore, for a finite group, there exists an integer n such that $A^n \in G$. The smallest integer for which this relation holds is the **order of the element A**.
- The ensemble $\{E, A, A^2, A^3 \ldots\}$ forms **the cyclic group of order n**. Cyclic groups are abelian !
- An ensemble $\{A, B, C, D \ldots\}$ of elements of G is an ensemble of **generators** of the group if every element of G is expressible as a finite product of powers of $\{A, B, C, D \ldots\}$.
  Note that a cyclic group is generated by a unique generator.
- G_S is a **subgroup** of G if it is itself a group with the same multiplication law $\circ$. Notation: $G \supset G_S$.

INVARIANT SUBGROUPS

- A subgroup H of a group G is an **invariant subgroup in G** when $g\{H\}g^{-1} = \{H\}, \forall g \in G$, i.e. $ghg^{-1} \in H, \forall g \in G$ and $\forall h \in H$.
- A group possessing no invariant subgroup apart from E and G itself is called **simple**.
- A group is called **semi-simple** if its invariant subgroups are non-abelian.

COSETS, CONJUGATED ELEMENTS AND CLASSES

- Be H a (proper) sub-group of G ($|H| < |G|$), and $g \in G$ ($g \notin H$).
  $\{g \circ H\}$ is called the **left coset** of H in G and
  $\{H \circ g\}$ is called the **right coset** of H in G, with respect to g.

- An element $B \in G$ is the **conjugated** of A if one can find $g \in G$ such that $B = gAg^{-1}$.

  Remark: since $A = g^{-1}Bg$, A is also the conjugated element of the element B.

- Conjugated elements form a **class of conjugated elements** or, simply, a **class**.

LINEAR AND MATRIX REPRESENTATIONS OF A GROUP

- An application F (which associates to each element g an image $F(g)$) is said to be **homomorphic** if

$$F(g_1)F(g_2) = F(g_1 g_2)$$

- Be now a linear vector space $\mathcal{V}$ with an ensemble of transformations $\mathcal{A} = \{T, T', T'', \ldots\}$ acting in $\mathcal{V}$, i.e. $T(\alpha u + \beta v) = \alpha Tu + \beta Tv$, $\forall \alpha, \beta \in \mathbb{R}$ and $u, v \in \mathcal{V}$.

  If $\mathcal{A}$ is homomorphic to a group G, then $\mathcal{A}$ is called a **linear representation** of G.

- If $\mathcal{V}$ is of finite dimension, the relation $v' = Tv$ can be expressed, within a given basis, as $v'_i = \sum_j D_{ij}(g) v_j$.

  The set of matrices $\{D(g), g \in G\}$ forms a group under matrix multiplication, and the correspondance $g \to D(g)$ is called a **matrix representation** of G.

REDUCIBLE/IRREDUCIBLE and EQUIVALENT REPRESENTATIONS

Reducible/irreducible representations

- $\mathcal{A}$ is said to be a **reducible representation** of a group G in a vector space $\mathcal{V}$ if there exists in $\mathcal{V}$ a subspace $\mathcal{V}'$ invariant with respect to the transformations $\mathcal{A}$.
- If $\mathcal{A}$ is not reducible (i.e. only $\mathcal{V}$ itself is invariant), then $\mathcal{A}$ is an **irrreducible representation (irrep)** of G.

Equivalent representations

- Be 2 matrix representations $T = \{T(E), T(A), T(B) \ldots\}$ and $T' = \{T'(E), T'(A), T'(B) \ldots\}$ of a group G.
- Suppose the existence of a non-singular matrix S such that $T(A) = S^{-1}T'(A)S$ (and identical relations with B, C ...).
- Then T and T' are 2 **equivalent representations** of G.

NOW TWO SHORT EXERCICES !

EXERCISE 1

Show that $T(E) = \mathbb{I}$ (unity matrix).

EXERCISE 2

Show that $T(A^{-1}) = \Big[T(A)\Big]^{-1}$.

THE SOLUTIONS !

SOLUTION TO EXERCISE 1

$\forall A \in G, EA = AE = A$ implies that

$$T(E)T(A) = T(A)T(E) = T(A)$$

If one supposes $\det T(A) \neq 0$, this matrix equation can only be satisfied for $T(E) = \mathbb{I}$, q.e.d.

SOLUTION TO EXERCISE 2

Since we have $A\,A^{-1} = E$, it follows that
$T(A\,A^{-1}) = T(A)\,T(A^{-1}) = T(E) = \mathbb{I}$.

Again, with the assumption $\det T(A) \neq 0$, we obtain immediately
$T(A^{-1}) = \left[T(A)\right]^{-1}$, q.e.d.

DIRECT PRODUCT OF GROUPS

- Be two groups G_1 and G_2. We define the **product of pair elements** as

$$(g_1, g_2) \times (g_1', g_2') \equiv (g_1 \circ g_1', g_2 \bullet g_2')$$

for $g_1, g_1' \in G_1$ and $g_2, g_2' \in G_2$.

- The ensemble $G_1 \otimes G_2$ of pairs (g_1, g_2) form a group under the multiplication $\times$, called **direct product of G_1 and G_2**.

CHARACTERS

Let us start wit two equivalent representations T and T':
$\forall A \in G, T'(A) = S\,T(A)\,S^{-1}$ (similarity transformation).

EXERCISE: show that the trace is invariant with respect to the similarity transformation, i.e. $\mathrm{Tr}\,T' = \mathrm{Tr}\,T$.

SOLUTION:

We have $T' = S\,T\,S^{-1}$, and therefore

$$
\begin{aligned}
\operatorname{Tr} T' &= \sum_i T'_{ii} \\
&= \sum_i \left[S\,T\,S^{-1}\right]_{ii} \\
&= \sum_i \left[\sum_k S_{ik}\,(T\,S^{-1})_{ki}\right] \\
&= \sum_i \sum_k S_{ik} \sum_l T_{kl}\,(S^{-1})_{li} \\
&= \sum_{kl} T_{kl} \sum_i (S^{-1})_{li}\,S_{ik}
\end{aligned}
$$

Using now the fact that $S^{-1}\,S = \mathbb{I}$, or, explicitly,

$$(S^{-1}\,S)_{lk} = \delta_{lk} = \sum_i S_{ik}\,(S^{-1})_{li}$$

we end up with

$$\begin{aligned} \mathrm{Tr}\,T' &= \sum_{kl} T_{kl} \sum_i (S^{-1})_{li}\,S_{ik} \\ &= \sum_{kl} T_{kl}\,\delta_{lk} \\ &= \sum_k T_{kk} \\ &= \mathrm{Tr}\,T \quad \text{q.e.d.} \end{aligned}$$

CHARACTERS

Definition

Be $g \in G$ and $D(g)$ its representation, of matrix $\Big(D(g)\Big)_{ij}$. The **character** of $g \in G$ in the representation $D(g)$ is defined as the trace

$$\chi(g) \equiv \mathrm{Tr}\Big[D(g)\Big] \equiv \sum_i \Big(D(g)\Big)_{ii}$$

Theorem

Be $g, h, g' \in G$ such that $g' = h \circ g \circ h^{-1}$, meaning that g and g' belong to the same class of equivalence. One has $\chi(g') = \chi(g)$.

$\rightarrow$ One says that all elements in a class have the same character in a given representation.

$\rightarrow$ The character is therefore a function of classes, similarly to the fact that a representation is a function of the elements of a group.

SCHUR'S LEMMAS and CRITERIA OF IRREDUCIBILITY

Schur's lemma I (a)

If D and D' are two irreps of a group G of **different dimensions**, and if matrix A satisfies $D(g)A = AD'(g), \quad \forall g \in G$, then $A = 0$.

Schur's lemma I (b)

If D and D' are two irreps of a group G of **equal dimensions**, and if matrix A satisfies $D(g)A = AD'(g), \quad \forall g \in G$, then
i) Either $A = 0$,
ii) or D and D' are inequivalent, and det $A \neq 0$.

Schur's lemma II

If the matrices $D(g)$ form an irrep of a group G, and if
$D(g)A = AD(g), \quad \forall g \in G$, then $A = \lambda\mathbb{I}$ or $A = 0$ (λ being a constant).

PROPERTIES

Property 1

The number of non-equivalent irreducible representations of a given group is EQUAL to the number of classes in the group.

Property 2

If d_μ denotes the dimension of irrep $[\mu]$, $n_{irr.}$ the number of irreps and n_G the order of a group, it can be shown that

$$\sum_{\mu=1}^{n_{irr.}} d_\mu^2 = n_G$$

REPRESENTATIONS OF ABELIAN GROUPS

For an ABELIAN group, we have $\forall g, g' \in G$, $gg' = g'g$ and thus $g' = g\, g'\, g^{-1}$. This means that **for an abelian group, each element forms its own class**.

Consequently, **for an abelian group, the number of equivalence classes is equal to n_G, the order of the group** (=number of elements of the group).

Therefore, **for an abelian group, the number of non-equivalent irreducible representations is equal to the order of the group ($n_{irr.} = N_G$)**.

Using property 2 seen previously, we get $\sum_{\mu=1}^{n_G} d_\mu^2 = n_G$, which is only possible with $d_\mu = 1, \forall \mu$!

Thus, **for an abelian group, the irreducible representations are all one-dimensional**.

REPRESENTATIONS OF ABELIAN GROUPS

Consider now a FINITE abelian group. In such a case, the order of each element, say k, is finite, and we have the property

$$g^k = E \longleftrightarrow D(g^k) = D(E) \longleftrightarrow \Big[D(g)\Big]^k = 1$$

Of course, for one-dimensional representations, matrix and character will coincide:

$$\big[D(g)\big]_{11} = \chi(g).$$

Therefore we get the result

$$\chi(g) = \exp 2\pi i l/k, \quad l = 1, \ldots, k.$$

<u>In other words</u>: for such representations, the numerical values of the characters are the complex roots of unity.

A SIMPLE ILLUSTRATION

Let us consider the point-group $C_2 = \{E, \hat{C}_2\}$.

For this particular example we have $n_{irr.} = 2$, and each of these two irreps is one-dimensional, since the group is abelian. We denote them by $D^{[1]}$ and $D^{[2]}$.

We have $D^{[1]}(E) = \chi^{(1)}(E) = \mathbb{I}$ and $D^{[2]}(E) = \chi^{(2)}(E) = \mathbb{I}$.

Furthermore one has $\hat{C}_2^2 = E$, wherefrom $\left[\chi(\hat{C}_2)\right]^2 = 1$, and thus $\chi(\hat{C}_2) = \pm 1$. We will then attribute arbitrarily $\chi(\hat{C}_2) = +1$ to $\chi^{(1)}$, and $\chi(\hat{C}_2) = -1$ to $\chi^{(2)}$.

The results are usually summarized in a **character table**:

C_2	E	$\hat{C}_2$
$D^{(1)}$	$+1$	$+1$
$D^{(1)}$	$+1$	-1

QUANTUM MECHANICAL APPLICATIONS

SPECTROSCOPIC PROPERTIES

- Consider a hamiltonian H of a quantal system invariant under all symetry transformations g of a group G. One says also that G is the **symmetry group of H**: $[H, D(g)] = 0, \forall g \in G$.
- The irreps of the group are denoted by $D_{ij}^{[\mu]}(g)$, and the corresponding invariant subspaces by $\{\varphi^{[\mu]}; \mu = 1, \ldots, n_{irr.}\}$: $\{\varphi\} = \{\varphi^{[\mu_1]}\} \oplus \ldots \oplus \{\varphi^{[\mu_{n_{irr.}}]}\}$.
- In each sub-space one can introduce a **basis**: $B^{[\mu]} \equiv \{\psi_i^{[\mu]}; i = 1, \ldots, n_\mu\}$.

Using Schur's lemma, one can demonstrate the following theorem:

$$\langle\psi_i^{[\mu]}|H|\psi_j^{[\nu]}\rangle = \delta_{\mu\nu}\langle\psi_i^{[\mu]}|H|\psi_j^{[\mu]}\rangle$$

SPECTROSCOPIC PROPERTIES

One demonstrates the following property:

$$\sum_{g \in G} D_{lm}^{[\mu]^*} D(g) \psi_i^{[\nu]} = \frac{n_G}{n_\nu} \delta_{\mu\nu} \delta_{mi} \psi_l^{[\nu]}$$

Theorem

Be $\varphi_i^{[\mu]}$ a solution of the Schrödinger equation $H\varphi_i^{[\mu]} = e^{[\mu]}\varphi_i^{[\mu]}$.
One demonstrates that $H\varphi_j^{[\mu]} = e^{[\mu]}\varphi_j^{[\mu]}$, which means that:

- All members of the **multiplet** can be generated starting from one of it's member (this is demonstrated with the help of the above property). ($\rightarrow$ A multiplet is in fact an an irreducible invariant subspace of a given group).
- All members of the multiplet are **degenerate with respect to the same eigen-energy**.

LIE GROUPS

A **Lie group** G of order r is a special case of of continuous group whose elements are noted $R(a)$; $a \equiv (a_1, a_2, \ldots, a_r)$ represent r real parameters. It obeys the following 5 postulates:

- There exists an identity element $R(a_0)$ such that $R(a_0)R(a) = R(a)R(a_0) = R(a), \quad \forall R(a) \in G.$ NB: usually one takes $a_0 = 0$.
- For all a one can find $\bar{a}$ such that $R(\bar{a})R(a) = R(a)R(\bar{a}) = R(0)$, which means that for all $R(a)$ there exists an inverse $R(\bar{a}) = R^{-1}(a)$.
- For given parameters a and b one can find parameters c such that $R(c) = R(b)R(a)$, where c are real functions of a and b, i.e. $c = \varphi(a, b)$ (combination law for the group parameters).
- Associativity: $R(a)[R(b)R(c)] = [R(a)R(b)]R(c)$ and $\varphi(\varphi(c, b), a) = \varphi(c, \varphi(b, a))$.
- Parameters c above are analytical functions of a and b, and $\bar{a}$ are analytical functions of a.

NB: if the parameters are bounded the Lie group is called compact.

LIE ALGEBRAS

DEFINITION

A (real or complex) vector space $\mathcal{A}$ is called a **Lie algebra** if it has been defined a **Lie multiplication** or **commutator** $[X, Y]$ satisfying, $\forall X, Y, Z \in \mathcal{A}$:

- $[X, Y] \in \mathcal{A}$.
- $[\alpha X + \beta Y, Z] = \alpha[X, Z] + \beta[Y, Z], \forall \alpha, \beta \in \mathbb{R}$ or $\mathbb{C}$ (bilinearity).
- $[X, Y] = -[Y, X]$.
- $\Big[[X, Y], Z\Big] + \Big[[Y, Z], X\Big] + \Big[[Z, X], Y\Big] = 0$ (Jacobi associativity).

STRUCTURE CONSTANTS

Within the basis $\{e_i; i = 1, \ldots, n\}$, $X = \sum_i a_i^X e_i$ and $Y = \sum_j a_j^Y e_j$. One then writes $Z = [X, Y] = \sum_k a_k^Z e_k = \sum_{ij} a_i^X a_j^Y [e_i, e_j]$. Defining now the **structure constants** of the Lie algebra $[e_i, e_j] = \sum_k c_{ij}^k e_k$, one can write $a_k^Z = \sum_{ij} c_{ij}^k a_i^X a_j^Y$.

GENERATORS OF LIE GROUPS

With the requirement of analyticity, each element g in the neighborhood of the identity E can be expressed as

$$g(0, \ldots, \varepsilon_j, \ldots, 0) \simeq E + i\varepsilon_j I_j$$

where

$$I_j \equiv \frac{1}{i}\left(\frac{\partial g}{\partial \varepsilon_j}\right)_{(0)}$$

are called the **generators** of the Lie group.

By successive application of the product one can reach an element of the group at finite distance from the identity:

$$g(a) \equiv g(a_1, \ldots, a_r) = e^{i \sum_{i=1}^{r} a_i I_i}$$

NB: a Lie group with r parameters has r generators.

CASIMIR OPERATORS OF LIE GROUPS

- The maximal number of generators of a Lie group commuting with each other is it's **rank**.
- An operator commuting with all the generators of a Lie group is called a **Casimir operator**.

Theorem of Racah

The number of independent Casimir operators of a (semi-simple) Lie group is equal to the rank of this Lie group.

Fundamental interest: the eigenvalues of the Casimir operators can be used to label the irreps of a Lie group.

LINK WITH LIE ALGEBRAS

It can be shown that for a given r-parameter Lie group, the generators I_i have the following properties: if one defines the commutator (bracket) $[I_i, I_j] \equiv I_i I_j - I_j I_i$, then:

- $[I_i, I_j]$ is a linear combination of $I_1, I_2, \ldots, I_r$.
- $[I_i, I_j] = -[I_j, I_i]$.
- $\Big[[I_i, I_j], I_k\Big] + \Big[[I_j, I_k], I_i\Big] + \Big[[I_k, I_i], I_j\Big] = 0.$
- The operators I_i are independent, and can be chosen to form a basis of a vector space $\mathcal{A}$.

If, furthermore, one introduces the bracket $[\,,\,]$ as a product defined such that $K = \sum_i^r \alpha_i I_i, J = \sum_j^r \beta_j I_j \rightarrow [K, J] = \sum_{ij} \alpha_i \beta_j [I_i, I_j]$, then $\mathcal{A}$ is called the Lie algebra of the Lie group.

LINK WITH LIE ALGEBRAS

- $\mathcal{A}$ is the ensemble of linear combinations of the generators of its corresponding Lie group.
- The relation $a_k^Z = \sum_{ij} c_{ij}^k a_i^X a_j^Y$ seen previously defines the **multiplication table** of this algebra.
- The relation $[I_i, I_j] = \sum_k c_{ij}^k I_k$ defines the **structure constants** c_{ij}^k of the Lie group.
- Suppose now that one is able to find an ensemble of r matrices of order p satisfying the commutation relations of a Lie algebra. Then these matrices form a represenation of dimension p of the Lie group, i.e.

A representation of a Lie algebra can be used to generate a representation of the associated Lie group.

Remark: structure constants characterize a Lie group; they do not depend on a specific representation. However they are not unique, similarly to the group generators.

THE GROUP R_2

THE GROUP OF 2-DIMENSIONAL ROTATIONS

- Consider the ensemble of rotations of a circle around an axis perpendicular to the circle, passing through its center.
- Each element of this ensemble can be characterized by a certain parameter taken as the rotation angle $\theta \in [0, 2\pi]$.
- This ensemble of elements constitutes an example of a continous, abelian, compact, doubly connected, one parameter Lie group, the **group of axial rotations**, or **group of 2-dimensional rotations** R_2.

<u>EXERCISE</u>: find out what is meant by **doubly connected** by making a simple figure !

- Be $T(\theta)$ an element of this group. The composition law is given by

$$T(\theta)T(\phi) = T(\phi)T(\theta) = T(\theta + \phi) \quad \text{if} \quad \theta + \phi < 2\pi$$

$$T(\theta)T(\phi) = T(\phi)T(\theta) = T(\theta + \phi - 2\pi) \quad \text{if} \quad \theta + \phi \geqslant 2\pi$$

- The identity is $E = T(0)$ and the inverse of $T(\theta)$ is $T(2\pi - \theta)$

A REPRESENTATION OF R_2

- What can be a representation of this group ?
- Consider a transformation of the cartesian coordinates (x, y) of a point in a plane, under the rotations of R_2. This transformation is given (in a passive view) by

$$T(\theta)\begin{pmatrix} x \\ y \end{pmatrix} \equiv \begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}$$

- To every element $T(\theta)$ one can associate an orthogonal 2x2 matrix of determinant $+1$, this association being one-to-one. (Orthogonal matrix: $A^T = A^{-1}$).
- The ensemble of such matrices is called **SO(2)** (Special means det$= +1$), and is isomorphic to the group R_2. It provides therefore a **2-dimensional representation** of the group R_2.

IRREPS OF R_2

- We have already observed that R_2 is an abelian group, which implies that **its irreps must be one-dimensional**.
- To find them, we can make use of the composition law, and remark that the only numbers (matrices 1x1 !) that satisfy to it have the form

$$\chi(\theta) = e^{c\theta}$$

  where c is a given number and $\chi(\theta)$ the character of $T(\theta)$.
- Now, since $T(2\pi) = E$, and knowing that E has to be represented by 1 in any one-dimensional representation, we get $e^{2\pi c} = 1$, wherefrom $c = im$ with m integer, or

$$\chi^{(m)}(\theta) = e^{i\,m\,\theta}.$$

  $\rightarrow$ **For all integer value m, this equation provides an irrep of R_2 !**

GENERATORS OF R_2

- Since SO(2) is a 1-parameter group, **it has only 1 generator**.
- However, this generator will depend on the group that has been taken as isomorphic to R_2.

EXAMPLE 1: the group SO(2) itself. The generator is then given by

$$I = \frac{1}{i} \lim_{\phi \to 0} \left\{ \frac{\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}}{\phi} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\} = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} = \sigma_y$$

(Pauli matrix).

Any orthogonal 2x2 matrix with det$= +1$ can be written as

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = e^{i\,\phi\,\sigma_y}$$

EXAMPLE 2:

- Consider a certain function $f = f(x,y)$ and an orthogonal transformation of the coordinates as seen previously:

$$T(\phi)\begin{pmatrix} x \\ y \end{pmatrix} \equiv \begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}$$

- The action of $T(\phi)$ on the function f reads

$$T(\phi)f(x,y) = f(x\cos\phi + y\sin\phi, -x\sin\phi + y\cos\phi)$$

- The generator can be obtained using the relations

$$\begin{aligned} I\,f(x,y) &= \frac{1}{i}\lim_{\phi\to 0}\left\{\frac{f(x\cos\phi + y\sin\phi, -x\sin\phi + y\cos\phi) - f(x,y)}{\phi}\right\} \\ &= \frac{1}{i}\lim_{\phi\to 0}\left\{\frac{y\phi\frac{\partial f}{\partial x} - x\phi\frac{\partial f}{\partial y}}{\phi}\right\} \end{aligned}$$

GENERATORS OF R_2

- This expression then reduces to

$$I\, f(x,y) = \frac{1}{i}\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right) f(x,y)$$

- Introducing the z component of the orbital angular momentum operator

$$L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = \frac{\hbar}{i}\frac{\partial}{\partial \phi}$$

  it is seen that an orthogonal transformation of the coordinates in the (x, y) plane is given by

$$T(\phi) = e^{-\frac{i}{\hbar}\,\phi\, L_z}$$

- The rank of SO(2) is 1, because there is only 1 generator L_z. The eigenvalues are given by m.

THE GROUP R_3

THE GROUP OF 3-DIMENSIONAL ROTATIONS

- The group of all orthogonal spatial transformations in 3-dimensional space is usually denoted by O(3).
- Alternatively, O(3) can be defined as the group of all 3x3 orthogonal matrices.
- These two groups are isomorphic.
- In fact, one has $O(3) = SO(3) \otimes (E, \hat{I})$.

<u>EXERCISE</u>: explain why the ensemble of matrices of O(3) with det$= -1$, does NOT form a group, in contrast to SO(3) !

PARAMETERS OF SO(3)

- According to the isomorphism between orthogonal matrices and orthogonal transformations, it is seen that an orthogonal matrix with det$= +1$ corresponds to a pure or **proper rotation** of the coordinate system.
- Orthogonal matrices with det$= -1$ correspond **improper rotation** of the coordinate system.
- SO(3) is a 3-parameter group which can be taken as follows: 2 angles (polar and azimuthal) characterizing the position of the rotation axis, plus the angle of rotation about this axis. This is known as the Darboux parametrization.

PARAMETERS OF SO(3)

Another choice is given by the 3 Euler angles (α, β, γ): rotation about the *z* axis by angle α, followed by a rotation about the y' axis by angle β, followed by a rotation about the z'' axis by angle γ.

The Euler matrix rotation (general element of SO(3)) is

$$R(\alpha,\beta,\gamma)=\begin{pmatrix} \cos\alpha\cos\beta\cos\gamma-\sin\alpha\sin\gamma & \sin\alpha\cos\beta\cos\gamma+\cos\alpha\sin\gamma & -\sin\beta\cos\gamma \\ -\cos\alpha\cos\beta\sin\gamma-\sin\alpha\cos\gamma & -\sin\alpha\cos\beta\sin\gamma+\cos\alpha\cos\gamma & \sin\beta\sin\gamma \\ \cos\alpha\sin\beta & \sin\alpha\sin\beta & \cos\beta \end{pmatrix}$$

GENERATORS OF SO(3)

- The generators of SO(3) can be obtained by considering an infinite rotation of angle ε about an axis $\vec{u}$.
- The group of rotations $R_{\vec{u}}(\phi)$ $(0 \leqslant \phi < 2\pi)$ is in fact a sub-group of SO(3), isomorphic to SO(2) and therefore we have

$$I_{\vec{u}} = -\frac{1}{\hbar} L_u, \quad L_u = \vec{L} \cdot \vec{u}$$

- Since any rotation can be expressed as the product of 3 rotations about the cartesian axes, we need the 3 operators

$$I_x = -\frac{1}{\hbar} L_x, \quad I_y = -\frac{1}{\hbar} L_y, \quad I_z = -\frac{1}{\hbar} L_z$$

- Any rotation operator reads then

$$R_{\vec{u}}(\phi) = e^{-\frac{i}{\hbar}\phi \vec{L}\cdot\vec{u}}$$

LABELLING IRREPS OF SO(3)

- There are 3 generators, but each of them commutes with itself: the rank of SO(3) is 1.

- The only Casimir operator for SO(3) is $\vec{L}^2$. Its eigenvalues $l(l+1)$, or simply the label l, serve to characterize the irreps $\mathcal{D}^{(l)}$, which are of dimensions $(2l+1)$.

- The common eigenstates $|lm\rangle$ of $\vec{L}^2$ and L_z are introduced in quantum mechanics. The group-theoretical justification for their use is very simple, and stems from the group chain

$$SO(3) \supset SO(2)$$

$\rightarrow$ l and m are labels for the Casimir operators of SO(3) and SO(2), respectively !

IRREPS OF THE 3-DIMENSIONAL ROTATION GROUP

- Using Dirac ket notations, one can write

$$\begin{aligned} R(\alpha\beta\gamma)|lm\rangle &= \sum_{m'} |lm'\rangle\langle lm'|R(\alpha\beta\gamma)|lm\rangle \\ &= \sum_{m'} \mathcal{D}^{l}_{m'm}(\alpha\beta\gamma)\,|lm'\rangle \end{aligned}$$

- $\mathcal{D}^{l}_{m'm}$ are called **Wigner functions**.
- <u>EXERCISE</u>: give a justification for this relation !
- Projecting onto $|\theta\phi\rangle$, one gets for the spherical harmonics $Y_{lm}(\theta\phi) \equiv \langle\theta\phi|lm\rangle$:

$$R(\alpha\beta\gamma)Y_{lm}(\theta\phi) = \sum_{m'=-l}^{+l} Y_{lm'}(\theta\phi)\,\mathcal{D}^{(l)}_{m'm}(\alpha\beta\gamma)$$

- **The spherical harmonics span/generate an irrep of dimension** $(2l+1)$ denoted by $\mathcal{D}^{(l)}$.

IRREDUCIBLE SPHERICAL TENSORS

- An **irreducible spherical tensor** T^k, of rank k, is defined such that its $(2k+1)$ components transform under rotations as

$$T'^k_q = \sum_{q'=-k}^{+k} T^k_{q'} \, \mathcal{D}^{(k)}_{q'q}(\alpha\beta\gamma)$$

- An alternative (and equivalent) definition has been given by Racah:

$$[J_z, T^k_q] = q\, T^k_q, \quad [J_\pm, T^k_q] = \hbar\sqrt{k(k+1) - q(q\pm 1)}\, T^k_{q\pm 1}$$

SO(3) VERSUS SU(2)

Let us make a short intermezzo at this point !

Consider the Special Unitary Group SU(2) composed of all 2x2 unitary matrices ($U^\dagger = U^{-1}$) with det$= +1$. They can be expressed as

$$\begin{pmatrix} a & -b^* \\ b^* & a^* \end{pmatrix}, \quad aa^* + bb^* = 1.$$

- SU(2) is a 3-parameter group (a and b are called the Cayley-Klein parameters).
- One can show that each SU(2) matrix can be put into correspondence with a unique rotation of SO(3).
- However, the inverse is only partly true, since to each rotation of SO(3) correspond 2 different SU(2) matrices ! For example, to a rotation about Euler angles ($\alpha = 0, \beta = 0, \gamma = 0$) and ($\alpha = 0, \beta = 2\pi, \gamma = 0$) (NO ROTATION AT ALL !) one associates the 2 different SU(2) matrices $+(I)_{2\times2}$ and $-(I)_{2\times2}$.
- One says that there is a 1 to 2 homomorphisme between SO(3) and SU(2).

CLEBSH-GORDAN SERIES

- It is well known from the theory of angular momentum that the coupled and uncoupled bases are related by

$$|JM\rangle = \sum_{m_1 m_2} |j_1 m_1; j_2 m_2\rangle \langle j_1 m_1; j_2 m_2 | JM\rangle$$

- The brackets $\langle j_1 m_1; j_2 m_2 | JM\rangle = C^{JM}_{j_1 m_1; j_2 m_2}$ are the **Clebsh-Gordan** coefficients.
- It can be shown that the direct product of two SU(2) irreps $\mathcal{D}^{(j_1)}$ and $\mathcal{D}^{(j_2)}$, denoted by $\mathcal{D}^{(j_1)} \otimes \mathcal{D}^{(j_2)}$ can be decomposed into the **Clebsh-Gordan series**

$$\mathcal{D}^{(j_1)} \otimes \mathcal{D}^{(j_2)} = \sum_{J=|j_1-j_2|}^{J=j_1+j_2} \mathcal{D}^{(J)}$$

- Group theory gives the full justification for the angular momentum coupling procedure !

DIRECT AND IRREDUCIBLE TENSOR PRODUCTS

- Two irreducible spherical tensors R^k and $S^{k'}$ can be coupled to an **irreducible spherical tensor** $T^K = \left[R^k \otimes S^{k'}\right]^K$ according to the rule

$$T_Q^K = \sum_{qq'} C_{kq;k'q'}^{KQ} \, R_q^k \, S_{q'}^{k'}$$

- The **direct product** of R^k and $S^{k'}$ is defined as the set of $(2k+1)(2k'+1)$ components $R_q^k \, S_{q'}^{k'}$.
- The direct product is in general reducible and can be decomposed as a sum of irreducible tensors according to

$$R_q^k \, S_{q'}^{k'} = \sum_{K=|k-k'|}^{K=k+k'} C_{kq;k'q'}^{KQ} \, T_Q^K$$

DYNAMICAL SYMMETRIES

DYNAMICAL SYMMETRIES

- We have seen previously some examples of **geometrical symmetries**.
- They arise in many branches of physics: molecular, atomic, nuclear physics...
- In the context of nuclear physics, they arise for example in the context of mean-field theories through the symmetry properties of the mean-field potential.
- There exist other forms of symmetries, called **dynamical symmetries**, as they stem from particular forms of the interactions in the system.

  We will give now two well known example.

DYNAMICAL SYMMETRY OF THE HYDROGEN ATOM

- We have noticed already that for a physical system, the bunching of levels (eigenstates) is related to the dimensions of the irreps of the corresponding symmetry group.
- The hamiltonian of the reduced problem for the hydrogen atom reflects spherical symmetry, thus the bound states should show the typical $(2l+1)$ degeneracy characteristic for the SO(3) irreps.
- Eigenenergies are $E_n = -\frac{1}{n^2} E_I$ $(n = 1, 2, 3, \ldots)$, with ionization energy $E_I \simeq 13.6$ eV.
- Each shell, characterized by n, is composed of subshells corresponding to the values $l = 0, 1, 2, \ldots, (n-1)$.
- Each subshell with given l is composed of $(2l+1)$ magnetic substates: $-l \leqslant m \leqslant +l$.
- Therefore, each level of energy E_n has degeneracy $g_n = \sum_{l=0}^{n-1}(2l+1) = n^2$.
- It can be shown that in fact the dynamical symmetry of the hydrogen atom is O(4), which contains SO(3) as a subgroup.

DYNAMICAL SYMMETRY OF THE ISOTROPIC HARMONIC OSCILLATOR

- The 3-dimensional isotropic harmonic oscillator is another example where the degeneracies of the bound states are larger than expected from the geometrical SO(3) symmetry group.
- Eigenenergies are $E_n = (n + \frac{3}{2})\hbar\omega$ with $n = n_x + n_y + n_z$, and thus the degeneracy of the level E_n is $(n+1)(n+2)/2$.
- It can be shown that the dynamical symmetry group of the 3-dimensional isotropic harmonic oscillator is in fact SU(3), and, more generally, the dynamical symmetry group of a n-dimensional isotropic harmonic oscillator is SU(n).

THE UNITARY GROUP U(n)

THE UNITARY GROUP U(n)

DEFINITION

The unitary group U(n) is the ensemble of $n \times n$ complex matrices satisfying $UU^\dagger = U^\dagger U = \mathbb{I}_n$.

One can observe that any unitary matrix U can be expressed with the help of Cartan-Weyl matrices e_{ij} (element in line i and column j equal to 1, all other elements null) as

$$U = \exp\left(i \sum_{ij} a_{ij} e_{ij}\right)$$

where a_{ij} are complex numbers satisfying $a_{ij} = a_{ji}^*$.

STRUCTURE CONSTANTS

The structure constants of the U(n) can be evaluated with the help of the Cartan-Weyl matrices :

$$[e_{ij}, e_{kl}] = \delta_{jk} e_{il} - \delta_{il} e_{kj}, \quad i, j, k, l = 1, \ldots, n.$$

THE UNITARY GROUP U(n) AND THE MANY-BODY PROBLEM

- Let us introduce the bosonic or fermionic creation $a_i^\dagger$ and annihilation a_i operators satisfying the commutation or anti-commutation relations

$$\{a_i, a_j^\dagger\}_\pm = \delta_{ij} \quad \text{and} \quad \{a_k^\dagger, a_l^\dagger\}_\pm = 0.$$

- Define the operators $A_{ij} = a_i^\dagger a_j$.
- It is straightforward to show that these operators satisfy the commutation rules characteristic for the unitary group U(n) :

$$[A_{ij}, A_{kl}] = \delta_{jk} A_{il} - \delta_{il} A_{kj}, \quad i, j, k, l = 1, \ldots, n,$$

showing that :

The operators $A_{ij} = a_i^\dagger a_j$ $(i, j = 1, \ldots, n)$ can be considered as generators of the unitary group U(n).

CONSTRUCTING BASIS FOR U(n) IRREPS

- We begin by constricting an ensemble of polynomials P of order $p = \sum_{i=1}^{n} \rho_i$ in the operators $a_i^\dagger$:

$$P = {a_1^\dagger}^{\rho_1} {a_2^\dagger}^{\rho_2} {a_3^\dagger}^{\rho_3} \ldots {a_n^\dagger}^{\rho_n}.$$

- It can be shown that this ensemble constitutes a basis of representations for the algebra of U(n). These representations are however in general not irreducible.
- From now on we will identify each polynomial with its **weight** $w = [\rho_1, \rho_2 \ldots, \rho_n]$, and we call **i-th partial weight** in P the value ρ_i.
- Consider now two polynomials P and P' with weights w and w', respectively and construct the difference $w'' = w - w' = [(\rho_1 - \rho_1'), (\rho_2 - \rho_2') \ldots, (\rho_n - \rho_n')]$.
- We say that the weight of P is greater than the weight of P' if, in w'', the first non-zero partial weight is positive.

CONSTRUCTING BASIS FOR U(n) IRREPS

- Polynomials P are eigenstates of the operators A_{ii} with eigenvalues ρ_i. The operators A_{ii} are therefore called **weight generators**.
- The operators A_{ij} **increase** the weights of polynomials if $i < j$.
- The operators A_{ij} **decrease** the weights of polynomials if $i > j$.
- A **highest weight polynomial** $P_{\max}$ is defined such that $A_{ij}P_{\max} = 0, i < j$, polynomials with lower weights can be generated by repeated action of lowering-weight operators.

Each symbol $[\rho_1, \rho_2 \ldots, \rho_n]_{\max}$ with $\rho_1 \geqslant \rho_2 \geqslant \ldots \geqslant \rho_n$ can serve to label an irrep of the group U(n). In each of these irreps, this symbol, called **highest weight**, is unique.

THE GELFAND AND ZETLIN CONSTRUCTION

The so-called **Gelfand-Zetlin** approach is based on the following properties:

- As seen previously, each irrep of U(n) can be characterized by its unique highest weight vector $[m_{1\,n}, m_{2\,n}, \ldots, m_{n\,n},]$ where $m_{1\,n} \geqslant m_{2\,n} \geqslant \ldots \geqslant m_{n\,n}$.

- Owing to the group chain $U(n) \supset U(n-1) \supset U(n-2) \supset \ldots \supset U(2) \supset U(1)$, it follows that each representation space of U(n) can be decomposed into irreps with respect to U(n-1), and so on. Therefore, in the irreps of U(n) one only finds irreps of U(n-1) where the partial weights of the heighest weights satisfy the **betweeness conditions** $m_{i\,n} \geqslant m_{i\,n-1} \geqslant m_{i+1\,n}, \quad i = 1, \ldots, n-1$.

THE GELFAND AND ZETLIN CONSTRUCTION

One represents graphically the Gelfand-Zetlin states as follows

$$(m)_n = \begin{pmatrix} m_{1\,n} & & m_{2\,n} & & m_{3\,n} & & \dots & & m_{n\,n} \\ & m_{1\,n-1} & & m_{2\,n-1} & & \dots & & m_{n-1\,n-1} & \\ & & \dots & & \dots & & \dots & & \\ & & & m_{1\,2} & & m_{2\,2} & & & \\ & & & & m_{1\,1} & & & & \end{pmatrix}$$

or, in more compact form

$$|(m)_n\rangle = \left| \begin{pmatrix} [m]_n \\ (m) \end{pmatrix} \right\rangle$$

AN APPLICATION FOR MULTIFERMIONIC SYSTEMS

Consider a multifermionic hamiltonian with one-body and two-body interaction terms describing for example a mean-field plus a residual term:

$$H = \sum_{\alpha\beta} \langle \alpha | h_1 | \beta \rangle a^\dagger_\alpha a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | h_2 | \gamma\delta \rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma .$$

QUESTION: what are the basis states allowing for the diagonalisation process of the many-body hamiltonian, in the case there are $p = 2$ fermions located on $n = 4$ valence orbitals ?

ANSWER: take the Gelfand-Zetlin construction for U(4), labelled by the highest weight [1 1 0 0] !

AN APPLICATION FOR MULTIFERMIONIC SYSTEMS

$$|GZ\rangle_1 = \begin{pmatrix} 1 & & 1 & & 0 & & 0 \\ & 1 & & 1 & & 0 & \\ & & 1 & & 1 & & \\ & & & 1 & & & \end{pmatrix}, |GZ\rangle_2 = \begin{pmatrix} 1 & & 1 & & 0 & & 0 \\ & 1 & & 1 & & 0 & \\ & & 1 & & 0 & & \\ & & & 1 & & & \end{pmatrix},$$

$$|GZ\rangle_3 = \begin{pmatrix} 1 & & 1 & & 0 & & 0 \\ & 1 & & 0 & & 0 & \\ & & 1 & & 0 & & \\ & & & 1 & & & \end{pmatrix}, |GZ\rangle_4 = \begin{pmatrix} 1 & & 1 & & 0 & & 0 \\ & 1 & & 1 & & 0 & \\ & & 1 & & 0 & & \\ & & & 0 & & & \end{pmatrix},$$

$$|GZ\rangle_5 = \begin{pmatrix} 1 & & 1 & & 0 & & 0 \\ & 1 & & 0 & & 0 & \\ & & 1 & & 0 & & \\ & & & 0 & & & \end{pmatrix}, |GZ\rangle_6 = \begin{pmatrix} 1 & & 1 & & 0 & & 0 \\ & 1 & & 0 & & 0 & \\ & & 0 & & 0 & & \\ & & & 0 & & & \end{pmatrix}.$$

A SIMPLE INTERPRETATION

Let us define the quantities

$$\rho_0(m) = 0 \quad \text{and} \quad \rho_k(m) = \sum_{j=1}^{k} m_{j\,k}, \;\; k = 1, \ldots, n.$$

Now, omitting the labels m, one defines the **Gelfand-Zetlin weight vectors** $|GZ\rangle_i$ as

$$|GZ\rangle_i = \begin{pmatrix} \rho_n - \rho_{n-1} \\ \vdots \\ \rho_2 - \rho_1 \\ \rho_1 - \rho_0 \end{pmatrix}$$

A SIMPLE INTERPRETATION

In the case of the previous example, it is straightforward to get

$$|GZ\rangle_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \quad |GZ\rangle_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$

$$|GZ\rangle_3 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad |GZ\rangle_4 = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

$$|GZ\rangle_5 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |GZ\rangle_6 = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$\rightarrow$ **Occupation representation !!!**

THANK YOU FOR YOUR ATTENTION !