# Lecture notes: Group theory and its applications in physics

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Part 1

Finite and discrete groups

#### LECTURE 1

### Symmetries in Physics

#### 1. Classical physics

What does it mean that a dynamical system has symmetries? Consider standard dynamical equations:

(1.1) 
$$\frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{q}} \right) = \frac{\partial \mathcal{L}}{\partial q}, \qquad S = \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}) dt$$

for a time evolution of a number of classical particles. To find solution q(t) we have to solve a complicated (system) of differential equations, which in exact form only in few exceptional cases (of integrable systems) is possible. On the other hand, it often happens that given an arbitrary solution q(t) one can construct a family of solutions by application of certain transformation to it:

$$q(t,\epsilon) := g_{\epsilon} \cdot q(t)$$
, such that  $q(t) = q(t,0)$ .

In such a case the transformations  $g_{\epsilon}$ , form a symmetry group G of the system. By the definition  $g_{\epsilon_1} \cdot g_{\epsilon_2} \in G$  if  $g_{\epsilon_1}, g_{\epsilon_2} \in G$  and there exists an inverse transformation  $g_{\epsilon}^{-1}$  for each  $g_{\epsilon} \in G$ . In mathematical language the last two properties in combination with the associativity of transformations imply that G is a group.



FIGURE 1. Symmetry transformation.

**Example** 1.1. **Continuous symmetries:** Translational symmetries  $q(t, \epsilon) = q(t) + \epsilon$ . Rotation symmetries  $q(t, \epsilon) = R(\epsilon) \cdot q(t)$ ,  $R(\epsilon)R^{T}(\epsilon) = I$ .

The existence of such symmetries is directly follows from the invariance of the action S under the transformation  $g_{\epsilon}$ :

(1.2) 
$$S(q(t)) = S(g_{\epsilon} \cdot q(t)).$$

This is clear, since  $g_{\epsilon}$  transforms extremum of S into another extremum, see figure 1. In its own turn the invariance of the action would follow from the invariance of the Lagrangian:

(1.3) 
$$\mathcal{L}(q(t), \dot{q}(t))dt = \mathcal{L}\left(g_{\epsilon} \cdot q(t), g_{\epsilon} \cdot \dot{q}(t)\right) d(g_{\epsilon} \cdot t).$$

Here we can also add an additional dF which changes transformed action by a constant (and therefore does not affect the above arguments). This leads to the following (sufficient) symmetry condition:

(1.4) 
$$\mathcal{L}(q(t), \dot{q}(t)) = \mathcal{L}(g_{\epsilon} \cdot q(t), g_{\epsilon} \cdot \dot{q}(t)) \frac{d(g_{\epsilon} \cdot t)}{dt} + \frac{dF}{dt}.$$

To summarize, the transformations  $g_{\epsilon}$  leaving  $\mathcal{L}dt$  invariant up to a closed form dF form a group of symmetries of the system. They transform one solution of the dynamical equation to another:

$$q(t) \rightarrow q(t,\epsilon), \qquad q(t,0) = q(t).$$

Note that typically we do not know explicitly any solution of this family. Nevertheless, knowledge of symmetries of the system might be very useful:

With any *continues symmetry* of a Lagrangian system we can associate a conserved quantity.

#### 2. Continues symmetries & Noether theorem

Let  $g_{\epsilon}$  be a continues symmetry, i.e.,  $\epsilon \in \mathbb{R}$ . Consider an infinitesimal transformation

$$q \to q + \epsilon \eta(q)$$
  $q(t, \epsilon) = q(t) + \epsilon \eta(q(t))$ 

which leaves  $\mathcal{L}$  invariant up to a full time derivative, see (1.4):

(2.1) 
$$\mathcal{L}(q(t) + \epsilon \eta(t), \dot{q}(t) + \epsilon \dot{\eta}(t)) = \mathcal{L}(q(t), \dot{q}(t)) + \epsilon \left(\frac{\partial \mathcal{L}}{\partial q} \eta(t) + \frac{\partial \mathcal{L}}{\partial \dot{q}} \dot{\eta}(t)\right).$$

It follows immediately from eq. (1.1) that:

(2.2) 
$$\mathcal{J} = \frac{\partial \mathcal{L}}{\partial \dot{q}} \eta(t) + F(t), \qquad \frac{d\mathcal{J}}{dt} = 0$$

From this also follows that

(2.3) 
$$\{H, \mathcal{J}_{\eta}\} = \frac{d\mathcal{J}_{\eta}}{dt} = 0,$$

where  $\{f,g\} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}$  is the Poisson bracket. Currents  $\mathcal{J}_{\eta}$  form Lie algebra with the Poisson brackets playing the role of "commutator operation".

Symmetry transformations including time. Considering more general transformation:

$$t \to t + \epsilon \phi(q, t) = t'; \qquad q_i \to q_i + \epsilon \eta_i(q, t) = q'_i$$

leaving S invariant (one can also consider  $\phi$  and  $\eta$  depending on time derivatives of  $\mathbf{q} = (q_1, \dots, q_n)$ ) we can get a generalized version of Noether theorem:

(2.4) 
$$\mathcal{J} = \sum_{i} \left[ \frac{\partial \mathcal{L}}{\partial \dot{q}_{i}} \eta_{i}(\mathbf{q}, t) + \left( \mathcal{L} - \frac{\partial \mathcal{L}}{\partial \dot{q}_{i}} \dot{q}_{i} \right) \phi(\mathbf{q}, t) \right] + F(t), \qquad \frac{d\mathcal{J}}{dt} = 0.$$

*Proof*: If the system is invariant under the above transformation

(2.5) 
$$\mathcal{L}\left(q_{i},\frac{dq_{i}}{dt}\right)dt + dF =$$
$$= \mathcal{L}\left(q_{i}',\frac{dq_{i}'}{dt'}\right)dt' = \mathcal{L}\left(q_{i} + \epsilon\eta_{i}(\mathbf{q},t),\dot{q}_{i}(1 - \epsilon\phi(\mathbf{q},t)) + \epsilon\dot{\eta}_{i}(\mathbf{q},t)\right)(1 + \epsilon\phi(\mathbf{q},t))dt.$$

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#### 2. CONTINUES SYMMETRIES & NOETHER THEOREM

After expansion of the right hand side we have:

(2.6) 
$$\sum_{i} \left[ \partial_{q_i} \mathcal{L} \eta_i + \partial_{\dot{q}_i} \mathcal{L} (\dot{\eta}_i - \dot{q}_i \phi) \right] + \mathcal{L} \dot{\phi} = \dot{F}$$

Now using the equation of motion (1.1) the left part of this equation can be written down as full time derivative:

$$\frac{d}{dt}\sum_{i}\left[\frac{\partial \mathcal{L}}{\partial \dot{q}_{i}}\eta_{i} + \underbrace{\left(\mathcal{L} - \frac{\partial \mathcal{L}}{\partial \dot{q}_{i}}\dot{q}_{i}\right)}_{Hamiltonian}\phi\right].$$

Applications  $\mathcal{L} = \sum_i m \dot{\mathsf{q}}_i^2/2 + \sum_{i \neq j} V(|\mathsf{q}_i - \mathsf{q}_j|)$ 

A) Shift in space:

$$q_i^{(x)} \to q_i^{(x)} + \epsilon, \qquad \mathcal{J}_x = \sum_i p_i^{(x)} \qquad (\text{Momentum}).$$

B) Rotations:

$$q_i \rightarrow R_{x,y,z}q_i$$

(2.7) 
$$R_z = \begin{pmatrix} \cos(\epsilon) & \sin(\epsilon) & 0\\ -\sin(\epsilon) & \cos(\epsilon) & 0\\ 0 & 0 & 1 \end{pmatrix} = I + \epsilon \begin{pmatrix} 0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0 \end{pmatrix} + O(\epsilon^2)$$

(2.8)  $\mathcal{J}_z = \sum_i -p_i^{(x)} q_i^{(y)} + p_i^{(y)} q_i^{(x)} \qquad \text{(Angular Momentum)}.$ 

C) Shift in time:

t

$$\rightarrow t + \epsilon, \qquad \mathcal{J}_t = \mathcal{L} - \sum_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \dot{q}_i = H$$
 (Energy).

D) Some less standard example for the potential  $V(\mathbf{q}) \sim 1/|\mathbf{q}|^2$ . The transformation:

$$t \to \lambda^2 t, \qquad q_i \to \lambda q_i$$

is an obvious symmetry of the action (consider  $\mathcal{L}dt$ ). In the infinitesimal form  $\lambda = 1 + \epsilon$  this symmetry is given by:

$$t \to \lambda^2 t(1+2\epsilon), \qquad q_i \to q_i(1+\epsilon),$$

implying that

$$\mathcal{J} = (1/2)d_t \sum q_i^2 - 2Ht, \quad \mathcal{J} = const.$$

This leads to the conclusion that

$$\sum q_i^2 = 2Et^2 + t \cdot const.$$

Depending on the sign of energy the particle either flies away with a constant radial velocity or collapses to the center in a finite time!

#### 3. Quantum mechanics

Now consider action of symmetry group in the framework of quantum mechanics. By the same principle, if  $\Psi(x,t)$  is solution of the Schrödinger equation:

(3.1) 
$$i\hbar\partial_t\Psi(x,t) = \widehat{H}\Psi(x,t)$$

the function  $\Psi'(x,t) = g \cdot \Psi(x,t) \equiv \Psi(g \cdot x,t)$  is also solution of the same equation. This is automatically satisfied if

$$(3.2) g \cdot H = H \cdot g.$$

#### 4. Continues symmetries

As in the classical case we can consider an infinitesimal group action:

(4.1) 
$$g \cdot \Psi(x) \approx \Psi(x) + \epsilon J \Psi(x).$$

By (3.2) we then immediately obtain:

(4.2) 
$$[\widehat{H},\widehat{J}] = \frac{d\widehat{J}}{dt} = 0$$

Example 1.2. Translation and rotation symmetries:

(a) Translation symmetry

$$\Psi(x+\epsilon) = \Psi(x) + \epsilon \partial_x \Psi, \qquad -i\hbar \widehat{J} = -i\hbar \partial_x = \hat{p}, \quad d_t \hat{p} = 0.$$

(b) Rotation symmetry

$$\Psi(x+\epsilon y, y-\epsilon x) = \Psi(x) + \epsilon(y\partial_x - x\partial_y)\Psi, \qquad -i\hbar\widehat{J} = \widehat{L}, \quad d_t\widehat{L} = 0$$

#### 5. Discrete symmetries

So far we considered continues groups of symmetries. For discrete groups of symmetries there are no associated conserved quantities (no associated Lie algebras). So at first it seems that existence of discrete symmetries provides little additional information about time evolution of the system. Nevertheless, the use of group theory becomes of great importance when we consider stationary (spectral) problem.

Example 1.3. Reflection and rotation symmetries:

(a) Reflection symmetry 
$$V(x) = PV(x) = V(-x)$$
:  
(5.1)  $\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x) = E_n\psi(x).$ 

If  $\psi(x)$  is solution then  $P\psi(x)$  is also solution. From this and non-degeneracy of the spectrum follows that either  $P\psi(x) = \psi(x)$  or  $P\psi(x) = -\psi(x)$ . The first case corresponds to symmetric functions while the second one to antisymmetric one. Thus the whole spectrum can be decomposed in accordance to symmetry group.



FIGURE 2. Discrete symmetries.

(b) Rotation symmetry  $V(x) = g \cdot V(x)$ ,  $G = \{e, g, g^2\}$ : By the same argument we have three possibilities:

 $g \cdot \psi(x) = \psi(x);$   $g \cdot \psi(x) = e^{i2\pi/3}\psi(x);$   $g \cdot \psi(x) = e^{-i2\pi/3}\psi(x).$ 

In addition, by the time reversal symmetry if  $\psi(x)$  is solution then  $\psi^*(x)$  is solution with the same eigenvalue as well. From this follows that the spectrum must be degenerate. The spectrum can be split into real eigenfunctions  $\{\psi_1(x)\}$  invariant under rotations and degenerate pairs of real eigenfunctions:

$$\psi_2(x) = \psi(x) + \psi^*(x); \psi_3(x) = i(\psi(x) - \psi^*(x)), \text{ where } g \cdot \psi(x) = e^{i2\pi/3}\psi(x).$$

#### **Example** 1.4. Symmetry groups in physics:

- (a) Translations T.
- (b) Rotations SO(3).
- (c) Point groups, i.e., subgroups of O(3).
- (d) Point groups + discrete translations e.g., symmetry groups of crystals.
- (e) Lorentz group O(3,1) the group of linear transformations  $\Lambda(t,x,y,z) \rightarrow (t',x',y',z')$ , which preserve bilinear form

$$t^{2} - x^{2} - y^{2} - z^{2} = t^{\prime 2} - x^{\prime 2} - y^{\prime 2} - z^{\prime 2}.$$

- (f) Poincaré group: Lorentz group + translations in space-time.
- (g) Permutation groups

$$S\Psi(x_1, x_2, \dots, x_n) = \Psi(x_2, x_1, \dots, x_n).$$

(h) Boson wavefunctions are symmetric while fermion wavefunctions are anti-symmetric under exchange of variables.

#### LECTURE 2

### **Basics of Group Theory**

#### 1. Groups definitions

DEFINITION 1.1. A set G with a multiplication  $(\cdot)$  is a group if:

- Closer: For any  $g_1, g_2 \in G$  it follows that  $g_1 \cdot g_2 \in G$ .
- Associativity:  $g_1 \cdot (g_2 \cdot g_3) = (g_1 \cdot g_2) \cdot g_3$ .
- Unit element: There exists  $e \in G$  such that  $e \cdot g = g$  for any  $g \in G$ .
- Inverse: For each  $g \in G$  there exists  $g^{-1} \in G$  such that  $g^{-1} \cdot g = e$

Two groups are **isomorphic**  $G \cong H$  if there is an equivalence relation between elements of the group  $g \sim h$  which is preserved under the matrix multiplication  $g_1 \cdot g_2 \sim h_1 \cdot h_2$  if  $g_1 \sim h_1$ ,  $g_2 \sim h_2$ . Order of groups |G| is a number of elements in G. If  $|G| < \infty$  the group is called **finite**.

#### Example 2.1. Infinite groups, matrix groups:

- (1) GL(n,F)  $(F = \mathbb{R}, \mathbb{C})$  group of invertible matrices, SL(n,F) is the subgroup of the matrices with det equals one.
- (2) O(n), group of real orthogonal matrices leaving euclidean product  $(x, x) = \sum_{i} x_i^2$  invariant:  $O \cdot O^T = 1$ . Its subgroup SO(n) contains all matrices with the det 1. Physics: Rotation group SO(3).
- (3) O(n-q,q) group of real matrices leaving scalar product  $(x,x) = \sum_{i=1}^{q} x_i^2 \sum_{i=q+1}^{n} x_i^2$  invariant. Lorentz group SO(3,1).
- (4) Unitary groups U(n), SU(n):  $U \cdot U^* = 1$ . Physics: Strong interaction. Weak interaction.
- (5) Symplectic group Sp(2n). Group of symplectic matrices:

$$M^T \cdot \Omega \cdot M = \Omega, \qquad \Omega = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}.$$

Physics: In Hamiltonian mechanics symplectic matrices describe transformations from one set of canonical coordinates to another.

#### Example 2.2. Finite groups:

(1) Cyclic group  $\mathbb{Z}_n$ . For the elements  $m \in \{0, 1, \dots, n-1\}$  of cyclic group the multiplication is defined by

 $m_1 \cdot m_2 := m_1 + m_2 \mod n.$ 

where inverse is given by  $m^{-1} = n - m$  and unity element is represented by 0. This is abelian group.

- (2) Symmetry group of "directed" polygon  $C_n$ .  $C_n \cong \mathbb{Z}_n$ .
- (3) Symmetry group of polygons  $D_n$ . This is non-abelian group:

 $\sigma$ 

$$\sigma_2 \sigma_1 = g, \qquad \sigma_1 \sigma_2 = g^{-1}.$$

(4) Permutation group/Symmetric group  $S_n$ .

$$\sigma: i \to i' = \sigma(i), i = 1, \dots n \qquad \begin{pmatrix} 1 & 2 & \dots & N \\ \sigma(1) & \sigma(2) & \dots & \sigma(N) \end{pmatrix}, \quad |S_n| = n!$$



Symmetry group of "directed" (left) and "non-directed" (right) equilateral FIGURE 1. triangle.

**Example** 2.3. **Permutation group**  $S_3$ :

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} \cdot \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} .$$
$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 1 & 4 & 5 & 2 \end{pmatrix} = (1 \ 2) \begin{pmatrix} 3 & 4 & 5 \end{pmatrix} .$$

Cyclic decomposition:

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 1 & 4 & 5 & 3 \end{pmatrix} = \begin{pmatrix} 1 & 2 \end{pmatrix} \begin{pmatrix} 3 & 4 & 5 \end{pmatrix}.$$

Every permutation can be represented as product of transpositions:

$$(3 \ 4 \ 5) = (3 \ 5) (5 \ 4) = (3 \ 4) (4 \ 5) (3 \ 4) (4 \ 5)$$

This decomposition is not unique (as opposed to cyclic), but the number of transpositions always odd (even). To prove it we note isomorphism between  $\sigma$  and permutation matrices.

$$Ex: \begin{pmatrix} 1 & 2 & 3\\ 2 & 3 & 1 \end{pmatrix} \to \sigma = \begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0 \end{pmatrix}, \sigma \sigma \begin{pmatrix} x_1\\ x_2\\ x_3 \end{pmatrix} = \begin{pmatrix} x_2\\ x_3\\ x_1 \end{pmatrix}.$$

Parity of  $\sigma$  is determined by the sign of the determinant. Since each transposition has determinant -1 the parity is fixed by the number (whether it is even or odd) of entering transpositions. All even  $\sigma$  form a subgroup  $A_n$  of  $S_n$ . As we will see below permutations groups (subgroups of  $S_n$ ) play a special role.

#### 2. Subgroups

*H* is a **subgroup** of *G* if it is a group itself and  $H \subset G$ .

THEOREM 2.1. Cayley's Theorem. Any finite group G is isomorphic to a subgroup of  $S_N$ , N = |G|.

**Remark** 2.1. In many cases N can be smaller than |G|. For instance, the group of Rubik Cube is a subgroup of  $S_{43}$  while the order is  $|G| = 8! \cdot 11! \cdot 2^{12} \cdot 3^8$ .

The proof of the theorem is elementary. Let  $g_1, g_2, \ldots, g_N$  be elements of the group G. Consider now the action of an arbitrary element  $\sigma \in G$  on other elements of the group:

$$\sigma \cdot g_i = g_{i'}, \qquad i' = \sigma(i) \text{ for all } i = 1, \dots N,$$

where we introduced notation  $\sigma(i)$  for the corresponding index. Since  $\sigma_2 \cdot \sigma_1 \cdot g_i = g_{\sigma_2 \sigma_1(i)}$  we have isomorphism:

$$\sigma \leftrightarrow \begin{pmatrix} 1 & 2 & \dots & N \\ \sigma(1) & \sigma(2) & \dots & \sigma(N) \end{pmatrix},$$

with the unit element corresponding to the trivial permutation.

#### 3. Conjugate classes. Normal subgroups

Given a subgroup H, G can be decomposed into **cosets**:

(3.1) 
$$G = \{g_1H, g_2H, \dots, g_kH\}, \quad k = (G:H) -$$
index.

From this immediately follows:

THEOREM 3.1. Lagrange Theorem:  $|G|/|H| = k \in \mathbb{N}$ .

Analogously, we can consider right hand decomposition:

(3.2) 
$$G = \{Hg'_1, Hg'_2, \dots Hg'_k\}.$$

In general these are two different decompositions. However, if  $gHg^{-1} \in H$  for any g then two decompositions coincide. Such subgroups are called **normal**. For a normal subgroup we can define **factor group** (also called quotient group) G/H whose elements are cosets of H:

$$[g_i] \cdot [g_j] = [g_i g_j], \qquad [g_i] = \{g_i H\}, \quad [e] = \{H\}.$$

Example 2.4. Normal subgroups and factor groups:

- (1) If n is a prime number no subgroups exist. Any subgroup is normal (since the group is abelian)  $\mathbb{Z}_n/\mathbb{Z}_m \cong \mathbb{Z}_{n/m}$ .
- (2) The set  $H = \{e, g, g^2\}$  is the normal subgroup of  $D_3$ . Two non-equivalent cosets are:

$$[e] = \{H\}, [\sigma] = \{\sigma_1 H\}, \qquad \Longrightarrow G/H \cong \mathbb{Z}_2.$$

- (3) The set of even permutations  $A_n$  is normal subgroup of  $S_n$ ,  $S_n/A_n \cong \mathbb{Z}_2$ .
- (4) U(1) is normal (and abelian) subgroup of U(n),  $U(n)/U(1) \cong SU(n)$ .
- (5) Group of translations is normal (and abelian) subgroup of Poincaré group.

An "inverse" operation – **direct product**  $G \times F$  of groups G and F is defined in the following way. The elements of the group are all possible pairs  $[g, f], g \in G, f \in F$ . The product is then  $[g_1, f_1] \cdot [g_2, f_2] =: [g_1g_2, f_1f_2]$ , with the unit element given by  $[e_G, e_F]$ . It is easy to see that  $G \cong [G, e_F]$  and  $F \cong [e_G, F]$  are normal subgroups of  $G \times F$  and

$$G \cong G \times F/F, \qquad F \cong G \times F/G.$$

Is it always true that from G/H = F follows that  $G = F \times H$ ? Not in general!  $D_3/C_3 = C_2$ , but  $D_3 \neq C_3 \times C_2$ , since  $D_3$  is non-abelian as opposed to the right hand side.

**Homeomorphism. Kernels as normal subgroups.** Homeomorphism  $\phi : G \to H$  is a map from G to H which preserves the group structure. Kernel of G is a subgroup of G such that  $\phi(g) = e$ if  $g \in Ker_{\phi}(G)$ . It is straightforward to see that  $Ker_{\phi}(G)$  is normal and  $G/Ker_{\phi}(G) \cong H$ . It follows from identification of  $\phi(g)$  with  $\{g \cdot Ker_{\phi}(G)\}$ . If  $Ker_{\phi}(G) = e$  then  $\phi$  is isomorphism.

**Example** 2.5. A kernel as normal subgroup:  $A \in U(n)$ ,  $\phi(A) = \det(A) \Longrightarrow Ker_{\phi}(U(n)) = SU(n)$ .

#### 4. Point groups

Point groups are finite subgroups of O(3). Play very important role in physics: they are groups of symmetries of molecules as well as crystals. We will first consider finite subgroups G of SO(3) and then add special transformations.

1) Let  $H_A$  be a subgroup of a discrete group G which leaves invariant a point (pole) A on the unit sphere.  $H_A \cong Z_{n_A}$ , where  $n_A$  is the order of  $H_A$ . Consider the decomposition of G, |G| = N into cosets:

(4.1) 
$$G = \{g_1 \cdot H_A, g_n \cdot H_A, \dots g_{m_A} \cdot H_A\}, \qquad m_A n_A = N.$$

each coset  $g_i \cdot H_A$  transfers the point  $A = A_1$  to some another point  $A_i \neq A$  which is the same for all elements of the coset. Different cosets generate different points. The set:  $\{A_1, A_2, \ldots, A_{m_A}\}$ 



FIGURE 2. (a) Star of a point A. (b) Star system of the tetrahedron group.

is called **star** of A. If we start from another point  $A_i$  of the star we produce the same star. The transformations leaving  $A_i$  invariant have the form  $g_i H_A g_i^{-1}$  form a subgroup of G isomorphic to  $H_A$ .

**Example** 2.6. **Star system of a tetrahedron:** The point group T of a tetrahedron has 4 axes of symmetries of 3rd order and 3 axes of 2nd order, see figure 4 (b). The corresponding star system is therefore:

$$A = (A_1, A_2, A_3, A_4), [n_A = 3, m_A = 4]$$
  

$$B = (B_1, B_2, B_3, B_4), [n_B = 3, m_B = 4]$$
  

$$C = (C_1, C_2, C_3, C_4, C_5, C_6), [n_C = 2, m_C = 6]$$

2) Let us count the number of pairs (A, g) such that  $g \neq e$  leaves invariant the pole A. On one side, since each element g leaves invariant precisely two poles, this number is 2(N-1). On the other hand for each pole A there are exactly  $(n_A - 1)m_A$  such pairs. As a result we have

$$\sum_{X=\{A,B,\dots,Z\}} (n_X - 1)m_X = 2(N-1),$$

where the sum is over all stars. Using (4.1) one gets:

(4.2) 
$$\sum_{k=1}^{l} \frac{1}{n_k} = l - 2 + \frac{2}{N},$$

where  $n_k$  is the order of k-th star and l is the total number of stars.

#### 5. NON-SPECIAL TRANSFORMATIONS

3) As it turns out this equation has a finite number of solutions. To see this let us first note that since  $n_k \ge 2$ ,  $l \le 3$  (otherwise right side of (4.2) is too large.

A) l = 2.

$$\frac{1}{n_1} + \frac{1}{n_2} = \frac{2}{N} \Longrightarrow m_1 + m_2 = 2$$

From this follows  $m_1 = m_2 = 1$  and

•  $n_1 = n_2 = N$ , while N is arbitrary.  $G \cong C_N$  - Symmetry of the **pyramid** with N-side polygon in the foundation.

B) 
$$l = 3$$
.

$$\frac{1}{n_1} + \frac{1}{n_2} + \frac{1}{n_3} = 1 + \frac{2}{N}.$$

Without loss of generality we can assume  $n_1 \leq n_2 \leq n_3$ . One can see then that  $n_1 = 2$ . The only possible solutions of the above equation:

- $n_1 = 2, n_2 = 2, n_3 = N/2$ .  $G \cong D_{N/2}$  Symmetry group of **prism** with N/2-side polygon in the foundation.
- $n_1 = 2, n_2 = 3, n_3 = 3, N = 12$ .  $G \cong T$  Symmetry group of tetrahedron.
- $n_1 = 2, n_2 = 3, n_3 = 4, N = 24. G \cong O$  Symmetry group of cube.
- $n_1 = 2, n_2 = 3, n_3 = 5, N = 60. G \cong Y$  Symmetry group of icosahedron.



FIGURE 3. Platonic solids. The different point groups basically classify all possible (symmetries of) platonic solids. Note that Octahedron and Cube have the same symmetry group. The same goes for Icosahedron and Dodecahedron.

#### 5. Non-special transformations

The above considerations can be generalized to the case when non-special transformations are present. If the inversion  $\iota$  is present then the resulting symmetry group G is (since  $\iota$  commutes with all other elements of the group) just the direct product  $I \times G_0$  where  $I = \{e, \iota\}$  and  $G_0$  is one of the groups  $\{C_n, D_n, O, T, Y\}$ . In the case when  $\iota \notin G$  the symmetry group is the union  $G_0 \cup \iota G'_0$ where  $G_0, G'_0$  are proper transformations. Note that the set  $G_0$  is a group (from the above list) itself while  $G'_0$  is not (since it contains no unite element). The number of elements in both sets  $G_0, G'_0$  must coincide and  $G_0 \cap G'_0 = \emptyset$  (otherwise  $\iota$  would belong to G). Furthermore, since  $\iota$ commutes with all elements, the group G is isomorphic to the union  $G_0 \cup G'_0$ , and therefore is, in fact, one of the groups  $\{C_n, D_n, O, T, Y\}$ . A standard notation for groups from O(3) is:

$$(G, G_0), \quad G, G_0 \in \{C_n, D_n, O, T, Y\}.$$

The condition  $|G| = 2|G_0| = 2|G_0'|$  leaves only few possibilities:

$$(D_n, C_n),$$
  $(C_{2n}, C_n),$   $(D_{2n}, D_n),$   $(O, T).$ 

For instance the full group of symmetries of tetrahedron is (O, T).

#### LECTURE 3

### Representation Theory I

#### 1. Basic notions

It is clear that the same group e.g.,  $S_n$  can appear in different disguises (permutations, matrices, geometrical transformations of a points set etc.). Representation theory studies groups by representing their elements as linear transformations of vector spaces. In essence, a representation makes an abstract group more concrete by describing its elements as matrices with a standard multiplication. We have seen already with the example of  $S_n$  that such representation might be quite useful – the notion of determinant allowed us to define even and odd permutations in a simple way.

From the physics point of view the representation theory appears naturally in quantum mechanics. Since quantum mechanics is a "linear theory" any symmetry operation  $g \in G$  acts as a linear transformation on the corresponding Hilbert space V:

(1.1) 
$$g \cdot (|\psi_1\rangle + |\psi_2\rangle) = g \cdot |\psi_1\rangle + g \cdot |\psi_2\rangle, \qquad |\psi_i\rangle \in V$$

By choosing some basis  $\{\phi_i\}$  in V we have

(1.2) 
$$g \cdot |\phi_i\rangle = \sum_{j=1}^{\dim V} D(g)_{ij} |\phi_j\rangle, \quad i = 1, 2..., \dim V.$$

So we have a map  $D: g \to D(g)$  of the group elements g into matrices D(g).

DEFINITION 1.1. Formal definition of N-dimensional representation:

- (1)  $D(g), g \in G$  is a linear operator acting on the N-dimensional Hilbert space.
- (2) D is a homeomorphism:  $D(g_1 \cdot g_2) = D(g_1)D(g_2)$ .

**Remark** 3.1. Matrix representations. For a finite N, D(g) can be seen as N-dimensional matrix.

**Example** 3.1. **2-element group:** Group  $G = \{e, \sigma\}$ ,  $\sigma^2 = e$ . One-dimensional representation:  $D^{(1)}(e) = 1$ ,  $D^{(1)}(\sigma) = 1$  and  $D^{(2)}(e) = 1$ ,  $D^{(2)}(\sigma) = -1$ . Two-dimensional representation:

$$D(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad D(\sigma) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Two representations D, D' are equivalent if

$$V^{-1}D(g)V = D'(g)$$
, for all  $g \in G$ .

In this case one can transform D to D' just by changing the basis in V.

Representation is called **unitary** if D(g) is unitary for all  $g \in G$ . Important fact: each representation of a finite group is equivalent to unitary (proof is simple but not completely trivial). Therefore, we need to consider only unitary representations.

Main goal of the representation theory is to classify possible representations. We need however to impose some restriction on the type of representations we consider. The representation is called **reducible** if there exists  $V_1 \subset V$ , such that

$$D(g)V_1 \subset V.$$

If the representation is reducible

$$U^{-1}D(g)U = D^{(1)}(g) \oplus D^{(2)}(g) \dots \oplus D^{(k)}(g).$$

When k = 1 the representation is called **irreducible**. They are building blocks of a general representation.

It is straightforward to see that any **abelian group has only one-dimensional representations**. This just follows from a simple fact that all elements of such a group are commuting matrices and can be diagonalized simultaneously.

**Motivation:** For a given group we aim to *classify all possible irreducible representations* Why do we need such a classification? The main reason is due to the following fact:

PROPOSITION 1.2. (Informal form of Wigner's theorem.) If G is a symmetry of the Hamiltonian H, then [H, D(g)] = 0, for all  $g \in G$ . Consider decomposition of the Hilbert space  $V = V_1 \oplus V_2 \oplus \cdots \oplus V_k$  and the corresponding decomposition D(g) into (different) irreducible representations:

$$U^{-1}D(g)U = \begin{pmatrix} D^{(1)}(g) & 0 & \dots & 0\\ 0 & D^{(2)}(g) & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \dots & D^{(k)}(g) \end{pmatrix}$$

With the same transformation U we can bring H into the diagonal form

$$U^{-1}HU = \begin{pmatrix} H^{(1)} & 0 & \dots & 0\\ 0 & H^{(2)} & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \dots & H^{(k)} \end{pmatrix}, \qquad H^{(i)} = h_i I_{N_i \times N_i}.$$

This means H multiply by a constant  $(h_i)$  vectors from  $V_i$ .

In other words we managed <u>"almost" diagonalize H</u> without actually solving the eigenvalue problem. If all the entering representations are one dimensional then D(g) is diagonal and the above statement becomes obvious: Eigenvectors of D(g) and H coincide because these are commuting matrices. The Wigner theorem can be seen as a generalization of this fact. In order to prove it in full generality we will need a couple of auxiliary lemmas. The same mathematics is also necessary for classification of irreducible representations.

#### 2. Schur's lemmas

We now prove two auxiliary statements.

LEMMA 2.1. First Schur's lemma. Let [M, D(g)] = 0, for all  $g \in G$  with D being a Ndimensional irreducible representation. Then  $M = \lambda I_{N \times N}$ .

#### 3. ORTHOGONALITY THEOREM

*Proof:* Let v be an eigenvector of M (at least one always exists) with an eigenvalue  $\lambda$ . Consider now the subspace  $V' \subseteq V$ , of all eigenvectors v' with the same eigenvalue  $\lambda$ , i.e.,  $Mv' = \lambda v'$ . By construction  $D(g)V' \subseteq V'$  for all  $g \in G$ . This implies that the dimension of V' must be N, since D is an irreducible representation.

LEMMA 2.2. Second Schur's lemma. Let  $D^{(1)}(g)$ ,  $D^{(2)}(g)$  be two non-equivalent irreducible representations of dimension  $N_1$  and  $N_2$ , respectively. Let M be  $N_1 \times N_2$  matrix such that

$$MD^{(1)}(g) = D^{(2)}(g)M, \qquad for all \ g \in G.$$

Then M = 0.

*Proof:* Taking conjugate and change 
$$g$$
 to  $g^{-1}$  we obtain

$$D^{(1)}(g)M^* = M^*D^{(2)}(g), \Rightarrow MM^*D^{(2)}(g) = D^{(2)}(g)MM^*.$$

By first Schur's lemma:

$$MM^* = \lambda I_{N_2 \times N_2}.$$

a)  $N_1 = N_2$ . If det  $M \neq 0$  then

$$MD^{(1)}(g)M^{-1} = D^{(2)}(g)$$

and two representations are equivalent.

b)  $N_1 < N_2$ . In this case we extend matrix M by zeros to square  $\tilde{M}$ , such that

$$MM^* = \tilde{M}\tilde{M}^*$$

and by using det  $\tilde{M} = 0$  conclude that  $\lambda = 0$ .

#### 3. Orthogonality theorem

We will prove now the group orthogonality theorem which plays a fundamental role in the representation theory.

THEOREM 3.1. For two representations  $D^{(i)}$ ,  $D^{(j)}$  of the dimensions  $n_i$ ,  $n_j$  we have

(3.1) 
$$\frac{1}{|G|} \sum_{g \in G} D^{(i)}_{\mu,\nu}(g) \bar{D}^{(j)}_{\alpha,\beta}(g) = \frac{1}{n_i} \delta_{\mu,\alpha} \delta_{\nu,\beta} \delta_{ij}.$$

**Interpretation:** Consider |G|-component vectors  $\{D_{\mu,\nu}^{(i)}(g_i), i = 1... |G|\}$ . There are  $\sum_i n_i^2$  such vectors. By the group orthogonality theorem all these vectors orthogonal. In particular, from this follows  $\sum_i n_i^2 \leq |G|$  the number of irreducible representations is restricted by the order of the group (actually, as we show the equality holds).

*Proof:* For an arbitrary matrix X of the dimension  $n_i \times n_j$ , construct the following matrix:

$$M = \sum_{g \in G} D^{(i)}(g) X D^{(j)}(g^{-1}).$$

It is easy to see that  $MD^{(j)}(g) = D^{(i)}(g)M$ . Thus by the second Schur's lemma we have M = 0 if  $i \neq j$ . After taking matrix X in the form  $X_{s,t} = \delta_{s,\beta}\delta_{t,\nu}$  we obtain:

$$\sum_{g \in G} D^{(i)}_{\mu,\nu}(g) D^{(j)}_{\beta,\alpha}(g^{-1}) = 0$$

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If i = j then by the first Schur's lemma:

$$\sum_{g \in G} D^{(i)}_{\mu,\nu}(g) D^{(i)}_{\beta,\alpha,}(g^{-1}) = \lambda(\nu,\beta) \delta_{\mu,\alpha}.$$

Fixing now  $\alpha = \mu$  and summing up over the index  $\mu$  gives:

$$\sum_{g \in G} D^{(i)}_{\beta,\nu}(e) = n_i \lambda(\nu,\beta).$$

Since the sum on the left hand side is  $\delta_{\nu,\beta}|G|$ , we have  $\lambda(\nu,\beta) = \delta_{\nu,\beta}|G|/n_i$ .

#### LECTURE 4

### **Representation Theory II**

#### 1. Characters

There is a convenient way to distinguish non-equivalent representations. To this end we introduce **characters**:

$$\chi(g) := \operatorname{Tr}(D(g))$$

The characters provide minimal piece of information which we need to know about the irreducible representations in order to distinguish/classify them. If we know characters of a representation D we also know what/how many irreducible representations enter D.

- (1) Equivalent representations have the same characters.
- (2) By the group orthogonality theorem

(1.1) 
$$\frac{1}{|G|} \sum_{g \in G} \chi^{(i)}(g) \bar{\chi}^{(j)}(g) = \delta_{ij}.$$

From this immediately follows that different irreducible representations have different set of characters. Note that different group elements might have the same characters. For each element g define its **class**  $C(g) = \{hgh^{-1}, h \in G\}$ . All elements from the same class have the same character. Thus we need to know only restricted number of characters. The group orthogonality relation (1.1) can be rewritten as:

$$\frac{1}{|G|} \sum_{C(g)} |C(g)| \chi^{(i)}(g) \bar{\chi}^{(j)}(g) = \delta_{ij}.$$

(3) The characters of a reducible representation D is the sum over characters of irreducible representations entering D:

$$\chi(g) = \sum_{i} r_i \chi^{(i)}(g),$$

where  $r_i$  is the number of times  $D^{(i)}$  enters D. By the group orthogonality theorem we have:

THEOREM 1.1. Decomposition:

$$r_i = \frac{1}{|G|} \sum_{g \in G} \bar{\chi}^{(i)}(g) \chi(g).$$

#### 2. Classification of irreducible representations

To get an information on the number of irreducible representations, we will make use of the regular representation  $\sigma$  considered in the second lecture:

$$h \cdot g_i = g_{\sigma(i)}, \qquad G = \{g_1, g_2 \dots g_{|G|}\}; \qquad h \to \sigma(h).$$

For this representation we have:

$$\chi^{(\sigma)}(g) = 0$$
 if  $g \neq e$ , and  $\chi^{(\sigma)}(e) = |G|$ .

Now, let us decompose this representation into irreducible:

$$\chi^{(\sigma)}(g) = \sum_{i} r_i \chi^{(i)}(g), r_i = \frac{1}{|G|} \sum_{g \in G} \bar{\chi}^{(i)}(g) \chi^{(\sigma)}(g) = m_i.$$

From this follows simple conclusion: every irreducible representation enters  $\sigma$ . Furthermore the number of times it enters  $\sigma$  equals to its dimension. We therefore get:

(2.1) 
$$\chi^{(\sigma)}(e) = \sum_{i} m_i \chi^{(i)}(e) \Longrightarrow |G| = \sum_{i} m_i^2.$$

In some cases of groups with low order the above equation (2.1) is sufficient in order to recover dimensions of all irreducible representations.

#### 3. How to find characters of irreducible representations?

**Example** 4.1. **Permutations of three objects:** Dihedral group  $D_3$ . Here |G| = 6 and the only possible solutions of (2.1) are  $m_i = 1, i = 1...6$  or  $m_1 = m_2 = 1, m_3 = 2$ . The group contains three classes:  $G = \{[e], [g, g^2], [\sigma_1, \sigma_2, \sigma_3]\}$ . First of all we look for one dimensional representations. There are only two possibilities:

 $\chi^{(1)}([e]) = 1, \chi^{(1)}([g]) = 1, \chi^{(1)}([\sigma]) = 1; \qquad \chi^{(2)}([e]) = 1, \chi^{(2)}([g]) = 1, \chi^{(2)}([\sigma]) = -1.$ For the remaining two-dimensional representation we have by the group orthogonality theorem:

The remaining two-dimensional representation we have by the group orthogonality theor $1 \cdot \chi^{(3)}([e]) + 2 \cdot \chi^{(3)}([g]) \pm 3 \cdot \chi^{(3)}([\sigma]) = 0.$ 

Using  $\chi^{(3)}([e]) = 2$  we get  $\chi^{(3)}([\sigma]) = 0$  and  $\chi^{(3)}([g]) = -1$ .

<b>D</b> <sub>3</sub>	[e]	2[g]	3[σ]
$A_1$	1	1	1
$A_2$	1	1	-1
Е	2	-1	0

FIGURE 1. Character table for  $D_3$ .

A standard (physics) notation is A for one-dimensional representation, E for two-dimensional and F for three-dimensional representations.

**Remark** 4.1. Different groups can have the same character tables. It is worth noting that, in general, a group is not defined by its character table. For example, compare  $D_4$  and the quaternion group of example 4.2.

#### 4. Dual orthogonality relationship

Note that the sum in the orthogonality relation is running over the group elements. There is in fact a dual connection, where the sum is running over the irreducible representations. To show it we need the following simple fact:

#### 5. THREE TYPES OF REPRESENTATIONS

THEOREM 4.1. The number of irreducible representations equals to the number of the group classes.  $^{1}$ 

Using this we can define the square matrix:  $B_{ij} = \sqrt{C_i/|G|}\chi^{(j)}(C_i)$ , where  $C_i, i = 1, ... l$ . Then orthogonality relation implies:  $BB^* = I$ . Changing the order, i.e.,  $B^*B = I$  implies:

(4.1) 
$$\sum_{j=1}^{l} \chi^{(j)}(C_k) \bar{\chi}^{(j)}(C_m) = \frac{|G|}{C_k} \delta_{k,m}$$

#### 5. Three types of representations

There are three types of representation: **Real**, **Pseudo-real** and **Complex**. For real representations matrices D(g) can be brought into real form such that  $D_{ij}(g) = \overline{D}_{ij}(g)$ . This implies in particular that all the characters are real. For pseudo real representation the characters are also real but matrices D(g) cannot be brought into real form. Finally, for complex representations the characters are complex. In the last case D(g) and the conjugate  $\overline{D}(g)$  constitute two different representation (since they characters are different), while in the real and pseudo-real case both representations are equivalent, i.e.,  $\overline{D}(g) = UD(g)U^{\dagger}$ .

**Indicator.** To distinguish between three types of representations one looks at the indicator:

$$\operatorname{Ind}(\alpha) = \frac{1}{|G|} \sum_{g \in G} \chi^{(\alpha)}(g^2) \in \{1, 0, -1\},\$$

where 1, -1, 0 are obtained for real, complex and pseudo-real representations, respectively.

*Proof:* For a general irreducible representation we have

(5.1) 
$$D^{(\alpha)}(g) = U\bar{D}^{(\beta)}(g)U^{\dagger},$$

where  $\alpha \neq \beta$  for a complex representation (since  $\chi^{(\alpha)}(g) \neq \bar{\chi}^{(\alpha)}(g)$ ) and  $\alpha = \beta$  for real and pseudo-real representations. From  $D^{(\alpha)}(g^2) = D^{(\alpha)}(g)D^{(\alpha)}(g)$  follows

$$\operatorname{Ind}(\alpha) = \sum_{i,j=1}^{m_{\alpha}} \sum_{k,n=1}^{m_{\alpha}} \sum_{g \in G} \frac{1}{|G|} \sum_{g \in G} U_{k,j} D_{i,k}^{(\alpha)}(g) \bar{D}_{j,n}^{(\beta)}(g) U_{ni}^{\dagger},$$

with  $m_{\alpha}$  being dimension of  $\alpha$ . By the orthogonality theorem this expression is zero for  $\alpha \neq \beta$  which is the case of complex  $\alpha$ . For real and pseudo-real representations we have

$$\operatorname{Ind}(\alpha) = \frac{1}{m_{\alpha}} \operatorname{Tr}\left(U\bar{U}\right).$$

Now note, that for  $\alpha = \beta$  eq. (5.1) yields

$$D^{(\alpha)}(g)U\bar{U} = U\bar{U}D^{(\alpha)}(g).$$

By the first Schur's lemma it follows then that  $U\bar{U} = \gamma I$ , or  $U = \gamma U^{\top}$  which also implies  $\gamma^2 = 1$ . This leaves only two possibilities  $\gamma = 1$  for real and  $\gamma = -1$  for pseudo-real representations. In the first case we have  $UU^{\top} = I$  and  $Ind(\alpha) = 1$ , while in the second one  $UU^{\top} = -I$  and  $Ind(\alpha) = -1$ . Note finally, that  $1 = \det (U\bar{U}) = \gamma^{m_{\alpha}}$ . So  $\gamma = -1$  might appear only if  $m_{\alpha}$  is even. In other words, a pseudo-real irreducible representation must be of even dimension.

<sup>&</sup>lt;sup>1</sup> I give the proof of this statement at the end of this lecture

**Example** 4.2. **Quaternions:** *Quaternion multiplication table is* 

$$\{\pm 1, \pm i, \pm j, \pm k\}$$
  $i^2 = j^2 = k^2; \quad ij = k.$ 

This group has five conjugate classes:

 $\{1\}, \{-1\}, \{\pm i\}, \{\pm j\}, \{\pm k\}.$ 

The only possible solution for the equation  $\sum_{i=1}^{5} m_i^2 = 8$  is  $m_i = 1, i = 1, \dots, 4, m_5 = 2$ . In addition to fully symmetric representation, the other three one-dimensional representations are easy to find:  $\chi(1) = 1, \chi(-1) = 1$ , while  $\chi(i) = -1, \chi(j) = -1, \chi(k) = 1; \chi(i) = -1, \chi(k) = -1, \chi(j) = 1$  or  $\chi(k) = -1, \chi(j) = -1, \chi(i) = 1$ . The two-dimensional representation can be find by the orthogonality relation:

$$2 + \chi(-1) \pm \chi(k) \pm \chi(i) \pm \chi(j) = 0, \Longrightarrow \chi(-1) = -2, \chi(k) = \chi(i) = \chi(j) = 0$$

Since the indicator equals

$$Ind = (2\chi(1) + 6\chi(-1))/8 = -1,$$

the last representation is pseudo-real. Note that this representation can be realized using Pauli matrices:

 $\{\pm I, \pm \sigma_x, \pm \sigma_y, \pm \sigma_z\}.$ 

#### 6. Representations of cross products

If we have two different irreducible representations  $D^{(i)}$ ,  $D^{(j)}$  of a group G acting on the spaces  $V^{(i)}$ ,  $V^{(j)}$  we can generate (in general) reducible representation:

$$D^{(ij)}(g) = D^{(i)}(g) \otimes D^{(j)}(g),$$

which acts on the space  $V^{(i)} \otimes V^{(j)}$ . The characters  $\chi^{(i)}(g)\chi^{(j)}(g)$  of this representation can be decomposed into irreducible:

$$\chi^{(i)}(g)\chi^{(j)}(g) = \sum_{k=1}^{l} r_k \chi^{(k)}(g), \qquad r_k = \frac{1}{|G|} \sum_{g \in G} \chi^{(i)}(g)\chi^{(j)}(g)\bar{\chi}^{(k)}(g).$$

**Example** 4.3.  $D_3$ : Consider representation  $E \times E$ . The corresponding characters are then

$$\chi^{(2,2)}([e]) = 4, \qquad \chi^{(2,2)}([g]) = 1, \qquad \chi^{(2,2)}([\sigma]) = 0.$$

and the multiplicities are:

$$r(A_1) = r(A_2) = r(E) = 1$$
, *i.e.*,  $E \times E = A_1 \oplus A_2 \oplus E$ 

Note: the above construction can be used in order to construct higher dimensional irreducible representations from lower one. The same idea is used for continues groups, i.e., SU(2).

For  $G = H \times F$  all irreducible representations can be constructed from the irreducible representations of H and F:

$$D^{(ij)}(g) = D^{(i)}(h) \otimes D^{(j)}(f), \qquad g = (h, f).$$

It is an easy exercise to check that  $D^{(ij)}$  is indeed irreducible.

#### 7. Representations of subgroups

Let *H* be a subgroup of *G*. Any representation *D* of *G* restricted to *H* gives representation  $D|_H$  (or  $\operatorname{Res}_G^H(D)$  in mathematical notation) of *H*, which is called restrictive representation.

In the opposite direction having a representation of H we can lift it to a representation  $\operatorname{Ind}_{G}^{H}(D)$  of G. This representation is called induced.<sup>2</sup>

<sup>&</sup>lt;sup>2</sup>The precise construction is not trivial and we do not provide it here (for a while)

#### 8. Appendix. Proof of the theorem (4.1)

*Proof idea:* Construct some linear space  $V_0$  (see below) of the dimension given by the number of classes, and then show that  $V_0$  can be also spanned by characters of the irreducible representations. Hence

#### Number of Classes = $\dim V_0$ = Number of Irreducible representation.

*Proof:* Let V be N = |G| dimensional vector space. For each v we label its components by the group elements:

$$v = (v(g_1), v(g_2), \dots v(g_N)).$$

Consider the subspace  $V_0$  of V composed of vectors which remain invariant under all group transformations:

$$h \cdot v = (v(hg_1h^{-1}), v(hg_2h^{-1}), \dots v(hg_Nh^{-1}))$$
 for all  $h \in G$ 

It is straightforward to see that  $V_0$  is a linear subspace itself. i.e., if  $h \cdot v_1 = v_1, h \cdot v_2 = v_2 \Rightarrow h \cdot (v_1 + v_2) = v_1 + v_2$  and dim $V_0$  equals the number of the conjugate classes. Indeed, all elements of the invariant vectors from the same conjugate class must be equal. This means that vectors from  $V_0$  are of the form:

$$v = (\underbrace{a_1 \dots a_1}_{C_1}, \underbrace{a_2 \dots a_2}_{C_2}, \dots, \underbrace{a_k \dots a_k}_{C_k}),$$

where  $C_i$  are conjugate classes.

Note that any irreducible representation  $\alpha$  defines an invariant vector with the components given by its characters:

$$\vec{\chi}^{(\alpha)} = (\chi^{(\alpha)}(g_1), \chi^{(\alpha)}(g_2), \dots \chi^{(\alpha)}(g_N)).$$

Let us show that any vector from  $V_0$  can be represented as a linear combination:

$$v = \sum_{\alpha} c_{\alpha} \vec{\chi}^{(\alpha)}.$$

A g component of an arbitrary vector  $v \in V$  can be represented as:

$$v(g) = \sum_{\alpha,i,j} \gamma^{\alpha}_{i,j} D^{(\alpha)}_{ij}(g).$$

If  $v \in V_0$  then v(g) = hv(g) for all  $h \in G$  and we can take the average over the group:

$$v(g) = \frac{1}{|G|} \sum_{h \in G} v(hgh^{-1}).$$

By the group orthogonality theorem:

(8.1) 
$$v(g) = \frac{1}{|G|} \sum_{h \in G} \sum_{\alpha, i, j} \gamma_{ij}^{\alpha} D_{ik}^{(\alpha)}(h) D_{k,m}^{(\alpha)}(g) D_{mj}^{(\alpha)}(h^{-1}) =$$

$$=\sum_{\alpha}\frac{1}{m_{\alpha}}\left(\sum_{i}\gamma_{ii}^{\alpha}\right)\chi^{(\alpha)}(g).$$

#### LECTURE 5

### Applications I. Vibration modes

#### 1. Vibration spectrum of molecules

In the linear approximation the classical dynamics of the molecule is governed by the Hamiltonian:

$$H = \sum_{i=1}^{N} \frac{m}{2} \dot{x}_{i}^{2} + \sum_{i,j=1}^{N} \mathcal{V}_{ij} x_{i} x_{j}.$$

By making a linear transformation we can bring it to the diagonal form

$$x \rightarrow y = Ux, \qquad H = \sum_{i=1}^{N} \frac{m}{2} \left( \dot{y}_i^2 + \omega_i^2 y_i^2 \right).$$

If the system is invariant under the group of symmetries G we have:

$$[\mathcal{V}, D(g)] = 0, \qquad g \in G.$$

Using Wigner's theorem we can diagonalize H through the decomposition of D into irreducible representations.

THEOREM 1.1. Wigner's theorem. Let  $[H, D(g)] = 0, g \in G$  for some representation D of G, and let

$$D = \bigoplus_k I_{r_k \times r_k} \otimes D^{(k)}$$

be its decomposition into irreducible representations, where  $r_k$  is the number of times representation  $D^{(k)}$  enters D. Then H takes the form:

$$H = \bigoplus_k H^{(k)} \otimes I_{n_k \times n_k},$$

where  $H^{(k)}$  is a matrix of the dimension  $r_k \times r_k$  and  $n_k$  is the dimension of  $D^k$  (pay attention to the different order in the cross products).

*Proof:* The proof of the theorem is straightforward by using Schur's lemmas. For the sake of clearness we will give a proof for a particular case of two irreducible representations, with one representation appearing twice. In this case Wigner's theorem tells that if [H, D(g)] = 0, for all  $g \in G$ , then both matrices can be simultaneously brought to the block-diagonal form:

(1.1) 
$$D(g) = \begin{pmatrix} D^{(1)} & 0 & 0\\ 0 & D^{(1)} & 0\\ 0 & 0 & D^{(2)} \end{pmatrix} \qquad H = \begin{pmatrix} h_{11}^{(1)}I & h_{12}^{(1)}I & 0\\ h_{21}^{(1)}I & h_{22}^{(1)}I & 0\\ 0 & 0 & h^{(2)}I \end{pmatrix}$$

To prove it assume that D(g) has the above block-diagonal form and write H a:

$$H = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}.$$

The commutation relationship [H, D(g)] = 0 then reads as:

$$\begin{pmatrix} H_{11}D^{(1)} & H_{12}D^{(1)} & H_{13}D^{(2)} \\ H_{21}D^{(1)} & H_{22}D^{(1)} & H_{23}D^{(2)} \\ H_{31}D^{(1)} & H_{32}D^{(1)} & H_{33}D^{(2)} \end{pmatrix} = \begin{pmatrix} D^{(1)}H_{11} & D^{(1)}H_{12} & D^{(1)}H_{13} \\ D^{(1)}H_{21} & D^{(1)}H_{22} & D^{(1)}H_{23} \\ D^{(2)}H_{31} & D^{(2)}H_{32} & D^{(2)}H_{33} \end{pmatrix}.$$

By application of Schur's lemmas now follows (1.1).

**Projection operators.** By Wigner's theorem we know that H becomes block-diagonal in the same basis where D(g) takes the block-diagonal form. We thus need to know how to construct such a basis. To this end for each irreducible representation i we define **projections**:

(1.2) 
$$P_i = \frac{n_i}{|G|} \sum_{g \in G} \bar{\chi}^{(i)}(g) D(g).$$

satisfying the following properties:

- Orthogonality: P<sub>i</sub>P<sub>j</sub> = δ<sub>ij</sub>P<sub>i</sub>.
  Completeness: Σ<sup>l</sup><sub>i=1</sub>P<sub>i</sub> = 1.
  Let D = ⊕<sub>i</sub>r<sub>i</sub>D<sup>i</sup> be the decomposition of D into irreducible representations and let V =  $\oplus_i r_i V^{(i)}$  be the decomposition of the space V, where D acts (such that  $DV^{(i)} = D^{(i)}V^{(i)}$ ). then  $P_i$  acts as unity on  $V^{(i)}$ :

$$P_i v = v$$
, if  $v \in V^{(i)}$  and  $P_i v = 0$  if  $v \in V^{(j)}, j \neq 0$ .

*Proof:* Consider  $P_i$  in the basis where D has the block-diagonal form. Proof then follows immediately by a simple application of the group orthogonality theorem.





FIGURE 1. a) Chain with circular symmetry. b) Dependance of frequency on the representation wavenumber k. c) Molecule with  $D_3$  symmetry.

The interaction is given by the potential  $\mathcal{V} = \sum_i k_1 (x_i - y_i)^2 + k_2 (x_{i+1} - y_i)^2$  whose matrix form is: vibModes - 2016-01-04

$$(1.3) \qquad \mathcal{V} = \begin{pmatrix} k_1 + k_2 & -k_1 & 0 & 0 & 0 & \dots & 0 & 0 & -k_2 \\ -k_1 & k_1 + k_2 & -k_2 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & -k_2 & k_1 + k_2 & -k_1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & -k_1 & k_1 + k_2 & -k_2 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & -k_2 & k_1 + k_2 & -k_1 \\ -k_2 & 0 & 0 & 0 & 0 & \dots & 0 & -k_1 & k_1 + k_2 \end{pmatrix}$$

(1.4) 
$$\underbrace{\begin{pmatrix} 0 & 0 & \dots & 0 & I \\ I & 0 & \dots & 0 & 0 \\ 0 & I & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & I & 0 \end{pmatrix}}_{D(T)} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_n \end{pmatrix} = \begin{pmatrix} z_n \\ z_1 \\ z_2 \\ \vdots \\ z_{n-1} \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad z_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix}$$

The characters of the representation D:

$$\chi(T^l)=0, \,\,$$
 if  $l
eq 0,\,\,$  and  $\chi(e)=2n,$ 

have to be decomposed into the characters of the irreducible representations:

$$\chi^{(k)}(T) = \exp\left(\frac{2\pi i k}{n}\right), \qquad k = 0, \dots n - 1.$$

The result is

$$\chi = \sum r_k \chi^{(k)}, \qquad r_k = \frac{1}{n} \sum_{g \in G} \bar{\chi}^{(k)}(g) \chi(g) = 2,$$

where each irreducible representation enters twice. The corresponding projection matrices are given by:

(1.5) 
$$P^{(k)} = \begin{pmatrix} I & \bar{\alpha}I & \bar{\alpha}^{2}I & \dots & \bar{\alpha}^{n-2}I & \bar{\alpha}^{n-1}I \\ \alpha I & I & \bar{\alpha}I & \dots & \bar{\alpha}^{n-3}I & \bar{\alpha}^{n-2}I \\ \alpha^{2}I & \alpha I & I & \dots & \bar{\alpha}^{n-4}I & \bar{\alpha}^{n-3}I \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \alpha^{n-2}I & \alpha^{n-3}I & \alpha^{n-4}I & \dots & I & \bar{\alpha}I \\ \alpha^{n-1}I & \alpha^{n-2}I & \alpha^{n-2}I & \dots & \alpha I & I \end{pmatrix}, \qquad \alpha = \exp\left(\frac{2\pi ik}{n}\right)$$

To find the eigenmodes we apply  $P^{(k)}$  to the whole Hilbert space. The resulting space is spanned by two vectors:

$$\eta_{1} = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 \\ 0 \\ \alpha \\ 0 \\ \vdots \\ \alpha^{n-1} \\ 0 \end{pmatrix}, \qquad \eta_{2} = \frac{1}{\sqrt{n}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \alpha \\ \vdots \\ 0 \\ \alpha^{n-1} \end{pmatrix}.$$

In order to find eigenfrequences we have to consider action of  ${\mathcal V}$  on these two vectors:

$$\mathcal{V}\eta_1 = (k_1 + k_2)\eta_1 - (k_1 + k_2\alpha)\eta_2, \qquad \mathcal{V}\eta_2 = (k_1 + k_2)\eta_2 - (k_1 + k_2\bar{\alpha})\eta_1.$$

The corresponding eigenfrequences are determined by the equation:

(1.6) 
$$\det \left( \begin{pmatrix} k_1 + k_2 & -(k_1 + k_2 \alpha) \\ -(k_1 + k_2 \bar{\alpha}) & k_1 + k_2 \end{pmatrix} - \frac{\omega^2}{2} I \right) = 0, \implies \frac{\omega_{\pm}^2(k)}{2} = k_1 + k_2 \pm |k_1 + k_2 \alpha(k)|.$$

It is worth noticing that in the case when there are m particles in one cell, the corresponding representation is given by the direct sum

$$\underbrace{D \oplus D \oplus \cdots \oplus D}_{m},$$

where D is the representation obtained for one particle (in one cell). This means for m particles each irreducible representation enters m times and we have to consider m-dimensional eigenvalue problem, in order to find eigenfrequences. These leads to m branches of  $\omega(k)$  - one acoustic and the rest optical, see figure 1. (In 3 dimensions we would have 3m branches of which 3 are acoustic  $\omega(0) = 0$ ).

**Example** 5.2.  $D_3$  symmetry:

$$(1.7) D(T) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}, D(\sigma_1) = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$$(1.8) D(\sigma_2) = \begin{pmatrix} 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, D(\sigma_3) = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$G = \{[e]; [g, g^2]; [\sigma_1, \sigma_2, \sigma_3]\}, \qquad \chi^{(1)} = \{1, 1, 1\}, \chi^{(2)} = \{1, 1, -1\}, \chi^{(3)} = \{2, -1, 0\}$$
$$r_i = \chi(e)\chi^{(i)}(e)/6; \qquad r_i = \{1, 1, 2\} \implies D = 2E \oplus A_1 \oplus A_2.$$

$$P_i = \frac{1}{3} \sum_{g \in G} \chi^{(i)}(g) D(g)$$

(1.9) 
$$P_{1} = \frac{1}{3} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix}, \qquad P_{2} = \frac{1}{3} \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The vibration modes associated with the two one-dimensional representations are given by

$P_1V = \alpha \left($	$\begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$	and	$P_2V = \beta$	$\begin{pmatrix} 1\\0\\1\\0\\1\\0 \end{pmatrix}$	,
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respectively. Here  $P_1V$  represents symmetric mode shown in figure (red). The second mode  $P_2V$  corresponds to the rotations of the whole system. Finally the projection operator for the two-dimensional representation is

#### 1. VIBRATION SPECTRUM OF MOLECULES

(1.10) 
$$P_{3} = \frac{2}{6}(2D(I) - D(T) - D(T^{2})) = \frac{1}{3} \begin{pmatrix} 2 & 0 & -1 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 & 0 & -1 \\ -1 & 0 & 2 & 0 & -1 & 0 \\ 0 & -1 & 0 & 2 & 0 & -1 \\ -1 & 0 & -1 & 0 & 2 & 0 \\ 0 & -1 & 0 & -1 & 0 & 2 \end{pmatrix}$$

From this we have to separate two vectors corresponding to shift in x and y directions.

$$\eta_{x} = \begin{pmatrix} 1 \\ 0 \\ -1/2 \\ \sqrt{3}/2 \\ -1/2 \\ -\sqrt{3}/2 \end{pmatrix}, \qquad \eta_{y} = \begin{pmatrix} 0 \\ 1 \\ -\sqrt{3}/2 \\ -1/2 \\ \sqrt{3}/2 \\ -1/2 \end{pmatrix}$$
$$P_{3}V = \begin{cases} \alpha \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \end{pmatrix} + \beta \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \end{pmatrix} + \gamma \frac{1}{\sqrt{6}} \begin{pmatrix} 0 \\ 2 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \\ -1 \end{pmatrix} + \delta \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ \xi_{4} \end{pmatrix}$$

where  $\eta_x = \sqrt{3/2}(\xi_4 + \xi_1)$ ,  $\eta_y = \sqrt{3/2}(\xi_3 - \xi_2)$  ( $\xi_i$  are just columns of  $P_3$  and their linear combinations.) The orthogonal vectors are given by

$$\nu_{1} = \sqrt{3/2}(\xi_{1} - \xi_{4}) = \begin{pmatrix} 1\\0\\-1/2\\-\sqrt{3}/2\\-1/2\\\sqrt{3}/2 \end{pmatrix}, \qquad \nu_{2} = \sqrt{3/2}(\xi_{2} + \xi_{3}) = \begin{pmatrix} 0\\1\\\sqrt{3}/2\\-1/2\\-\sqrt{3}/2\\-1/2 \end{pmatrix}.$$



FIGURE 2. Different modes of molecule with  $D_3$  symmetry.

#### 2. 3-dimensional symmetries

Let G be a point group of symmetries for a molecule composed of n atoms. In general a group element from G acts on the vectors of local displacements of atoms as:

$$D(g)\begin{pmatrix} r_1\\r_2\\\vdots\\r_n \end{pmatrix} = \begin{pmatrix} R(\varphi)r_{\sigma(1)}\\R(\varphi)r_{\sigma(2)}\\\vdots\\R(\varphi)r_{\sigma(n)} \end{pmatrix}, \quad r_i = (x_i, y_i, z_i),$$

where  $R(\varphi)$  is a 3-dimensional rotation and  $\sigma$  is some permutation of the indices  $1, \ldots n$ . For the trace of D(g) to be non-zero the transformation g must leave invariant at least one atom. If  $n_q$ atoms are left invariant under a transformation g then

$$\chi(g) = \operatorname{Tr} D(g) = n_q(\pm 1 + 2\cos(\varphi)),$$

where plus and minus signs stand for rotations (det  $R(\varphi) = 1$ ) and improper rotations (det  $R(\varphi) =$ (-1), respectively. After we calculated all characters for group elements we can easily find the decomposition of D into irreducible representations.

Example 5.3. Tetrahedral symmetry group: 
$$\mathbf{T} = \{[e], [g], [g^{-1}], [\sigma]\}\$$
  
 $\chi([e]) = 4 \cdot 3(\varphi = 0), \chi([g]) = 0(\varphi = 2\pi/3), \chi([g^{-1}]) = 0(\varphi = -2\pi/3), \chi([\sigma]) = 0$   
 $D = 3F \oplus A_1 \oplus B_1 \oplus B_2 = \underbrace{2F}_{\substack{\text{rotations}\& \\ \text{translations}}} \oplus \underbrace{F \oplus A_1 \oplus B_1 \oplus B_2}_{\substack{\text{vibration modes}}}$ 

Among the set of modes obtained in this way there exist modes with zero frequencies. These modes correspond to rotations and translation of the whole molecule. In order to separate them from the rest of the spectrum we need to construct the corresponding vectors and subtract the respective irreducible representations. The translations in x, y, z directions are represented by the vectors:

(0)

$$v_{1} = \frac{1}{\sqrt{3n}} \begin{pmatrix} 1\\0\\0\\\vdots\\1\\0\\0 \end{pmatrix}, \quad v_{2} = \frac{1}{\sqrt{3n}} \begin{pmatrix} 0\\1\\0\\\vdots\\0\\1\\0 \end{pmatrix}, \quad v_{3} = \frac{1}{\sqrt{3n}} \begin{pmatrix} 0\\0\\1\\\vdots\\0\\1\\0 \end{pmatrix}.$$

The subspace  $V_{tr}$  spanned by these vectors remains invariant under any group transformation D(g). We thus have a representation  $D_{tr}$  of G (which enters into D) acting on  $V_{tr}$  with the corresponding character:

$$\chi_{tr}(g) = \sum_{i=1,2,3} (v_i, D(g)v_i) = \operatorname{Tr} R(\varphi) = \pm 1 + 2\cos(\varphi).$$

A similar reasoning gives for the rotation part  $D_{rot}$ :

$$\chi_{rot}(g) = 1 \pm 2\cos(\varphi),$$

with plus in case of proper rotations and minus in case of improper rotations. To subtract  $D_{tr}$  and  $D_{rot}$  from D we just need to use the "reduced" characters:

$$\chi(g) - \chi_{rot}(g) - \chi_{rot}(g) = \begin{cases} (n_g - 2)(1 + 2\cos(\varphi)) & \text{rotation}, \\ n_g(-1 + 2\cos(\varphi)) & \text{improper rotation} \end{cases}$$

instead of  $\chi(g)$ . In the case of the group T this leads to subtraction of two F representation from D.

#### LECTURE 6

### **Applications II. Quantum Mechanics**

#### 1. Spectral decomposition

First point of view: If G is a symmetry group of the Hamiltonian H, then:

$$HD(g) = D(g)H, \qquad g \in G$$

where D(g) acts on the Hilbert space V of the system. Since we can split V and respectively D(g) into irreducible representations:

$$V = \bigoplus_{k} V^{(k)}, \qquad D(g) = \bigoplus_{k} D^{(k)}(g), \qquad D(g)V^{(k)} \subseteq V^{(k)}$$

it follows immediately (by the second Schure's lemma) that

$$H = \bigoplus_{k} H^{(k)}, \qquad HV^{(k)} \subseteq V^{(k)},$$

where  $H^{(k)} = P_k H, V^{(k)} = P_k V$  and

(1.1) 
$$P_{k} = \frac{m_{k}}{|G|} \sum_{g \in G} D(g) \chi^{(k)}(g)$$

is the projection operator on the k-th sector of the system. Accordingly, the **spectrum** of H can be split into subspectra with degeneracies given by dimensions  $m_k$  of the irreducible representations of G.

**Example** 6.1. Reflectional symmetry  $G = \{e, \sigma\}$ : There are two irreducible representations of G. Correspondingly:

$$v = V^{(1)} \cup V^{(2)}, \text{ where}$$
 Even:  $V^{(1)} = \{\phi | \phi(x) = \phi(-x)\}, \qquad \text{Odd: } V^{(2)} = \{\phi | \phi(x) = -\phi(-x)\}.$ 

Second point of view: We consider the eigenstates of the Hamiltonian H corresponding to the same energy level:

$$H\varphi_n^{(i)} = E_n \varphi_n^{(i)}, \qquad i = 1, \dots m.$$

Generically the situation where m > 1 arises only if H has some symmetry G. In such a case the set of eigenfunctions  $\varphi_n^{(i)}$  form a linear space  $V^{(n)}$  of m-dimensional representation of the group G:

$$\sum_{i=1}^{m} D_{ji}(g)\varphi_n^{(i)}(x) = \varphi_n^{(j)}(g \cdot x) \in V^{(n)}.$$

Furthermore the representation D must be in general irreducible. If D(g) would be reducible, a generic small perturbation would break  $V^{(n)}$  into invariant (under action of D(g)) subspaces, thereby lifting (at least partially) degeneracy of  $E_n$ . **Summary:** If G is a symmetry group of the system its energy spectrum can be split into sectors in accordance to the irreducible representations  $D^{(\alpha)}$  of G:

$$\{E_n\} = \bigcup_{\alpha} \{E_n^{(\alpha)}\}.$$

• Each sector has degeneracy equal to the dimension of the representation  $m_{\alpha}$ .

Additional information for one particle Hamiltonian systems (no statistics):

- The density of states is proportional to the dimension of representation  $m_{\alpha}$  i.e., for a system with high symmetry singlets appear rearer then dublets etc., see 4.
- Spectra of different sectors are generally uncorrelated. Spectral statistics within sectors might depend on the type of representation (complex, real, pseudo-real), see 5.

**Example** 6.2.  $D_3$  versus  $C_3$ : Both systems posses doublets and singlets with degenerate levels consti-



FIGURE 1. Tables of characters for  $C_3$  and  $D_3$ .

tuting 2/3 of all levels. However, the spectral statistics of doublets are different: GUE in the first case and GOE in the second case. This is because  $C_3$  has two conjugate complex representations, while all representations of  $D_3$  are real.<sup>1</sup>

#### 2. Perturbation theory

Let  $H' = H + \lambda H_1$ , where H has a symmetry G while  $H_1$  has a lower symmetry  $G_1$ . A natural question: how the degeneracies in the spectrum of H are affected, when  $G_1 \subset G$ ? Let  $E_n$  be an m-degenerate eigenvalue of H corresponding to an m-dimensional irreducible representation D of G. Restricted to  $G_1$ , D provides in general reducible representation of  $G_0$ , which can be decomposed into irreducible ones:

$$D = \bigoplus_{k=1}^{l} D^{(k)}, \qquad \sum_{k=1}^{l} \dim(D^{(k)}) = m.$$

 $<sup>^{1}</sup>$ 1) This is true if the classical dynamics of the system are chaotic. 2) GUE, GOE means spectral statistics of Gaussian unitary and orthogonal ensembles, respectively. This terminology comes from random matrix theory.
#### 3. SELECTION RULES

This decomposition corresponds to splitting  $E_n$  into l different levels  $E_n^{(k)}$ ,  $k = 1, \ldots l$  with the degeneracies given by dim $(D^{(k)})$ .

Т	[e]	4[g]	4[g-1]	<b>3</b> [σ]		=
$A_1$	1	1	1	1	•{≡ // -	_
$A_2$	1	ε	ε <sup>2</sup>	1		
$\bar{A}_2$	1	ε <sup>2</sup>	ε	1		
F	3	0	0	-1		

FIGURE 2. Splitting of an energy level in two-particle system.

**Example** 6.3. Two interacting particles: Consider first two non-interacting particles subject to a potential with the T symmetry:

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + W(x_1) + W(x_2).$$

The total symmetry group of the system is  $G = T \times T$ . Assuming now that there is a weak interaction between the particles we have

$$H' = H + \lambda w(x_1 - x_2)$$

and the reduced symmetry of the system is  $G_0 = T$ . We need to calculate how the irreducible representations of G given by  $D^{(i)}(g) \times D^{(j)}(g)$  are split into irreducible representations of  $G_0$ . By the group orthogonality theorem we have:

$$r_k = \frac{1}{|T|} \sum_{g \in T} \chi^{(i)}(g) \chi^{(j)}(g) \bar{\chi}^{(k)}(g).$$

For i = j = F (representation of the dimension 3) we get  $r_k = 1$  for all  $k \neq F$  and  $r_F = 2$ , i.e.,

$$F \times F = A^{(1)} \oplus A^{(2)} \oplus \overline{A}^{(2)} \oplus 2F.$$

The corresponding splittings are shown in the figure (2).

#### 3. Selection rules

Consider a particle which is in an eigenstate

$$H_0\phi_n = E_n\phi_n,$$

of a Hamiltonian  $H_0$  whose symmetry is given by a point group G. If a weak external timedependent potential  $\lambda \hat{f}_i \cos(\omega t)$  is added to  $H_0$ , the particle might undergo transition from the state  $\phi_n$  to another eigenstate  $\phi_m$  of  $H_0$ . The corresponding transitional rate is then proportional to the matrix elements:

$$P_{n,m} \sim |\langle \phi_n | \hat{f}_i | \phi_m \rangle|^2.$$

What are the condition under which  $P_{n,m} \neq 0$ ? In other words which transitions are possible?

Let  $\hat{f}_i$  be a tensorial quantity (scalar, vector etc.) which transforms according to a certain representation of G:

$$\hat{f}_i = \sum_j D_{ij}^{(f)} \hat{f}_j.$$

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If  $\alpha, \beta$  are irreducible representations corresponding to  $\phi_n$  and  $\phi_m$  then the whole combination  $\langle \phi_n | \hat{f}_i | \phi_m \rangle$  transforms in accordance with the representation:

$$D = \bar{D}^{(\alpha)} \times D^{(f)} \times D^{(\beta)}.$$

LEMMA 3.1. The average

(3.1) 
$$O_{\mathbf{s}} = \langle \phi_n | \hat{f}_i | \phi_m \rangle = \int dx \phi_n^*(x) \hat{f}_i \phi_m(x), \qquad \mathbf{s} = (n, i, m)$$

is zero if D does not contain trivial representation.

*Proof:* Since  $O_{\mathbf{s}}$  is invariant under any group transformation, we have

$$O_{\mathbf{s}} = \frac{1}{|G|} \left( \sum_{g \in G} D_{\mathbf{s}\mathbf{s}'}(g) \right) O_{\mathbf{s}'}, \quad O_{\mathbf{s}} = \langle \phi_n | \hat{f}_i | \phi_m \rangle, \ O_{\mathbf{s}'} = \langle \phi_{n'} | \hat{f}_{i'} | \phi_{m'} \rangle,$$

where

$$D_{\mathbf{ss}'}(g) = \bar{D}_{n,n'}^{(\alpha)}(g) D_{i,i'}^{(f)}(g) D_{m,m'}^{(\beta)}(g), \quad \mathbf{s} = (n, i, m), \mathbf{s}' = (n', i', m').$$

By the group orthogonality theorem the above sum is zero if D contains no trivial representation.<sup>2</sup>

Example 6.4. Scalar time-dependent potential: If  $\hat{f}$  is scalar e.g.,  $\hat{f} \sim w(|r|)$  then  $P_{n,m} \neq 0$  only if  $\alpha = \beta$ .

**Example** 6.5. Vector time-dependent potential: Let  $\hat{f}$  be a vector e.g.,  $\hat{f}_i \sim \hat{x}, \hat{p}_x$ , and  $G = \mathbf{T}$ . In this case  $D^{(f)} = F$  is the three-dimensional representation. Finding all possible transition reduces to the problem of finding the decomposition of the product representation  $F \times D^{(\beta)}$  into irreducible ones. We have:

 $F \times A^{(1)} = F \times A^{(2)} = F \times \bar{A}^{(2)} = F, \qquad F \times F = A^{(1)} \oplus A^{(2)} \oplus \bar{A}^{(2)} \oplus 2F.$ 

Which means that the following transitions are possible:

$$A^{(1)}, A^{(2)}, \overline{A}^{(2)}, F \leftrightarrow F.$$

# 4. Appendix A: Density of states or why singlets are rare in the energy spectrum of systems with high symmetry

Consider spectrum of a particle confined by a bounded potential V(x) in an arbitrary dimension. If V(x) has a non-abelian symmetry then at least some eigenenergies  $E_n$  of the Hamiltonian  $H = \frac{p^2}{2m} + V(x)$  have degeneracies. How often will these degeneracies occur in the energy spectrum when  $n \to \infty$ ?

Let us look at the density of eigenvalues within each sector separately:

(4.1) 
$$\rho_{\alpha}(E) = \sum_{n=1}^{\infty} \delta(E - E_n^{(\alpha)}) = \frac{1}{\pi} \lim_{\epsilon \to 0} \operatorname{ImTr}\left(\frac{P_{\alpha}}{H - E + i\epsilon}\right)$$

where  $P_{\alpha}$  is projection (1.1) on the  $\alpha$  sector of the spectrum. We can right down this trace explicitly in the coordinate representation as the sum over different group elements:

(4.2) 
$$\rho_{\alpha}(E) = \frac{m_{\alpha}}{\pi |G|} \lim_{\epsilon \to 0} \operatorname{Im} \sum_{g \in G} \int dx \left\langle x \left| \frac{1}{H - E + i\epsilon} \right| g \cdot x \right\rangle$$

The leading order contribution (in E) to this integral arrives from x satisfying  $g \cdot x \approx x$ . This implies that only the term g = e might be left out of the sum. As a result we obtain:

$$\rho_{\alpha}(E) = \frac{m_{\alpha}}{|G|}\rho(E)(1+o(E^0)),$$

<sup>&</sup>lt;sup>2</sup> For more examples see Landau & Lifshitz [1].

## REFERENCES

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where  $\rho(E)$  is the total density of the eigenenergies.

## 5. Appendix B: Spectral statistics or why compex representation matter

[to be added]

#### References

 L. Landau and E. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon Press, Oxford, 1959).

#### LECTURE 7

# **Applications III. Energy Band Structure**

#### 1. Lattice symmetries

1.1. Bravais lattice symmetries. Before considering the group of Crystal symmetries one should first to define possible symmetry group G for "empty lattices"  $\mathcal{L}$ . The group G has as a (normal abelian) subgroup the discrete group of translational symmetries:

$$t_{\mathbf{a}} \cdot x = x + \mathbf{a}, \qquad \mathbf{a} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3, \quad n_i \in \mathbb{Z}.$$

Together with a point group  $G_0$  they form a group of symmetries of the corresponding **Bravais** lattice  $\mathcal{L}$ .

The fact that lattice must remain invariant under the action of both  $G_0$  and  $\{t_a\}$  imposes strong restriction on the possible form of  $G_0$ . Recall that an arbitrary element  $R \in G_0$  in (an appropriate) orthonormal basis takes the form:

(1.1) 
$$R = \begin{pmatrix} \cos\varphi & \sin\varphi & 0\\ -\sin\varphi & \cos\varphi & 0\\ 0 & 0 & \pm 1 \end{pmatrix}.$$

On the other hand this element  $URU^{-1}$  written in the basis  $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$  must contain only integer entries (since it transforms vectors of integers to vectors of integers). From this follows that:

$$\operatorname{Tr} R = 2\cos\varphi \pm 1 \in \mathbb{Z}, \qquad \Longrightarrow \varphi = \pi, \frac{\pi}{2}, \frac{\pi}{3}, \frac{2\pi}{3}.$$

In 3 dimensions this leaves only 7 possibilities for the point group  $G_0$  (see the pictures in Landau & Lifshitz [1]):<sup>1</sup>

$$S_2, C_{2h}, D_{2h}, D_{4h}, D_{3d}, D_{6h}, O_h$$

**1.2.** Space group. Since atoms fill cells of Bravais lattice, the rotational part of the crystal symmetry, might be less than the symmetry of empty lattice (due to the presence of an "internal" structure). Most general element of crystal symmetry group  $\tilde{G}$  has the form:

$$\tilde{g} = t_{\alpha} R,$$

where  $t_{\alpha}$  is translation by a vector  $\alpha$  (which is not necessarily from Bravais lattice). It is easy to show (see e.g., Petrashen' & Trifonov [2]) that rotational part R must form a subgroup  $\tilde{G}_0$ of  $G_0$ . To each of 32 such subgroups, there exists corresponding **class of crystals**. In addition elements of each class can be distinguished by translational part of the group. In total there exist 230 different space groups  $\tilde{G}$ .<sup>2</sup>

<sup>&</sup>lt;sup>1</sup> Since  $-\mathbf{a} \in \mathcal{L}$  whenever  $\mathbf{a} \in \mathcal{L}$ , inversion always belongs to  $G_0$ .

<sup>&</sup>lt;sup>2</sup> For further detail see Landau & Lifshitz [1]

#### 2. Band structure

Assume that we have a potential W(x) having a space group symmetry G of a crystal. Our goal is to construct irreducible representations of G and thus classify the spectrum of a particle moving in such a potential. We first have to start with translational symmetry subgroup.

**2.1. Translational symmetry.**  $t_{\mathbf{a}}W(x) = W(x + \mathbf{a}) = W(x)$ . Since  $T = \{t_{\mathbf{a}}\}$  is an abelian group all its irreducible representations  $\alpha$  are one dimensional:

$$t_{\mathbf{a}}\phi(x) = e^{i\alpha(\mathbf{a})}\phi(x).$$

By  $t_{\mathbf{a}_1+\mathbf{a}_2}\phi(x) = t_{\mathbf{a}_1}t_{\mathbf{a}_2}\phi(x) = e^{i(\alpha(\mathbf{a}_1)+\alpha(\mathbf{a}_2))}\phi(x)$  we also have

$$\alpha(\mathbf{a}_1) + \alpha(\mathbf{a}_2) = \alpha(\mathbf{a}_1 + \mathbf{a}_2), \quad \Longrightarrow \alpha(\mathbf{a}) = (\mathbf{k}, \mathbf{a}),$$

where **k** is a vector. We will denote by  $V^{(\mathbf{k})}$  the linear space of vectors with the fixed quasimomentum **k**, i.e.,  $V^{(\mathbf{k})} = \{\phi | t_{\mathbf{a}}\phi(x) = e^{i(\mathbf{k},\mathbf{a})}\phi(x)\}.$ 

Let  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  be defined by

$$(\mathbf{a}_i, \mathbf{b}_j) = 2\pi\delta_{ij}, \qquad i, j = 1, 2, 3$$

The  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  triplet form reciprocal lattice

$$\bar{\mathcal{L}} = \{ p_1 \mathbf{b}_1 + p_2 \mathbf{b}_2 + p_3 \mathbf{b}_3, \qquad p_i \in \mathbb{Z} \}.$$

One can show that point symmetries of  $\overline{\mathcal{L}}$  are given by the point symmetry group of  $\mathcal{L}$ . Indeed if R is a point symmetry of  $\mathcal{L}$  and  $b \in \overline{\mathcal{L}}$  then  $(Ra, b) = 2\pi n'$ , or equivalently  $(a, R^{-1}b) = 2\pi n$ . From this follows that  $R^{-1}b$  belongs to  $\overline{\mathcal{L}}$  as well.

Two vectors  $\mathbf{k}$ ,  $\mathbf{k}'$  are equivalent (give the same representation) iff  $\mathbf{k} - \mathbf{k}' \in \mathcal{L}$ . We can define then the fundamental domain which contains only non-equivalent vectors  $\mathbf{k}$ . This is so-called **Brillouin zone**. Since W(x) is invariant under translation symmetry of  $\mathcal{L}$  we can decompose the Hilbert space and the Hamiltonian accordingly:

(2.1) 
$$V = \bigoplus_{\mathbf{k}} V^{(\mathbf{k})}, \qquad H = \bigoplus_{\mathbf{k}} H^{(\mathbf{k})},$$

where  $\mathbf{k}$  runs over the Brillouin zone.

**2.2. Point group symmetry.** In general, in addition to translational symmetries the potential W(x) also obeys point group symmetries which will be denoted by  $R \in G_0$ . Consider how these symmetries act on the functions from the space  $V^{(\mathbf{k})}$ : Since  $t_{\mathbf{a}}R = Rt_{R^{-1}\mathbf{a}}$  we get:

(2.2) 
$$t_{\mathbf{a}}(R\varphi_{\mathbf{k}}) = e^{i(R\mathbf{k},\mathbf{a})}(R\varphi_{\mathbf{k}}) \implies R\varphi_{\mathbf{k}} \in V^{(R\mathbf{k})}$$

By applying all possible elements of  $R \in G_0$  we obtain star of k:

$$[\mathbf{k}] = \{\mathbf{k}_1 = \mathbf{k}, \mathbf{k}_2, \dots \mathbf{k}_l\}.$$

For each vector  $\mathbf{k}$  one also defines the stabilizer  $G_{\mathbf{k}}$ . This is the subgroup of  $G_0$  which leaves vector  $\mathbf{k}$  invariant:

$$G_{\mathbf{k}}\mathbf{k} = \mathbf{k}, \qquad |G_{\mathbf{k}}|l = |G_0|.$$

Any irreducible representation of G leaves the subspace  $\bigcup_{i=1}^{l} V^{(\mathbf{k}_i)}$  invariant.

#### 2. BAND STRUCTURE

For a typical value of **k** taken from the Brillouin zone, the group  $G_{\mathbf{k}}$  is trivial, i.e., consists only of the unity element. In this case if  $\varphi_{\mathbf{k}} \in V^{(\mathbf{k})}$  is an eigenvector of the Hamiltonian:

(2.3) 
$$H\varphi_{\mathbf{k}} = E(\mathbf{k})\varphi_{\mathbf{k}}$$

then  $R\varphi_{\mathbf{k}} = \varphi_{R\mathbf{k}}, R \in G_0$  are also eigenvectors with the same eigenvalue. Therefore all vectors from the star have the same eigenvalues:

$$E(\mathbf{k}_1) = E(\mathbf{k}_2) = \dots = E(\mathbf{k}_l), \qquad l = |G_0|.$$

However, for some values of the quasi-momenta  $\mathbf{k}$  the group  $G_{\mathbf{k}}$  might be non-trivial. In such a case the number of elements in the star  $l < |G_0|$ . This reduced symmetry of  $E(\mathbf{k})$  is "compensated" by the degeneracies between different bands. Indeed for any  $\sigma \in G_{\mathbf{k}}$  applied to an eigenvector  $\varphi_{\mathbf{k}}$  the vector  $\sigma \varphi_{\mathbf{k}}$  is also eigenvector of H. Since

$$\sigma\varphi_{\mathbf{k}} \in V^{(\mathbf{k})},$$

it must belong to a different band. The vectors  $\sigma \varphi_{\mathbf{k}}, \sigma \in G_{\mathbf{k}}$  therefore form a basis of irreducible representation. The number of sticking bands is therefore determined by the dimension of the irreducible representation of  $G_{\mathbf{k}}$ , see figure 1.

2.2.1. Note. Another way of thinking: First, consider only translational symmetry. This leads to the decomposition (2.1). Now if  $\sigma \in G_0$  is an element of crystal symmetry, we have

(a) 
$$[H^{(\mathbf{k})}, \sigma] = 0$$
, if  $\sigma \in G_{\mathbf{k}}$ , (b)  $H^{(\mathbf{k})}\sigma = \sigma H^{(\sigma\mathbf{k})}$  if  $\sigma \notin G_{\mathbf{k}}$ .

Therefore by (a),  $G_{\mathbf{k}}$  is a symmetry of  $H^{(\mathbf{k})}$  and the degeneracies of the energy levels in  $H^{(\mathbf{k})}$  (the number of sticking bands) are determined by the dimensions of irreducible representations of  $G_{\mathbf{k}}$ . From (b) it follows that  $E(\mathbf{k}) = E(\sigma \mathbf{k})$ .



FIGURE 1. Schematic plot of band structure. At  $\mathbf{k}_1$ ,  $\mathbf{k}_2$  the group  $G_{\mathbf{k}=\mathbf{k}_{1,2}}$  is trivial. At the point  $\mathbf{k}_0$ ,  $G_{\mathbf{k}=\mathbf{k}_0}$  has a 2-dimensional irreducible representation.

**Example** 7.1. **1-dim. potential:** *Consider 1-dim. potential which is symmetric under translations and reflection:* 

$$H = -\frac{\hbar^2}{2}\partial_x^2 + W(x), \qquad W(x+\mathbf{a}) = W(x), \quad W(x) = W(-x).$$

The Hilbert space can be decomposed in accordance with particle quasi-momenta:

$$\varphi^{(k)} = \{\varphi_k(x) = e^{ikx}\phi(x), \phi(x+a) = \phi(x)\}.$$

We look for eigenvalues of H with a fixed quasi-momentum k:

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$$H\varphi_k = E(k)H\varphi_k$$

After substituting function  $\varphi_k(x) = e^{ikx}\phi(x)$  we get an equivalent equation:

$$H^{(k)}\phi = E(k)\phi, \qquad H^{(k)} = -\frac{\hbar^2}{2}(\partial_x + ik)^2 + W(x).$$

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The Hamiltonian  $H^{(k)}$  is symmetric under the group  $G_k = \{e, \sigma\}$  for  $k = 0, \pi/a$ . Since the group is abelian, there are no sticking of the energy bands at these points. For other values of k, we get  $\sigma$ 

$$\sigma H^{(k)}\sigma = H^{(-k)} \implies E(k) = E(\sigma k) = E(-k).$$



#### 3. Band structure of graphene

FIGURE 2. Graphene lattice (left) and its band structure (right).

The lattice of graphene has hexagonal symmetry  $C_{6v}$ , see figure 2. Its band structure can be easily understood using tight binding model. The corresponding Hamiltonian is:

$$H = t \sum_{m,n} |m_A, n_A\rangle \left( \langle n_B, m_B | + \langle n_B, m_B - 1 | + \langle n_B - 1, m_B - 1 | \right) + C.C,$$

where  $(m_A, n_A)$ ,  $(m_B, n_B)$  are the (m, n)-site of the A and B lattice respectively. To find an eigenvalues we use a general procedure and look for eigenfunctions with a given momentum k:

$$\psi_{\mathbf{k}} = \sum_{m,n} a_{m,n} |m_A, n_A\rangle + b_{m,n} |m_B, n_B\rangle,$$

where

$$a_{m,n} = a_{m+p,n+l}e^{-i(\mathbf{k},p\mathbf{a}+l\mathbf{b})}, \quad b_{m,n} = b_{m+p,n+l}e^{-i(\mathbf{k},p\mathbf{a}+l\mathbf{b})}$$

with **k** being from the first Brillouin zone (see figure 3). Substituting it with  $a_{0,0} = A$ ,  $b_{0,0} = B$ into  $H\psi_{\mathbf{k}} = E(\mathbf{k})\psi_{\mathbf{k}}$  gives the following matrix equation for the energy band:

(3.1) 
$$\begin{pmatrix} 0 & th^*(\mathbf{k}) \\ th(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = E(\mathbf{k}) \begin{pmatrix} A \\ B \end{pmatrix}, \qquad h(\mathbf{k}) = 1 + e^{i(\mathbf{k},\mathbf{a})} + e^{i(\mathbf{k},\mathbf{a}+\mathbf{b})}.$$

Its solution is then

$$E(\mathbf{k}) = \pm |h(\mathbf{k})|, \qquad \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \pm \sqrt{h(\mathbf{k})} \\ \sqrt{h^*(\mathbf{k})} \end{pmatrix}.$$

The critical points where two bands approach each other are defined by the condition:

$$h(\mathbf{k}) = 0 \implies (\mathbf{k}, \mathbf{a}) = (\mathbf{k}, \mathbf{b}) = \pm 2\pi/3.$$

This gives two triplets of solutions denoted by the red and the blue points in figure 3. Note that the points of the same color represent the same quasi-momenta  $\mathbf{k}_1, \mathbf{k}_2$  (and therefore equivalent) as they differ only by a vector from reciprocal lattice. The corresponding band structure is shown in figure 2.

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FIGURE 3. Reciprocal lattice of graphene.

From the group theory prospective the above band structure can be understood as follows. For a generic quasi-momentum  $\mathbf{k}$  the stabilizer  $G_{\mathbf{k}}$  is trivial and we have 12 fold symmetry  $C_{6v}$  of the band energy  $E(\mathbf{k})$ . Here eigenstates with the same energy correspond to different elements of the star  $[\mathbf{k}]$ . For two special points  $\mathbf{k}_1$ ,  $\mathbf{k}_2$  the stabilizers  $G_{\mathbf{k}_1}$ ,  $G_{\mathbf{k}_2}$  are isomorphic to  $C_{3v}$ . Since  $C_{3v}$  allows two-dimensional irreducible representations, two different bands merge at these points.

#### References

- L. Landau and E. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon Press, Oxford, 1959).
- [2] M. I. Petrashen and E. D. Trifonov, *Applications of group theory in quantum mechanics* (Dover, New York, 2009).

Part 2

Continuous groups

#### LECTURE 8

# Lie groups & Lie algebras

#### 1. Basic definitions and properties

1. So far we have considered discrete symmetry groups with at most countable number of elements. In physics one often encounters systems where the symmetries are continuous, i.e.,  $g(x) \in G$  where elements can be parametrized by  $x \in \mathbb{R}^n$ . (Without loss of generality we can assume that g(0) = e.) In these cases G is n-dimensional manifold with an additional connection between elements provided by the group multiplication:

$$g(x_1)g(x_2) = g(x_3), \qquad \Longrightarrow \qquad x_3 = \phi(x_1, x_2).$$

Whenever  $\phi$  is differentiable, such groups are called **Lie Groups**.

**2.** For a given Lie group G we consider its local structure around the unit element e, i.e., elements of the tangent space TG at x = 0:

$$L_{\gamma} = \partial_t g(\gamma(t))|_{t=0},$$

where  $\gamma(t)$  is a differentiable path in the parameter space  $\mathbb{R}^n$  such that  $\gamma(0) = 0$ . By the definition the derivatives along *n* different directions form n-dimensional linear space  $\mathbf{g}$ , i.e., any element  $L \in TG$  can be represented as

$$L = \sum_{i} a_i L_i, \qquad L_i = \partial_i g(x)|_{x=0}, \quad i = 1, \dots n.$$

**3.** In an opposite direction, with each element L of g we can associate a family of elements from G:

$$\exp_t: L \to \exp(tL) = \sum_{k=0}^{\infty} \frac{t^k}{k!} L^k$$

(here we assume that G can be represented as a linear group, so  $L^k$  is defined.) To show that  $\exp(tL)$  is in G note that for large k we have approximation:

$$\exp(tL_{\gamma}/k + O(1/k^2)) = g_{\gamma}(t/k),$$

where  $g_{\gamma}(t/k)$  is a group element along the curve  $\gamma(t)$ . Taking now k-th power of both sides and sending k to infinity leads to:

$$\exp(tL_{\gamma}) = \lim_{k \to \infty} \left(g_{\gamma}(t/k)\right)^k \in G.$$

4. We can show now that g is in fact Lie algebra. For this it is sufficient to demonstrate that g is closed under the commutation operation.

THEOREM 1.1. If  $L_1, L_2 \in g$  then  $[L_1, L_2] \in g$  as well.

*Proof:* Consider element  $\exp(L_1t_1)\exp(L_2t_2)\exp(-L_1t_1)$ . By the differentiation over  $t_2$  we obtain that

 $\exp(L_1t_1)L_2\exp(-L_1t_1)\in \mathsf{g}$  for any  $t_1$ . We then differentiate over  $t_1$  and get  $[L_1,L_2]\in \mathsf{g}$  at  $t_1=0$ .

Since the commutation relation automatically satisfies the Jacobi identity,

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0,$$

g is Lie algebra. The coefficients  $C^{k}_{ij}$  in

$$[L_i, L_j] = C^k{}_{ij}L_k,$$

called **structural constants**, define the Lie algebra. The Lie algebra  $g_0$  generated by a subgroup  $G_0 \subset G$  is obviously subalgebra of g. If  $\dim(G_0) = \dim(G)$  then  $g_0 = g$ .

#### 5. Examples:

a) 
$$G = SO(n), OO^T = 1$$
. Representing  $O = \exp(tL) \Longrightarrow$   
 $\operatorname{so}(n) = \{L \in GL(n, \mathbb{R}) | L^T = -L\},$   
basis:  $L^{(km)}{}_{ij} = \delta_{ik}\delta_{jm} - \delta_{im}\delta_{jk}, \qquad \dim(\operatorname{so}(n)) = \frac{n(n-1)}{2}.$ 

b) 
$$G = SU(n), UU^* = 1, \det(U) = 1$$
. Representing  $U = \exp(tL) \Longrightarrow$   
 $su(n) = \{L = A + iB \in SL(n, \mathbb{C}) | A^T = -A, B^T = B, \operatorname{Tr}(B) = 0\},$   
 $\dim(su(n)) = \frac{n(n-1)}{2} + \frac{n(n+1)}{2} - 1 = n^2 - 1.$ 

6. Note that so(3) = su(2) = o(3), but  $SO(3) \not\cong SU(2) \not\cong O(3)$ . To what extent Lie algebra determines Lie group? It turns out that the local structure of the group around g(0) = e defines to a certain extent (only) its global structure.

Let G be a Lie group then define its maximal connected component  $G_0 \subset G$  which includes e. One can show (using local isomorphism between  $\exp(tL)$  and G) that  $G_0$  is subgroup of G with the same dimension. **Example:** G = O(n),  $G_0 = SO(n)$ . The elements  $g_0$  of the subgroup  $G_0$ can be represented as:

$$g_0 = \prod_i \exp(t_i L_i).$$

In other words, g completely determines connected component of G, but not the whole group if it is not simply connected like O(3). Note that SO(3), SU(2) are connected.

#### 2. Representations

Which results of the representation theory developed for finite groups can be exported to infinite groups? In order to use the machinery developed for finite groups we need to generalize the notion of invariance (group average):

$$\bar{f}(h) = \sum_{g \in G} f(gh) - \text{ is } h \text{ independent},$$

#### 2. REPRESENTATIONS

where  $\sum_{g \in G} \rightarrow \int d\mu(g)$  in the continues case. For this we need invariant measures:

$$\mu_r(gh) = d\mu_r(g), \qquad d\mu_l(hg) = d\mu_l(g),$$

which are called (left/right) Haar measures.

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**2.1. Haar measure.** This measure can be easily constructed if we know explicitly function  $\phi$ . Assuming  $d\mu_l(g) = p_l(x)dx^n$  we have:

$$x = 0 \rightarrow x_h = \phi(x_h, 0), \qquad \delta x \rightarrow \delta x' = \phi(x_h, \delta x),$$

where  $x_h$  is the coordinate of the element h. From this the condition of measure invariance is equivalent to:

$$p(0) \prod dx_i = p(x') \prod dx'_i = p(x_h) \det \left(\partial_{y_i} \phi_j(x_h, y)\right)|_{y=0} \prod dx_i.$$

Which implies:

$$p_l(x) = \det\left(\partial_{y_i}\phi_j(x,y)\right)|_{y=0}, \quad p_r(x) = \det\left(\partial_{y_i}\phi_j(y,x)\right)|_{y=0} \text{ (analog.)}$$

For compact groups two measures coincide and the total volume of the group is finite  $\int_G d\mu < \infty$ .<sup>1</sup>

Examples:

$$SO(2): \qquad g(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi\\ \sin\varphi & \cos\varphi \end{pmatrix}, \qquad d\mu = \frac{1}{2\pi}d\varphi.$$
$$SO(1,1): \qquad g(\varphi) = \begin{pmatrix} \cosh\varphi & \sinh\varphi\\ \sinh\varphi & \cosh\varphi \end{pmatrix}, \qquad d\mu = d\varphi, \quad \int_G d\mu = \infty$$

Equipped with an invariant measure one can prove for compact groups the same results as for finite groups:

- Every representation is equivalent to unitary
- Every irreducible representation  $\rho^{(i)}$  is finite dimensional
- Every representation is completely reducible:  $\rho = \oplus r_i \rho^{(i)}$
- Schur lemmas
- Orthogonality theorems:

$$\delta_{ij} = \int_G d\mu \bar{\chi}^{(j)}(g) \chi^{(i)}(g), \qquad r_i = \int_G d\mu \bar{\chi}(g) \chi^{(i)}(g),$$
$$P_i = \dim(\rho^{(i)}) \int_G d\mu \bar{\chi}^{(i)}(g) \rho(g).$$

**2.2. Representations of Lie algebras.** Every irreducible representation D of G induces an irreducible representation  $\rho$  of g by:

$$\rho(L_i) = \partial_t D(\exp(tL_i)|_{t=0}, \qquad [\rho(L_i), \rho(L_j)] = C^k{}_{ij}\rho(L_k).$$

Whether the converse is true: Can we lift each representation of Lie algebra to the representation of the corresponding Lie group? Yes, but only if the group is simply connected. Example: SO(3) and SU(2) have the same Lie algebra su(2). Each irreducible representation of su(2) provides an irreducible representation of SU(2), but not of SO(3) since it is not simply connected.

<sup>&</sup>lt;sup>1</sup> For linear groups (represented by matrices from GL(n)) compactness (probably) means that the group manifold is a bounded domain in  $\mathbb{R}^{n^2}$  (space of GL(n) elements).

#### LECTURE 9

# SU(2), SO(3) and their representations

#### 1. Connection between SU(2) and SO(3)

A rotation around z axis is given by the matrix:

(1.1) 
$$R_z(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0\\ \sin\varphi & \cos\varphi & 0\\ 0 & 0 & 1 \end{pmatrix} = \exp\left(\varphi \begin{pmatrix} 0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0 \end{pmatrix}\right).$$

In the same way an arbitrary rotation in  $\mathbb{R}^3$  can be represented by the matrix:

$$R_{\mathbf{n}}(\varphi) = \exp(-i\varphi(\mathbf{nL})), \qquad \mathbf{L} = (L_1, L_2, L_3)$$

where the normal vector **n** determines the plane and the direction of the rotation, and  $\varphi$  is the angle. Here  $L_1, L_2, L_3$  are generators of the rotation along x, y, z axes respectively:

(1.2) 
$$L_1 = i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad L_2 = i \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad L_3 = i \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

These matrices form Lie algebra with commutation relations:

$$[L_i, L_j] = i\varepsilon_{ijk}L_k.$$

To compare SO(3) with SU(2), note that an arbitrary element of SU(2) can be represented as

$$U = \exp(-iH), \qquad H = H^*, \quad \mathrm{Tr}H = 0.$$

Taking the basis of Pauli matrices an arbitrary matrix H can be represented as  $H = \alpha_i S_i$ :

$$S_1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_2 = \frac{1}{2} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad S_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Since the infinitesimal generators satisfy the same commutation relations

$$[S_i, S_j] = i\varepsilon_{ijk}S_k,$$

both groups have the same Lie algebra. On the other hand two Lie groups are not isomorphic. By  $\alpha_i = \varphi \mathbf{n}_i$  each element of SO(3) can be identified with an element of SU(2):

$$U_{\mathbf{n}}(\varphi) = \exp(-i\varphi(\mathbf{nS})), \qquad \mathbf{S} = (S_1, S_2, S_3)$$

This identification, however, is not one-to-one. Two matrices  $R_{\mathbf{n}}(\varphi)$ ,  $R_{-\mathbf{n}}(2\pi - \varphi)$  are equal and correspond to the same element of SO(3), while  $U_{\mathbf{n}}(\varphi) = -U_{-\mathbf{n}}(2\pi - \varphi)$ . One concludes from this that:

$$SO(3) \cong SU(2)/\mathbb{Z}_2,$$

where the normal subgroup  $\mathbb{Z}_2$  is formed by the matrices  $\pm I$ .



FIGURE 1. The groups SO(3) and SU(2) as manifolds. For SO(3) the diametrically opposite points on the surface are identical. Therefore the curve  $\gamma$  cannot be shrink to a point, i.e., the group is not simply connected. For SU(2) the whole surface of the ball represent one point -I, thus a curve  $\gamma$  can be continuously shrunk to a point.

#### **2.** Representations of SO(3) and SU(2)

To obtain representations of SO(3) and SU(2) it is useful to start from the representations of their Lie algebra su(2). To this end we first define raising and lowering operators  $L_{\pm} = L_1 \pm iL_2$  satisfying the following commutation relations:

$$[L_3, L_{\pm}] = \pm L_{\pm}, \qquad [L_+, L_-] = 2L_3$$

Note that if  $|v\rangle$  is an eigenvector of  $L_3$  with an eigenvalue  $\lambda$  then:

$$L_3|v\rangle = \lambda |v\rangle, \implies L_3 L_{\pm}|v\rangle = (\lambda \pm 1)L_{\pm}|v\rangle$$

and by induction  $L_{\pm}^{n}|v\rangle$  is an eigenvector of  $L_{3}$  with the eigenvalue  $\lambda \pm n$ . Since we are looking for finite representations, there exists an eigenvector  $|v_{0}\rangle$  (lowest weight) of  $L_{3}$ ,  $L_{3}|v_{0}\rangle = \lambda |v_{0}\rangle$  with the minimal value of  $\lambda$  such that:

$$L_{-}|v_{0}\rangle = 0, \qquad L_{+}^{n}|v_{0}\rangle = 0, \text{ and } L_{+}^{k}|v_{0}\rangle \neq 0, k \leq n.$$

From the following chain of equalities:

$$(2.1) \quad 0 = \langle v_0 | L_-^n L_+^n | v_0 \rangle = = -2 \langle v_0 | L_-^{n-1} L_3 L_+^{n-1} | v_0 \rangle + \langle v_0 | L_-^{n-1} L_+ L_- L_+^{n-1} | v_0 \rangle = \cdots = -2((\lambda + n - 1) + (\lambda + n - 2) + \cdots + \lambda) \langle v_0 | L_-^{n-1} L_+^{n-1} | v_0 \rangle$$

and  $\langle v_0 | L_{-}^{n-1} L_{+}^{n-1} | v_0 \rangle = || L_{+}^{n-1} | v_0 \rangle ||^2 \neq 0$  we conclude:

$$n\lambda + \frac{n(n-1)}{2} = 0 \implies -\lambda = \frac{n-1}{2}.$$

Because n is an integer all eigenvalues of  $L_3$  are either integer or half-integer numbers for a given irreducible representation, see fig. XXX. A **Casimir** of a Lie algebra is an operator from the enveloping algebra which commutes with all elements of the Lie algebra. For su(2) it is given by:

$$L^{2} = L_{1}^{2} + L_{2}^{2} + L_{3}^{2} = L_{3}^{2} + L_{3} + 2L_{+}L_{-}.$$

Its eigenvalues

$$L^2|v_0\rangle = l(l+1)|v_0\rangle, \qquad l = |\lambda|$$

label the irreducible representations.

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#### 3. APPLICATIONS

To obtain irreducible representations of SU(2) or SO(3) it remains to "exponentiate" irreducible representation of su(2). Note that half-integer representations of su(2) provide representations of SU(2) (simply connected group) but not of SO(3).

REMARK 2.1. In general each group G has a unique **universal cover** group  $\widetilde{G}$ . This is simply connected group such that  $G = \widetilde{G}/Z_k$ , where  $Z_k$  is a discrete group. Groups  $\widetilde{G}$  and G have the same Lie algebra  $\mathfrak{g}$ . Any irreducible representation of  $\mathfrak{g}$  can be lifted to a representation of  $\widetilde{G}$  and vice versa. However, a representation of  $\widetilde{G}$  is in general a multi-valued representation.  $\widetilde{G}$ . In our case SU(2) is the universal cover of  $SO(3) \cong SU(2)/Z_2$ . Another example: the universal cover of U(n) (which is not simply connected) is given by  $R \times SU(n)$  (which is simply connected), where Ris the additive group of real numbers.

Characters of group elements can be easily calculated using the fact that any rotation by an angle  $\varphi$  around an axis **n** can be represented as:

$$g_{\varphi} = RR_z(\varphi)R^{-1},$$

where R rotates **n** into z axis. Explicitly, for the representation l:

$$D^{(l)}(L_3) = \{-l, -l+1, \dots, 0, \dots, l-1, l\}$$

and the characters are given by

$$\chi^{(l)}(g_{\varphi}) = \operatorname{Tr} D^{(l)}(R_z(\varphi)) = \sum_{k=-l}^{l} e^{ik\varphi} = \frac{\sin(l+1/2)\varphi}{\sin(\varphi/2)}.$$

REMARK 2.2. 1) By the orthogonality theorem

$$\int_{SU(2)} \chi^{(l)}(g_{\varphi}) \, \chi^{(l')}(g_{\varphi}) d\mu_{\varphi} = \delta_{ll'}.$$

From this it is clear that  $\varphi$ -dependent part of measure must be  $d\mu_{\varphi} = \frac{1}{\pi} \sin^2(\varphi/2) d\varphi$ .<sup>1</sup>

2) Taking the limit  $\varphi \to 0$  in  $\chi^{(l)}(g_{\varphi})$  (i.e., taking the trace of the identity,  $d_l = \chi^{(l)}(e)$ ) we obtain  $\dim(D^{(l)}) = 2l + 1$ , as it should be.

#### 3. Applications

**3.1. Spectral degeneracies of rotation invariant systems,** SO(3) and O(3). In the coordinate representation the infinitesimal rotation acts on a quantum wavefunction (or any smooth function):

$$\psi(R_{\mathbf{n}}(\delta\varphi)x) \approx \psi(x) + i\delta\varphi(\mathbf{n}\hat{L})\psi(x),$$

where

$$\hat{L} = -ix \times \nabla,$$

is operator of angular momentum. The irreducible representations of SO(3) can be constructed by considering invariant subspaces of functions:

$$V = \oplus V^{(l)}, \qquad V^{(l)} = \{f(r)Y_l^{(m)}(\theta, \phi) | m = -l, \dots + l\},\$$

where spherical harmonics are simultaneous eigenfunctions of  $L^2, L_3$ ,

<sup>&</sup>lt;sup>1</sup>It is also clear that the "angular" part of the measure should be just  $d\Omega$ , where  $\Omega$  is the spherical measure for **n**.

$$\begin{split} \widehat{L}^2 Y_l^{(m)}(\theta,\phi) &= l(l+1) Y_l^{(m)}(\theta,\phi), \qquad \widehat{L}_z Y_l^{(m)}(\theta,\phi) = m Y_l^{(m)}(\theta,\phi), \\ Y_l^{(m)}(\theta,\phi) &= \frac{1}{\sqrt{2\pi}} e^{im\varphi} P_l^{(m)}(\cos\theta). \end{split}$$

If rotation invariant Hamiltonian posses in addition invariance under the inversion  $i: r \to -r$  (e.g., V(r) depends only on |r|), the full symmetry group of the quantum system becomes  $O(3) \cong SO(3) \times \{e, i\}$ . In this case the full set of the representations (l, w) can be labeled by angular momentum l and parity  $w = \pm 1$ . The representation (l, +1) correspond to D(i) = 1, i.e., symmetric functions  $\psi(x)$  under inversion  $\theta \to \pi - \theta, \phi \to \phi + \pi$ , while for the (l, -1), D(i) = -1 and the functions are antisymmetric. Note however that for the above coordinate representation, w is fixed by  $l, w = (-1)^l$ . For even (odd)  $l, Y_l^{(m)}(\pi - \theta, \phi + \pi) = \pm Y_l^{(m)}(\theta, \phi)$ .

**3.2.** Spectral degeneracies of hydrogen atom, SO(4). For the Coulomb potential  $-e^2/r$  the symmetry group is actually larger than SO(3). In addition to angular momentum there is another conserved quantity – Runge-Lenz vector:

$$M = \frac{1}{m}p \times L - e^2 \vec{r}/r.$$

After rescaling  $M' = M(-m/2H)^{1/2}$  the linear combinations  $J^{(1)} = (L+M')/2$ ,  $J^{(2)} = (L-M')/2$  satisfy the following commutation relation:

$$[J_i^{(1)}, J_j^{(1)}] = i\hbar\varepsilon_{ijk}J_k^{(1)}, \qquad [J_i^{(2)}, J_j^{(2)}] = i\hbar\varepsilon_{ijk}J_k^{(2)}, \qquad [J_i^{(1)}, J_j^{(2)}] = 0.$$

We conclude that the Lie algebra is  $\widehat{su}(2) \oplus \widehat{su}(2)$ , while the corresponding symmetry group is SO(4). The irreducible representations of SO(4) (which is double covered by  $SU(2) \otimes SU(2)$ ) are direct products of pairs of irreducible representations of SU(2):

$$D^{(l,k)} = D^{(l)} \otimes D^{(k)}, \quad \dim D^{(l,k)} = (2l+1)(2k+1).$$

Because of additional relationship:

$$(L \cdot M) = 0 \qquad \Longrightarrow \qquad \left(J^{(1)}\right)^2 = \left(J^{(2)}\right)^2$$

we have in fact l = k. This implies that the degeneracy of the *n*-th energy level  $E_n$  is  $n^2$ , n = 2l+1. Note that *l* runs over both integers and half-integers, since it labels representations of SU(2) rather then of SO(3).

**3.3.** Perturbation with discrete symmetry. Let  $H_0$  be rotational symmetric Hamiltonian. Consider its perturbation:

 $H = H_0 + \lambda W,$ 

where W has the symmetry of  $T \subset SO(3)$ . This situation arises e.g., in crystals. How the degeneracies of the energy levels are lifted? Take l = 2 representation of SO(3), which corresponds to 5-time degenerate energy level.  $D^{(2)}$  provides a reducible representation of T. We need to know ho it splits into irreducible representation of T. Recall that T has 12 elements corresponding to the rotations by the angle  $\varphi$ : 0 (1-time),  $\pi$  (3-times),  $2\pi/3$  (4-times),  $-2\pi/3$  (4-times). The corresponding characters are:

$$\chi^{(2)}(g_{\varphi}) = \{5, 1, -1, -1\}$$

which leads

$$D^{(2)} = \underbrace{\bar{A}_2 \oplus A_2}_{\text{c. cong.}} \oplus F \implies 5 \to \underbrace{1+1}_{\text{deg.}} +3.$$

where

#### 4. Spinors

Experiments show that for certain particles (e.g., electrons) application of magnetic field leads to the splitting of their energy levels into doublets. This suggests that internal angular momentum of these particles corresponds to half-integer representations of su(2). Correspondingly their states are transformed under the rotation at angle  $\varphi$  around **n** axis as

$$\sum_{j=1,2} U_{\mathbf{n}}(\varphi)_{ij} \chi_j = \chi_i.$$

The two component quantities  $\chi = (\chi_1, \chi_2)$ , which are transformed in this way are called **spinors**. Strictly speaking spinors do not provide representation for SO(3) since after rotation by  $2\pi$ ,  $\chi \rightarrow -\chi$ . This is however not a problem since the physical quantities  $\langle \chi | O | \chi' \rangle$  are, in fact, invariant.

Wavefunctions  $\Psi(x_1, \ldots x_n)$  of many-particle systems are spinors of rang n, i.e., they are transformed as products:

$$\chi_{i_1}^{(1)} \dots \chi_{i_n}^{(n)} \to U_{\mathbf{n}}(\varphi)_{i_1, j_1} \dots U_{\mathbf{n}}(\varphi)_{i_1, j_1} \chi_{i_1}^{(1)} \dots \chi_{i_n}^{(n)}.$$

In the same way as with vectors/tensors we can introduce tensor algebra for spinors. The conjugate spinors are transformed by the adjoints of  $U_{\mathbf{n}}(\varphi)$ . Because

$$U_{\mathbf{n}}(\varphi)\Sigma = \Sigma U_{\mathbf{n}}^{\dagger}(\varphi) \qquad \Sigma = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

we can use matrix  $\Sigma$  to rise indexes of the spinors. Namely, the transformation of the spinor:

$$\begin{pmatrix} \chi^1 \\ \chi^2 \end{pmatrix} := \Sigma \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} = \begin{pmatrix} \chi_2 \\ -\chi_1 \end{pmatrix}$$

is carried out by the adjoint of  $U_{\mathbf{n}}(\varphi)$ .

4.1. Time reversal invariance and Kramers degeneracies. For systems without spin the time reversal operation T is given in the coordinate basis by the complex conjugation K:

$$K\psi(x) = \psi^*(x).$$

This is easy to see, since  $\psi^*(x,t)$  satisfies the time dependent Schroedinger equation with  $t \to -t$ . For spinors, however this definition should be modified. The operator T is here a two-dimensional matrix satisfying:

$$T\hat{p}T^* = -\hat{p}, \qquad T\hat{x}T^* = \hat{x} \implies T\mathbf{S}T^* = -\mathbf{S},$$

From this follows that the time reversal operator is given by:

$$T\begin{pmatrix}\chi_1(x)\\\chi_2(x)\end{pmatrix} = i\begin{pmatrix}\chi_2^*(x)\\-\chi_1^*(x)\end{pmatrix}, \qquad T = i\Sigma K.$$

Important:

1) T is an **anti-unitary** operator, i.e.,

$$\langle T\psi|T\phi\rangle = \langle\psi|\phi\rangle^* = \langle\phi|\psi\rangle, \quad \text{Not!} \quad \langle T\psi|T\phi\rangle = \langle\psi|\phi\rangle$$

(this is always true for time reversal operator, since it involves complex conjugation).

2)

$$T^2 = -1$$

(this is different from scalar case).

Remark 4.1. A symmetry of a quantum system is represented by the linear operator S such that

$$|\langle S\psi|S\phi\rangle| = |\langle\psi|\phi\rangle|$$

By Wigner's theorem S must be either unitary or anti-unitary.

THEOREM 4.2. (Kramer's theorem). If system is time reversal invariant, i.e., [T, H] = 0 and  $T^2 = -1$  then spectrum is doubly degenerate.

*Proof:* Since

$$\langle \psi | T\psi \rangle = \langle T(T\psi) | T\psi \rangle = - \langle \psi | T\psi \rangle, \Rightarrow \langle \psi | T\psi \rangle = 0,$$

and  $\psi$ ,  $T\psi$  are orthogonal to each other.<sup>2</sup>

A non-trivial example of the Hamiltonian with double degeneracies:

$$H = H_0 + f(x)(\mathbf{L} \cdot \mathbf{S}),$$

where  $H_0$  has time reversal symmetry and does not contain spin operator.

If a system contains n particles with spin 1/2, then the time symmetry operator  $T = T_1 \times T_2 \times \cdots \times T_n$  and  $T^2 = -1$  iff n is odd. In this case the spectrum is doubly degenerate, while the total spin is half integer.

<sup>&</sup>lt;sup>2</sup>In the case  $T^2 = 1$ , we usually have  $\psi = T\psi$ .

#### **5.** Product representations of SO(3)

If the system is composed of a number of particles the Hilbert space has the structure of tensorial product. The symmetry group is then acts as:

$$D(g)\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_n = D^{(l_1)}(g)\psi_1 \otimes D^{(l_2)}(g)\psi_2 \otimes \cdots \otimes D^{(l_n)}(g)\psi_n$$

where each  $D^{(l_i)}(g)$  is an irreducible representation and  $l_i$  is the corresponding angular momentum of the particle *i*. As one can understand D(g) is not an irreducible representation itself. So it is important to know the decomposition of D(g) into irreducible representations:

$$(5.1) D = \bigoplus_k r_l D^{(k)}$$

This determines for example how energy levels of the system split in many-body systems when there is an interaction between particles. Exactly the same question can be asked about one particle with a spin s, e.g., s = 1/2. In that case an angular momentum l of the particle adds up with its spin. In mathematical language we are interested in the decomposition of the representation  $D^{(1/2)} \otimes D^{(l)}$  into irreducible one.

#### 6. Clebsch-Gordan series

To find coefficients  $r_k$  in the decomposition (5.1) we can use group orthogonality theorem:

(6.1) 
$$r_{k} = \int \bar{\chi}^{(k)}(\varphi)\chi^{(p)}(\varphi)\chi^{(m)}(\varphi)d\mu_{\varphi} =$$
$$= -\frac{1}{\pi}\int d\varphi \left(e^{-ik\varphi} + e^{-i(k-1)\varphi} + \dots e^{ik\varphi}\right)\sin\left(\left(m + \frac{1}{2}\right)\varphi\right)\sin\left(\left(p + \frac{1}{2}\right)\varphi\right) =$$
$$= \sum_{j=-k}^{k}\delta(m - p - j) - \delta(m + p + 1 - j) =$$
$$= 1 \text{ if } |m - p| \le k \le |m + p|, \text{ otherwise } 0.$$

In other words:

$$D^{(m)} \otimes D^{(p)} = \bigoplus_{k=|m-p|}^{p+m} D^{(k)}$$

#### 7. Clebsch-Gordan coefficients. Adding angular momenta

The basis states of the spinor representation  $D^{(l)}$  are given by

$$L_z|l,m\rangle = m|l,m\rangle, \qquad m = -l, \dots + l.$$

For applications we need to know how the tensor product of these states can be decomposed into such basis:

(7.1) 
$$|l,m\rangle \otimes |j,p\rangle = \sum_{L=|l-j|}^{l+j} C_{m,p,M}^{l,j,L} |L,M\rangle, \qquad M=m+p.$$

We can also invert this decomposition in order to express the eigenstates of total angular momentum in terms of eigenstates of individual angular momenta:

(7.2) 
$$|L,M\rangle = \sum_{m=-l}^{l} \bar{C}_{m,M-m,M}^{l,j,L} |l,m\rangle \otimes |j,p\rangle.$$

The **Clebsch-Gordan coefficients**  $C_{m,p,M}^{l,j,L} = C_{m,M-m}^{l,j,L}$  provide transformation matrices from the basis of  $|l,m\rangle \otimes |j,p\rangle$  to the basis  $|L,M\rangle$  where  $D^{(l)} \otimes D^{(j)}$  is block-diagonal. For SO(3),  $C_{m,p,M}^{l,j,L}$  can be chosen to be real.

7.1. Adding spin. As an example consider addition of angular momentum with the spin:

$$D^{(l)} \otimes D^{(1/2)} = D^{(l+1/2)} \oplus D^{(l-1/2)}.$$

The total angular momentum can take values  $j = l \pm 1/2$ . For the sake of concreteness consider the case j = l + 1/2:

$$|j M\rangle = C_{+}^{(m)} |l m\rangle |+\rangle + C_{-}^{(m)} |l m + 1\rangle |-\rangle, \quad M = m + 1/2.$$

Applying to the both sides of the equation  $J_+$  we obtain:

$$\begin{split} |j M + 1\rangle &= \left( C_{+}^{(m)} \left( \frac{l+m+1}{l+m+2} \right)^{1/2} + C_{-}^{(m)} \left( \frac{1}{(l-m)(l+m+2)} \right)^{1/2} \right) |l m + 1\rangle |+\rangle \\ &+ C_{-}^{(m)} \left( \frac{l-m-1}{l-m} \right)^{1/2} |l m + 2\rangle |-\rangle. \end{split}$$

From this follows recursion relationship:

$$\begin{pmatrix} C_{+}^{(m+1)} \\ C_{-}^{(m+1)} \end{pmatrix} = \begin{pmatrix} \left(\frac{l+m+1}{l+m+2}\right)^{1/2} & \left(\frac{1}{(l-m)(l+m+2)}\right)^{1/2} \\ 0 & \left(\frac{l-m-1}{l-m}\right)^{1/2} \end{pmatrix} \begin{pmatrix} C_{+}^{(m)} \\ C_{-}^{(m)} \end{pmatrix}$$

**Example** l = 1. Since  $|\frac{3}{2} \pm \frac{3}{2}\rangle = |\pm 1\rangle |\pm \frac{1}{2}\rangle \Rightarrow C_+^{(-2)} = 0$ ,  $C_-^{(-2)} = 1$ . By recursion we obtain:

$$|\frac{3}{2} - \frac{1}{2}\rangle = \sqrt{\frac{1}{3}}|-1\rangle|\frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|0\rangle| - \frac{1}{2}\rangle; \qquad |\frac{3}{2}\frac{1}{2}\rangle = \sqrt{\frac{1}{3}}|1\rangle| - \frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|0\rangle|\frac{1}{2}\rangle.$$

In the coordinate representation the above solutions can be written down in the spinor form as:

$$\begin{split} \Phi_{\frac{3}{2}}^{\frac{1}{2}}(x) &= \chi(r) \begin{pmatrix} \sqrt{\frac{2}{3}} Y_1^{(0)}(\theta,\varphi) \\ \sqrt{\frac{1}{3}} Y_1^{(1)}(\theta,\varphi) \end{pmatrix} \qquad \Phi_{\frac{3}{2}}^{-\frac{1}{2}}(x) &= \chi(r) \begin{pmatrix} \sqrt{\frac{1}{3}} Y_1^{(-1)}(\theta,\varphi) \\ \sqrt{\frac{2}{3}} Y_1^{(0)}(\theta,\varphi) \end{pmatrix} \\ \Phi_{\frac{3}{2}}^{\frac{3}{2}}(x) &= \chi(r) \begin{pmatrix} Y_1^{(1)}(\theta,\varphi) \\ 0 \end{pmatrix} \qquad \Phi_{\frac{3}{2}}^{-\frac{3}{2}}(x) &= \chi(r) \begin{pmatrix} 0 \\ Y_1^{(-1)}(\theta,\varphi) \end{pmatrix}. \end{split}$$

#### 8. Wigner-Eckart theorem

8.1. Motivation. In quantum mechanics we often consider interaction of systems with an external environment. Such interaction is described by adding a coupling term  $\lambda X$  to the system Hamiltonian H. By the perturbation theory this interaction induces transitions between eigenstates  $|m'\rangle$ ,  $|m'\rangle$  of H with the rates proportional to:

$$P_{m \to m'} \sim |\langle m | X | m' \rangle|^2.$$

Using the group theory we can often determine which transitions are possible (or prohibited) without making explicit calculations.<sup>3</sup> In addition, in some cases it is also possible to relate to each other the transition rates induced by different observables.

 $<sup>^{3}</sup>$  Are selection rules are restricted to the first order of the perturbation theory? Seems to depend on a particular case.

#### 8. WIGNER-ECKART THEOREM

As a simple example, let look at parity P. The transitions

$$\langle l|X|l'\rangle = \langle l|P^{-1}PXP^{-1}P|l'\rangle = (-1)^{l+l'}p(X)\langle l|X|l'\rangle$$

are zeroes if parity of X,  $p(X) \neq (-1)^{l+l'}$ . For example if X is a vector component, p(X) = -1 and the transitions between l = 0 to l = 2 are forbidden.

8.2. Scalar observable X. By definition a scalar observable is invariant under the rotation:

(8.1) 
$$\exp(-i\varphi(\mathbf{n}\hat{L}))X\exp(i\varphi(\mathbf{n}\hat{L})) = X.$$

For example this would be the case for any  $X = f(\hat{L}^2)$ . Note that

$$\langle m \, l | X | l' \, m' \rangle = f(l(l+1)) \delta_{l,l'} \delta_{m,m'}$$

where the prefactor depends only on l. The same statement can be proven for any X satisfying (8.1). Indeed first by inserting commutators:

(8.2) 
$$\langle m \, l | [X, \hat{L}_z] | l' \, m' \rangle = 0, \qquad \langle m \, l | [X, \hat{L}^2] | l' \, m' \rangle = 0$$

one obtains that m = m', l = l'. Second by using  $\hat{L}_+$  one gets

(8.3) 
$$\sqrt{(l+m)(l-m+1)} \langle m \, l | X | l \, m \rangle = \langle m \, l | X \hat{L}_{-} | l \, m+1 \rangle$$
  
=  $\langle m \, l | \hat{L}_{-} X | l \, m+1 \rangle = \sqrt{(l+m)(l-m+1)} \langle m+1 \, l | X | l \, m+1 \rangle.$ 

Therefore the result does not depend on m.

**8.3. General observable** X. Wigner-Eckart theorem generalizes the above statement to the case when  $X_i$  is transforming according to a representation of SO(3) (or some other symmetry group). For instance  $X_i$  might be a vector, tensor or spinor. In general case let  $X_i^{(l)}$ , i = -l, ... l be an observable which is transformed under rotation as:

(8.4) 
$$UX_i^{(l)}U^{-1} = D_{i,k}^{(l)}X_k^{(l)}, \qquad U = \exp(-i\varphi(\mathbf{n}\hat{L})),$$

where  $D_{i,k}^{(l)}$  is  $2l + 1 \times 2l + 1$  matrix representing rotation U in the spherical basis of the vectors  $\{|lm\rangle, m = -l, \ldots l\}$ . The set of observable  $X^{(l)} = \{X_i^{(l)}, i = -l, \ldots l\}$  is called **spherical tensor** of rank l. Its components are transformed exactly as spherical harmonics  $Y_l^m$  under the action of SO(3), which motivates the name.

For infinitesimal transformations (8.4) implies:

(8.5) 
$$[L_3, X_k^{(l)}] = k X_k^{(l)}, \qquad \sum_{i=1}^3 [L_i[L_i, X_k^{(l)}]] = l(l+1) X_k^{(l)}.$$

In other words, operators  $X_i^{(l)}$ ,  $i = -l, \ldots l$  provide spherical basis of so(3) representation with the angular momentum l.

**Example:** Vector like observable e.g.,  $\hat{x}$ ,  $\hat{p}$ . For a vector  $\{V_x, V_y, V_z\}$  the following three components  $X_0^{(1)} = V_z$ ,  $X_{\pm 1}^{(1)} = \mp (V_x \pm iV_y)/\sqrt{2}$  provide spherical basis for the representation  $D^{(1)}$ . Indeed it follows immediately from the defining property of vectors  $UV_iU^{-1} = R_{i,j}(\phi)V_j$ :

$$[L_3, V_i] = -i\varepsilon_{3ik}V_k \implies [L_3, X_0^{(1)}] = 0, \quad [L_3, X_{\pm 1}^{(1)}] = \pm X_{\pm 1}^{(1)}$$

THEOREM 8.1. (Wigner-Eckart theorem). Let  $X_m^{(l)}$  be an observable which transforms under rotation, as in eq. (8.4), then

$$\langle m'l'|X_m^{(l)}|l''m''\rangle = \langle l'||X^{(l)}||l''\rangle C_{m',m,m''}^{l',l,l''},$$

where  $\langle l' || X^{(l)} || l'' \rangle$  does not depend on m', m'' and m.

*Proof:* By using

(8.6) 
$$[L_{\pm}, X_m^{(l)}] = \sqrt{(l \mp m)(l \pm m + 1)} X_{m\pm 1}^{(l)}$$

we have

$$(8.7) \quad \sqrt{(l' \pm m')(l' \mp m' + 1)}Z(m' \mp 1, m, m'') = \sqrt{(l'' \mp m'')(l'' \pm m'' + 1)}Z(m', m, m'' \pm 1) + \sqrt{(l \mp m)(l \pm m + 1)}Z(m', m \pm 1, m''),$$

where  $Z(m', m, m'') = \langle m'l' | X_m^{(l)} | l''m'' \rangle$ . But exactly the same equation holds for the ClebschGordan coefficients  $C_{m',m,m''}^{l',l,l''}$ . Hence

$$\langle m'l'|X_m^{(l)}|l''m''\rangle \sim C_{m',m,m''}^{l',l,l''},$$

with the proportionality constant depending only on l', l, l''.

#### 9. Applications

Transitions induced by the operators x, y, z. It is easy to check that  $X_0 = z, X_{\pm 1} = (-x \pm iy)/\sqrt{2}$  are the eigenvectors of  $L_z$  (in adjoint representation):

$$[L_z, X_k] = kX_k$$

By Wigner-Eckart theorem

$$\langle m' l' | z | l m \rangle = a C_{m',0,m}^{l',1,l}.$$

From this follows that the only possible transitions are: m' = m,  $l = l' \pm 1$  (the transition l' = l is forbidden by parity). Analogously

$$\langle m' \, l' | x | l \, m \rangle = \langle m' \, l' | X_{-1} - X_1 | l \, m \rangle / \sqrt{2} = a / \sqrt{2} (C_{m',-1,m}^{l',1,l} - C_{m',1,m}^{l',1,l})$$

with the same a. So the possible transitions in this case are  $m' \pm 1 = m$ ,  $l = l' \pm 1$ .

**Zeeman effect.** In the presence of magnetic field an additional interaction term has to be added to the Hamiltonian of the system:



FIGURE 2. Zeeman effect. Without taking into account spin orbit-interactions the levels of an electron in a central potential are 2(2l + 1) times degenerate, where l is angular momentum and the factor 2 is due to the spin. After adding spin-orbit coupling  $L \cdot S$  the energy levels are determined by the total angular momentum  $j = l \pm 1/2$ . So the degeneracies are partially lifted. Note, however, that because of Kramers degeneracies, all energy levels must be (at least) twice degenerate. Finally, by adding magnetic field both time reversal symmetry and SO(3) symmetry are broken (to SO(2)) and the degeneracies are lifted completely.

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#### 9. APPLICATIONS

$$V = -\frac{eH}{2Mc}(L_z + 2S_z)$$

This leads to the splitting of degeneracies in the atomic energy levels. To account for such splittings in first order perturbation theory we need to calculate matrix elements:

$$\langle mj|S_z|jm\rangle$$

where  $\langle mj |$  are eigenstates of the total angular momentum  $J_z, J^2$ . By Wigner-Eckart theorem:

$$\frac{\langle mj|S_i|jm'\rangle}{\langle mj|J_i|jm'\rangle} = a(j), \Longrightarrow \qquad \langle mj|S_z|jm\rangle = ma(j).$$

It remains to find the constant a(j). For this note:

$$(9.1) \quad \langle mj|S \cdot J|jm \rangle = \sum_{i} \sum_{m'} \langle mj|S_i|jm' \rangle \langle m'j|J_i|jm \rangle = a(j) \sum_{i} \sum_{m'} \langle mj|J_i|jm' \rangle \langle m'j|J_i|jm \rangle = a(j) \langle mj|J^2|jm \rangle$$

Since  $2SJ = J^2 + S^2 - L^2$ , we have

$$a(j) = \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}.$$

Finally

$$\Delta E_{m,j} = -\frac{eH}{2Mc}m\left(1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}\right), \quad j = |l-s|, \dots l + s.$$

#### LECTURE 10

# Representations of simple algebras, general construction. Application to SU(3)

#### 1. Adjoint representation and Killing form

Let  $L_i, i = 1, \ldots n$  be generators of a Lie algebra g:

$$[L_i, L_j] = C^k{}_{ij}L_k.$$

Since  $L_i$ , i = 1, ..., n themselves form the linear space  $V = \{\sum_{i=1}^n a_i L_i\}$  we can consider action of  $L_i$  on V. This is so called **adjoint representation Ad**:

$$L_j \cdot \sum_{i=1}^n a_i L_i := \sum_{i=1}^n a_i [L_j, L_i] = \sum_{i=1}^n a'_i L_i, \qquad a'_k = C^k_{j,i} a_i.$$

Therefore:

$$(\mathbf{Ad}L_j)_{k,i} = C_{j,i}^k.$$

Note that coefficients  $C_{j,i}^k$  are antisymmetric in j, i.

We can also introduce scalar product (Killing form) on V through the adjoint representation:

$$(L_i, L_j) := \operatorname{Tr}(\mathbf{Ad}L_i \mathbf{Ad}L_j) = \sum_{l,k} C^k{}_{il} C^l{}_{jk} =: g_{ij}.$$

The **Cartan metric**  $g_{ij}$  is the object of the fundamental significance. In particular it determines whether the algebra is simple or semi-simple (condition A) and whether it is compact (condition B):

(1.1) Condition A: det 
$$(g) \neq 0$$
, Condition B:  $g < 0$ .

In the following we assume (1.1) hold. Under this assumption we can always chose a basis in V where  $g_{ij} = \delta_{ij}$  and

$$C^{k}{}_{il} = g_{ij}C^{j}{}_{il} =: C_{kil} = \operatorname{Tr}([\mathbf{Ad}L_k\mathbf{Ad}L_i]\mathbf{Ad}L_l)$$

is fully antisymmetric.

#### 2. Cartan sub-algebra and roots

We now define Cartan sub-algebra - a maximal set h of commuting generators:

$$[H_i, H_j] = 0, \qquad i = 1 \dots l,$$

where l is called the **rank** of the Lie algebra. The idea is to diagonalize simultaneously h in the adjoint representation:

(2.1) 
$$(\mathbf{Ad}H_i) \cdot E_{\alpha} = \alpha_i E_{\alpha}, \Longleftrightarrow C_i v_{\alpha} = \alpha_i v_{\alpha},$$

where  $C_i$  is the matrix with the elements  $[C_i]_{kl} \equiv C^k{}_{il}$ . Taking the basis where  $g_{ij} = \delta_{ij}$  (i.e.,  $(H_i, H_j) = \delta_{ij}$ ) we see that  $C_i$  is antisymmetric and its eigenvalues are purely real. Note that since

 $C_i$  has l zero eigenvalues corresponding to  $H_i$  the number of non-trivial solutions in eq. (2.1) is dim g - l. The theorem of Cartan asserts that all these solutions are non-degenerate.

Taking a general element  $H = \sum_{i=1}^{l} c_i H_i$  from h one has:

$$(\mathbf{Ad}H) \cdot E_{\alpha} = [H, E_{\alpha}] = \alpha(H)E_{\alpha}, \qquad \alpha(H) = \sum_{i=1}^{l} c_{i}\alpha_{i}.$$

The dim  $\mathbf{g} - l$  linear forms  $\alpha$  are called **roots** of the algebra.

After defining the roots of **g** we can chose the basis such that:

$$(H_i, H_j) = \delta_{ij}, \quad (E_\alpha, E_\beta) = \delta_{\alpha, -\beta}, \quad (H_i, E_\beta) = 0.$$

This is so called **Cartan-Weyl basis**. In this basis:

(2.2) 
$$[H_i, E_\alpha] = \alpha_i E_\alpha, \quad [E_\alpha, E_{-\alpha}] = \sum \alpha_i H_i, \quad [E_\beta, E_\alpha] = N_{\alpha,\beta} E_{\alpha+\beta}.$$

#### 3. Main properties of root systems

The root system  $\mathcal{R}(g)$  of a simple Lie algebra fulfills the following properties:

- If  $\alpha$  is root then  $-\alpha$  is root as well
- If  $\alpha, \beta$  are roots then either  $\alpha + \beta$  is also root or  $[E_{\beta}, E_{\alpha}] = 0$ .
- Weyl reflection (comes later). Give a root  $\beta$  it Weyl reflection:

$$\sigma_{\alpha}(\beta) = \beta - \frac{2(\alpha\beta)}{\alpha^2}\alpha$$

is also a root.

- The roots can be split into positive and negative  $\mathcal{R}(g) = \mathcal{R}_{-}(g) \cup \mathcal{R}_{+}(g)$ . The first component  $\alpha_1$  of a positive (negative) root is larger (resp. smaller) then 0.
- There is a basis of l (positive) simple roots  $\alpha^{(k)}, k = 1 \dots l$  such that any  $\alpha \in \mathcal{R}_+(g)$ :

$$\alpha = \sum_{k=1}^{l} n_k \alpha^{(k)}, \qquad n_k \ge 0.$$

#### 4. Building up representations of g

Using (2.2) we can construct an su(2) sub-algebra of g associated with any root  $\alpha$ . This sub-algebra  $g_{\alpha}$  is generated by the triplet:

$$\mathbf{g}_{\alpha} = \{ H_{\alpha} = \frac{\alpha_i}{|\alpha|^2} H_i, |\alpha|^{-1} E_{\alpha}, |\alpha|^{-1} E_{-\alpha} \}, \qquad \alpha \in \mathcal{R}(\mathbf{g}).$$

A general representation of g is constructed in the following way. Let  $|\lambda\rangle$  be an eigenvector of h, i.e.,

$$H_i|\lambda\rangle = \lambda_i|\lambda\rangle, \qquad i = 1, \dots l, \quad \Rightarrow \quad H_\alpha|\lambda\rangle = \frac{(\lambda, \alpha)}{|\alpha|^2}|\lambda\rangle$$

Since vectors  $|\alpha|^{-1}E_{-\alpha}|\lambda\rangle$  form representation of  $\mathbf{g}_{\alpha}$  the number  $\frac{\langle\lambda,\alpha\rangle}{|\alpha|^2}$  must be half integer:

(4.1) 
$$2\frac{(\lambda,\alpha)}{|\alpha|^2} \in \mathbb{Z}$$

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#### 5. REPRESENTATIONS OF SU(3)

In particular by taking the adjoint representation we obtain:

$$2rac{(eta,lpha)}{|lpha|^2}\in\mathbb{Z},\qquadeta,lpha\in\mathcal{R}(\mathsf{g}).$$

#### A general recipe for construction of the representations:

- Construct reciprocal lattice Λ = {Σ<sup>l</sup><sub>k=1</sub> m<sub>k</sub>λ<sup>(k)</sup>, m<sub>k</sub> ∈ Z} generated by fundamental weights λ<sup>(k)</sup>: 2<sup>(λ<sup>(i)</sup>,α<sup>(j)</sup>)</sup>/|α<sup>(j)</sup>|<sup>2</sup> = δ<sub>ij</sub>. All vectors from Λ obey (4.1).
  Take the highest weight λ ∈ Λ, which is annihilated by all raising operators:

$$H_i|\lambda\rangle = \lambda_i|\lambda\rangle, \qquad i = 1, \dots l, \qquad E_{\alpha}|\lambda\rangle = 0, \alpha \in \mathcal{R}_+(\mathsf{g}).$$

• Apply lowering generators, up to the point when it vanishes:

$$\{|\lambda_{\mathbf{n}}\rangle = \prod_{\alpha \in \mathcal{R}_{-}(\mathbf{g})} E_{\alpha}^{n_{\alpha}} |\lambda\rangle\}.$$

The corresponding weights are then given by:

$$H_i|\lambda_{\mathbf{n}}\rangle = \lambda_i + \sum_{\alpha} n_{\alpha} \alpha_i |\lambda_{\mathbf{n}}\rangle.$$

In other words all the weights are situated on the lattice generated by the roots of the system, shifted by the highest weight  $\lambda$ . In the basis free notation:

$$H|\lambda_{\mathbf{n}}\rangle = \lambda_{\mathbf{n}}(H)|\lambda_{\mathbf{n}}\rangle, \qquad \lambda_{\mathbf{n}} = \lambda + \sum_{\alpha \in \mathcal{R}_{-}(\mathbf{g})} n_{\alpha}\alpha.$$

#### 5. Representations of su(3)

5.0.1. Transition from su(3) to  $sl(3,\mathbb{C})$ . To find representation of the group SU(3) we look at the representations of its Lie algebra su(3). It is convenient to consider its complexification  $su(3)_{\mathbb{C}} \cong sl(3,\mathbb{C})$  which has the same representations as su(3) itself:

$$su(3) \to sl(3, \mathbb{C}).$$

5.0.2. Cartan-Weyl basis of  $sl(3, \mathbb{C})$ . : <sup>1</sup>

(5.1) 
$$H_1 = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad H_2 = \frac{1}{2\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

$$E_{1} = E_{-1}^{T} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad E_{2} = E_{-2}^{T} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \quad E_{3} = E_{-3}^{T} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The commutation relations are given by

$$[H_1, E_{\pm k}] = \pm \alpha^{(k)}(H_1)E_{\pm k}, \qquad [H_2, E_{\pm k}] = \pm \alpha^{(k)}(H_2)E_{\pm k}, \quad k = 1, 2, 3$$

where

$$\alpha^{(1)}(H_1) = 1, \alpha^{(2)}(H_1) = -1/2, \alpha^{(3)}(H_2) = 1/2$$

<sup>1</sup>Note:  $H_1 = I_3, H_2 = T_8 = \frac{\sqrt{3}}{2}Y$ 



FIGURE 1. Root system for su(3)

$$\alpha^{(1)}(H_2) = 0, \alpha^{(2)}(H_2) = \sqrt{3}/2, \alpha^{(3)}(H_2) = \sqrt{3}/2.$$

Note also that

$$[E_1, E_2] = E_3 \qquad \Rightarrow \qquad \alpha^{(3)}(H_i) = \alpha^{(1)}(H_i) + \alpha^{(2)}(H_i).$$

The corresponding roots  $\alpha_k, k = 1, 2, 3$  are shown in figure 1. The reciprocal lattice is generated by two weights:

$$\lambda^{(1)} = \frac{1}{3}(2\alpha^{(2)} + \alpha^{(1)}) \qquad \lambda^{(2)} = \frac{1}{3}(2\alpha^{(1)} + \alpha^{(2)}).$$

5.0.3. Adjoint representation [8]. This representation consists of 6 roots of the system and in addition contains 2 vectors with zero weights corresponding to  $H_1, H_2$ . The highest weight is  $\lambda = \alpha^{(3)}$ .

5.0.4. Fundamental representations [3],  $[\bar{3}]$ . These are the representations of minimal dimension (3) akin 1/2 representation for su(2). There are two such representations: [3] with the highest weight  $\lambda = \lambda^{(1)}$  and  $[\bar{3}]$  with the highest weight  $\lambda = \lambda^{(2)}$ .

5.0.5. General representation D(p,q). A general representation D(p,q) is constructed by fixing highest weight to be  $\lambda = p\lambda^{(1)} + q\lambda^{(2)}$ . The integers p and q show how many times we can apply operators  $E_{\alpha_1}$ ,  $E_{\alpha_2}$  to the highest weight, before it vanishes (see fig. XXX):

$$E_{\alpha_2}^{p+1}|\lambda\rangle = 0, \qquad E_{\alpha_1}^{q+1}|\lambda\rangle = 0.$$

The resulting representation diagram is a hexagon with  $D_3$  symmetry. This symmetry is easily understood if one considers the induced representations of  $g_{\alpha}$  groups. These representations must be symmetric under reflection about the line orthogonal to the root  $\alpha$  and passing through the origin. Note also that D(q, p) is complex conjugate representation for D(p, q). Note that the fundamental representations correspond to:  $D(1, 0) = [3], D(0, 1) = [\overline{3}]$ , while adjoint is D(1, 1) =[8].

The multiplicities of the weights in the representation are 1 at the outer layer and then increasing by one at each next layer before it reaches "triangular" part of the representation. At this



FIGURE 2. Construction of a general representation D(p,q). The multiplicity of each layer is increased up to the point when it reaches triangular structure, then the multiplicities stay the same.

point the multiplicities stay constant.<sup>2</sup> The resulting dimension of the representation is therefore given by (easy exercise in combinatorics):

$$\dim(D(p,q)) = \frac{1}{2}(p+1)(q+1)(p+q+2).$$

The number  $t := (p - q) \mod 3 = 2(\lambda, \alpha^{(1)} + \alpha^{(2)})$  is called *triality of the representation* It distinguishes between three classes of representations. All weights from the same representation have the same t. This is easy to see since adding of roots to  $\lambda$  does not change this number. For D(1,0), D(0,1) and D(1,1) this number is 1, -1 and 0, respectively.

**5.1. Tensor product representations.** It is also easy to multiply different representations using graphical picture. See the case  $[3] \otimes [\overline{3}] = [8] \oplus [1]$  in figure 3.



FIGURE 3. Tensor product of two fundamental representations:  $[3] \otimes [\overline{3}]$ .

 $<sup>^{2}</sup>$ The proof will be added later.

#### LECTURE 11

# Strong interactions: flavor SU(3)

In the classical physics elementary particles might have different characteristics: masses, charges, angular moments, energies, etc. Symmetries provide conservation laws but no organization principle in this zoo. From the point of view of 19th century physics there is no compelling reason reason to have any particular number of particles, specific charges or spins.

In quantum mechanics the symmetries play a much deeper role. Symmetries provide organization principles. To a large extent, a list of its symmetries defines the fundamental physics of the system. In particular, elementary particles can be associated with irreducible representation of *internal* symmetry groups. Assume that a system is governed by a Hamiltonian H whose continuous symmetry group is  $G = G_1 \times G_2 \times \cdots \times G_k$ . The states  $|\Lambda\rangle$  of isolated stable particles must be eigenvectors of H. But since H commutes with the generators  $Q_i$  of  $G_i$ ,  $i = 1, \ldots k$ , the states

$$|\Lambda\rangle = |\lambda_1\lambda_2\dots\lambda_k\rangle$$

must belong to a particular representation labeled by the numbers  $\lambda_1, \lambda_2, \ldots \lambda_k$ . Therefore knowledge of irreducible representations of the symmetry group of the system provides a valuable information on possible elementary particles. In opposite direction, knowledge of particles physical characteristics often allows their organization them into (approximate) multiplets (whose members have similar properties), allowing us to deduce the internal symmetry group from experimental data.

#### 1. Internal symmetries: isospin

When the neutron was discovered 1932, Heisenberg came up with a deep idea that in a profound way extended quantum mechanics to subatomic realm. Until then quantum theory was based on classical notions such as 3D rotations and translations of a particle, but now particles themselves became arranged into quantum multiplets. He posited that the proton and neutron, which appeared identical under strong interactions, are two possible states of a single particle in an abstract "isospin" space,

(1.1) 
$$|p\rangle = \begin{pmatrix} p\\ 0 \end{pmatrix}, \qquad |n\rangle = \begin{pmatrix} 0\\ n \end{pmatrix},$$

by analogy to the spin  $\pm 1/2$ . The strong interaction Hamiltonian  $H_s$  is assumed invariant under the "isospin" group SU(2), [H, I] = 0. Using the total isospin I and its third component  $I_3$  as quantum numbers  $|I, I_3\rangle$ , we can denote nucleons as

(1.2) 
$$|p\rangle = |\frac{1}{2}, \frac{1}{2}\rangle, \qquad |p\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$$

with the electromagnetic and weak interactions splitting them as a weak perturbation. The SU(3) symmetry then implies that there should exist states corresponding to I = 1, etc., with such states – pions

$$\pi^+ = |1,1\rangle, \qquad \pi^0 = |1,0\rangle, \qquad \pi^- = |1,-1\rangle$$

of nearly identical masses were discovered soon thereafter.

The assumed invariance of the strong interaction Hamiltonian  $H_s$  under the isospin group immediately constrains possible nuclear reactions. It connects different reaction amplitudes by the Wigner-Eckart theorem. For example, using this symmetry we can relate amplitudes of three different reactions:

$$\pi^0 p \to \pi^+ n, \quad \pi^0 p \to \pi^0 p, \quad \pi^+ n \to \pi^+ n \,.$$

The corresponding states can be decomposed as:

(1.3) 
$$|\pi^0 p\rangle := |10\rangle \otimes |\frac{1}{2}\frac{1}{2}\rangle = \sqrt{\frac{2}{3}}\frac{1}{2}\frac{1}{2}\rangle + \sqrt{\frac{1}{3}}\frac{1}{2}\frac{1}{2}\rangle$$

(1.4) 
$$|\pi^+n\rangle := |11\rangle \otimes |\frac{1}{2}\frac{-1}{2}\rangle = \sqrt{\frac{1}{3}}\frac{3}{2}\frac{1}{2}\rangle - \sqrt{\frac{2}{3}}\frac{1}{2}\frac{1}{2}\rangle$$

(1.5) 
$$|\pi^0 n\rangle := |10\rangle \otimes |\frac{1}{2} \frac{-1}{2}\rangle = \sqrt{\frac{2}{3}} |\frac{3}{2} \frac{-1}{2}\rangle + \sqrt{\frac{1}{3}} |\frac{1}{2} \frac{-1}{2}\rangle$$

Since H is invariant (a "scalar") under isospin transformations, [H, I] = 0, Wigner-Eckart theorem relates various scattering amplitudes:

$$\langle \pi^0 p | H(I) | \pi^+ n \rangle = I_{3/2} \frac{\sqrt{2}}{3} - I_{1/2} \frac{\sqrt{2}}{3}; \quad \langle \pi^+ n | H(I) | \pi^+ n \rangle = I_{3/2} \frac{1}{3} + I_{1/2} \frac{2}{3}$$
  
$$\langle \pi^0 p | H(I) | \pi^0 p \rangle = \langle \pi^0 p | H(I) | \pi^0 p \rangle = I_{3/2} \frac{2}{3} + I_{1/2} \frac{1}{3}$$

With an eye on the strangeness to follow, let's rephrase the SU(2) of isospin the way it is done today, in terms of "quarks." The 2-dimensional fundamental representation describes the approximate isospin symmetry of the u and d quarks. The pion triplet transforms as the  $\mathbf{2} \otimes \overline{\mathbf{2}} =$  $\mathbf{3} \oplus \mathbf{1}$  tensors constructed from the traceless part of the quark-antiquark outer products  $q \otimes \overline{q}$ ,

(1.6) 
$$\begin{pmatrix} u \\ d \end{pmatrix} \otimes \begin{pmatrix} \overline{u} & \overline{d} \end{pmatrix} = \begin{pmatrix} u\overline{u} & u\overline{d} \\ d\overline{u} & d\overline{d} \end{pmatrix} = \begin{pmatrix} \frac{u\overline{u} - d\overline{d}}{2} & u\overline{d} \\ \frac{d\overline{u}}{d\overline{u}} & -\frac{u\overline{u} - d\overline{d}}{2} \end{pmatrix} + \frac{1}{2}(u\overline{u} + d\overline{d})\mathbf{1}.$$

A generator of SU(2) transformations (an arbitrary traceless hermitian matrix) can be represented in terms of Pauli matrices

$$\sigma_1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \frac{1}{2} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

as

(1.7) 
$$\pi = \frac{1}{\sqrt{2}} \sum_{j=1}^{3} \pi_j \sigma_j = \frac{1}{\sqrt{2}} \begin{pmatrix} \pi_3 & \pi_1 - i\pi_2 \\ \pi_1 + i\pi_2 & -\pi_3 \end{pmatrix} = \begin{pmatrix} \frac{\pi^0}{\sqrt{2}} & \pi^+ \\ \pi^- & -\frac{\pi^0}{\sqrt{2}} \end{pmatrix}$$

where one can express the pion isospin 1 triplet (the adjoint rep of SU(2)) in terms of either real fields  $(\pi_1, \pi_2, \pi_3)$  or charged pion complex fields  $\pi^{\pm} = (\pi_1 \mp i\pi_2)/\sqrt{2}$ . The isospin 0 singlet in the decomposition (1.6)

(1.8) 
$$\eta = \begin{pmatrix} \frac{\eta^0}{\sqrt{2}} & 0\\ 0 & -\frac{\eta^0}{\sqrt{2}} \end{pmatrix}$$

is known as the  $\eta$  meson. If quarks are assigned quantum numbers

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## 2. INTERNAL SYMMETRIES: STRANGENESS



FIGURE 1. (a) The meson (pseudoscalars) octet. (b) The quark triplet, the anti-quark triplet and the gluon octet. (Wikipedia).

we can read off the isospin  $I_3$  of each pion in (1.7) by adding the quantum numbers of their quark constituents (1.6). Kaons and anitkaons form two further SU(2) meson doublets. We shall now incorporate all of them into a single flavor SUn3 octet, as in figure 1.

#### 2. Internal symmetries: strangeness

For Heisenberg, the nucleons (1.1) were the elementary constituents of matter. By 1956 Sakata has extended this list to  $(p, n, \Lambda)$  where  $\Lambda$  was a recently discovered heavy particle, a hyperon, and extended Heisenberg's symmetry from SU(2) to SU(3). Mesons were supposed to be extremely strongly bound states of these baryons (from Greek *bary*- meaning *heavy*).

This scheme did well for mesons, but failed for baryons. It took some courage to go to the next level of abstraction. In the process, Heisenberg's nucleons got demoted from their "elementary" status. In the modern parlance, nucleons are composed of the "up" and "down" "flavors" of quarks, p = uud, n = udd, with (1.2) replaced by

(2.1) 
$$|u\rangle = |\frac{1}{2}, \frac{1}{2}\rangle, \qquad |d\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$$

"Up" and "down" quark masses are nearly the same, making isospin a very good approximate symmetry. However, by 1940's and 1950's experimentalists have found a whole zoo of other slowly decaying particles produced by cosmic rays and accelerators. Nobody has asked for them (theoretical physicists have predicted about two yet fundamentally unexpected particles in the whole history of physics), so they appeared "strange." They could be made sense of if a new quantum number was added, strangeness S, and they obeyed the empirical Gell-Mann-Nishijima relation

(2.2) 
$$Q = I_3 + \frac{1}{2}(B+S),$$

where Q is electric charge, B is the baryon number. By late 1950's the known particles were empirically neatly arranged into baryon and meson octets of figure 2 (a) and figure 1 (a). Gell-Mann (and, somewhat later, Ne'eman and Zweig) took the apparent SU(3) symmetry seriously and took the next fundamental step.

**2.1. The Eightfold Way.** Within the sub-multiplets of particles e.g.,  $\{p,n\}, \{\pi^+, \pi^0, \pi^-\}$  the charge is growing by one. So to label each of these sub-multiplets one adds an additional number - hypercharge  $Y = Q_{max} + Q_{min}$  (Y/2 is then the average charge of a sub-multiplets), which is related to the charge,  $Q = Y/2 + I_3$ , by the Gell-Mann-Nishijima relation (2.2). If we label now each particle from the **baryon octet** by a point in Y-I<sub>3</sub> plane the resulting picture resembles



FIGURE 2. (a) The S = 1/2 ground state baryon octet. Particles along the same horizontal line share the same strangeness, s, while those on the same diagonals share the same charge, q. (b) The S = 3/2 baryon decuplet. Wikipedia.

TABLE 1. Quark quantum numbers.

	Q	Ι	$I_3$	Y	B
u	2/3	1/2	1/2	1/3	1/3
d	-1/3	1/2	-1/2	1/3	1/3
$\mathbf{S}$	-1/3	0	0	-2/3	1/3

the adjoint 8 representation for SU(3), see figure 2 (a). Equally simple picture is obtained for the meson octet, figure 1.

#### 3. Quarks

A surprising fact is that none of the observed particle multiplets correspond to the fundamental representation. While initially this was considered only a mathematical curiosity, today the fundamental representations are reserved for fundamental constituents of matter, the quarks (resp. anti-quarks)  $\{u, d, s\}$  (resp.  $\{\bar{u}, \bar{d}, \bar{s}\}$ ). The current belief -color confinement- is that such particles do not exist in isolation since they have a non-vanishing SU(3) color charge: only colorless particles can exist. This implies that the observed particles can be combinations of type  $q\bar{q}$  (mesons) or qqq,  $\bar{q}\bar{q}\bar{q}$  (baryons). In addition, recent experimentally measured decays are consistent with existence of  $qqqq\bar{q}$  (pentaquarks). Currently there is no evidence for existence of a  $qq\bar{q}\bar{q}$  (tetraquarks).

Gell-Mann and Ne'eman added a 'strange' quark to the up-down flavors (2.1)

(3.1) 
$$\begin{pmatrix} u \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ d \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ s \end{pmatrix}$$

and eliminated the baryon number B from the classification in favor of "hypercharge", the sum Y = B + S in (2.2). To be consistent with the quantum numbers of observed particles, quarks are assigned the quantum numbers listed in table 1.

Flavor SU(3) transformations are generated by eight Lie algebra generators  $U = \exp(\sum \phi_j \lambda_j)$ . Gell-Mann fundamental or defining representation basis  $\{\lambda_j\}$  for su(3) Lie algebra is handcrafted

# 3. QUARKS

(3.2)

for hypercharge Y symmetry breaking to isospin su(2) Pauli matrices (upper left corner):

$$\lambda_{1} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_{2} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_{3} = 2I_{0} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\lambda_{4} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \lambda_{5} = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}$$
$$\lambda_{6} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \lambda_{7} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$
$$\lambda_{8} = Y = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

They provide a metric for the adjoint representation

(3.3) 
$$\operatorname{tr}(\lambda_j \lambda_k) = 2\delta_{jk},$$

(factor 2 is Gell-Mann's normalization convention) and satisfy Lie algebra commutator relations

$$[\lambda_j, \lambda_k] = 2if_{jk\ell}\lambda_\ell$$

The 3-dimensional fundamental representation describes the approximate flavor symmetry of the three quarks u, d, and s. Individual isolated quarks are not observed in nature, but their mesonic and baryonic composite states are. The meson octet arises from the  $\mathbf{3} \otimes \overline{\mathbf{3}} = \mathbf{1} \oplus \mathbf{8}$  tensors constructed from the traceless part of the quark-antiquark outer products  $q \otimes \overline{q}$  (see figure 3),

(3.5) 
$$\begin{pmatrix} u \\ d \\ s \end{pmatrix} \otimes \begin{pmatrix} \overline{u} & \overline{d} & \overline{s} \end{pmatrix} = \begin{pmatrix} u\overline{u} & u\overline{d} & u\overline{s} \\ d\overline{u} & d\overline{d} & d\overline{s} \\ s\overline{u} & s\overline{d} & s\overline{s} \end{pmatrix}$$

For example, the pion  $\pi^+$  belongs to a non-vanishing entry in a  $3 \otimes \overline{3}$  tensor obtained by the outer product

(3.6) 
$$\pi^+ = u \otimes \overline{d} = \begin{pmatrix} u \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & \overline{d} & 0 \end{pmatrix} = \begin{pmatrix} 0 & ud & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

~

Filling in all  $q \otimes \overline{q}$  combinations and taking the traceless part yields a 8-parameter adjoint representation of SU(3) in terms of the traceless hermitian matrix (see (1.7) for the SU(2) example):

$$\Phi = \begin{pmatrix} \frac{\pi^{0}}{\sqrt{2}} + \frac{\eta}{\sqrt{6}} & \pi^{+} & K^{+} \\ \pi^{-} & -\frac{\pi^{0}}{\sqrt{2}} + \frac{\eta}{\sqrt{6}} & K^{0} \\ K^{-} & \overline{K^{0}} & -\frac{2\eta}{\sqrt{6}} \end{pmatrix}$$

$$(3.7) \qquad = \begin{pmatrix} \frac{\pi^{0}}{\sqrt{2}} & \pi^{+} & 0 \\ \pi^{-} & -\frac{\pi^{0}}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & K^{+} \\ 0 & 0 & K^{0} \\ K^{-} & \overline{K^{0}} & 0 \end{pmatrix} + \frac{\eta}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix},$$

where we have replaced the constituent  $q \otimes \overline{q}$  combinations by the names of the elementary particles they build. Similarly, the baryon octet and decuplet arise from the  $\mathbf{3} \otimes \mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{8} \oplus \mathbf{8} \oplus \mathbf{10}$ . In this way the meson and baryon octets are seen to correspond to the root system of the adjoint representation, in agreement with the empirical arrays of figure 2 (a) and figure 1 (a). **3.1. Gell-MannOkubo mass formula.** The "strange"  $\eta$  meson is heavier than pions, a phenomenological fact that we now use to split the masses of the approximate flavor SU(3) octet into pion, kaon and  $\eta$  sectors. Gell-Mann explicit basis (3.2), modulo some overall factors and *i*'s, is set up to break the symmetry by singling out the strangeness (hypercharge Y) in the su(3) space, and leaving as the residual non-trivial symmetry (the little group of Y) the su(2) of isospin.

 $\Phi$  is a  $q \otimes \overline{q}$  tensor which transforms as  $\Phi \to U^{\dagger} \Phi U$ . Hence we can write a flavor SU(3) invariant action bilinear in particle fields (the mass matrix for free relativistic particles at rest; a "Hamiltonian") as

(3.8) 
$$H_0 = \frac{1}{2}\mu^2 \mathrm{tr}\,\Phi^2 + M_0 \mathrm{tr}\,\overline{B}B\,,$$

with baryon mass  $M_0$  (baryons are fermions), and meson mass squared  $\mu^2$  (mesons are pseudoscalars).

Now we break the symmetry by singling out the Y direction. It suffices to consider a term whose only nonzero entry is

(3.9) 
$$\Delta = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

with perturbation mass matrix

(3.10) 
$$H_0 = \frac{\alpha}{2} \mu^2 \operatorname{tr} \Phi^2 \Delta + \beta \operatorname{tr} \overline{B} \Delta B \,,$$

To evaluate the mass matrix for mesons, take trace of  $\Phi$  squared, (3.7), using (3.3), etc. The three new, non-degenerate perturbed masses  $(m_{\pi}^2, m_{K}^2, m_{\eta}^2)$  will be parametrized by the perturbation strength  $\alpha$ . Eliminate  $\alpha$  to obtain a Gell-Mann-Okubo mass formula for the splitting of meson octet,

(3.11) 
$$m_{\eta}^2 = \frac{4\,m_K^2 - m_{\pi}^2}{3}\,.$$

This happens to be off by only 3.5%, which is great, considering that we do not know how to compute these masses from a fundamental theory. In all generality, this argument also leads to a sum rule for the masses of hadrons within a specific multiplet, determined by their isospin I and strangeness S:

(3.12) 
$$M_{I,S} = a_0 + a_1 S + a_2 \left[ I \left( I + 1 \right) - \frac{1}{4} S^2 \right],$$

where  $a_0$ ,  $a_1$ , and  $a_2$  are fitting parameters.

Gell-Mann received the 1969 Nobel prize for this work. He predicted existence of two new baryons, and in particular the mass of the strangeness spin S = 3/2 baryon  $\Omega^-$  whose existence was confirmed 6 years later. Gell-Mann calculation relied on the explicit  $\lambda$  matrix representations: the elegant calculation presented here, relying on invariance alone (in the spirit of Wigner 3n-jcoefficients) was Okubo's. Subsequent discoveries of other flavors of quarks: 'charm', 'bottom', and 'top', much heavier than u, d, and s, have made it clear that the flavor SU(3) is only an approximate symmetry, a useful guide to strong interaction properties of the particles composed of u, d, and s. The current "standard model" is a much more complicated, uglier affair.

The Gell-Mann-Okubo mass sum rules [1-3] are an easy consequence of the approximate SU(3) flavor symmetry. Determination of quark masses is much harder - they are parameters of the standard model, determined by optimizing the spectrum of particle masses obtained by lattice QCD calculations as compared to the experimental baryon and meson masses. The best



FIGURE 3. A lattice gauge theory calculation of the light QCD spectrum. Horizontal lines and bands are the experimental values with their decay widths. The  $\pi, K$  and and  $\Xi$  have no error bars because they are used to set the light and strange quark masses and the overall scale respectively. From Scholarpedia.

determination of the mass spectrum as of 2012 is given in figure 3. Up, down quarks are about 3 and 6 MeV, respectively, with strange quark mass about 100 MeV, all with large error brackets.

The 1/3 electric charge of quarks has lead to reappearance of SU(3) in yet another, still more profound guise, as the *exact* "color" SU(3) gauge symmetry, or QCD (Quantum ChromoDynamics), a conceptual advance that underpins almost all of the "fundamental" physics since 1970's. To understand that, you need to take a full-fledged QFT course.

# References

- [1] M. Gell-Mann, *The eightfold way: a theory of strong interaction symmetry*, Synchrotron Laboratory Report CTSL-20 (CalTech, 1961).
- [2] M. Gell-Mann, "Symmetries of baryons and mesons", Phys. Rev. 125, 1067–1084 (1962).
- [3] S. Okubo, "Note on unitary symmetry in strong interactions", Prog. Theor. Phys. 27, 949–966 (1962).

## LECTURE 12

# Many particle systems. Young tableaux

Motivation for Young tableaux is coming from two primary sources:

- First, they provide an effective way to classify all irreps of the symmetric group  $S_n$ . This is of great importance on its own, since by Cayley's theorem any finite group can be seen as a subgroup of  $S_n$ .
- Second, the same construction (with some minor adjustments) provides irreps of SU(n).

Before looking at the details of the Young tableau construction, let us briefly discuss the reason for connections between representations of SU(N) and  $S_n$ . A system of *n* identical particles forms a tensor representation of a symmetry group e.g., SU(N):

$$D(g)\psi_1(x_1)\otimes\psi_2(x_2)\otimes\cdots\otimes\psi_n(x_n)=D^{(l)}\psi_1(x_1)\otimes D^{(l)}\psi_2(x_2)\otimes\cdots\otimes D^{(l)}\psi_n(x_n).$$

In order to split this representation into a sum of irreducible representations one can use the following trick. A tensor representation is invariant under the action of a permutation

$$\sigma\psi_1(x_1)\otimes\psi_2(x_2)\otimes\cdots\otimes\psi_n(x_n)=\psi_{\sigma(1)}(x_1)\otimes\psi_{\sigma(2)}(x_2)\otimes\cdots\otimes\psi_{\sigma(n)}(x_n)$$

This just follows from a simple fact that, D(g) commutes with any  $\sigma \in S_n$ . In the reverse direction, each irreducible representations of  $S_n$  remains invariant under the action of the symmetry group. In this way the irreducible representations for SU(N) can be constructed by finding irreducible subspaces of the tensor products under the action of symmetry group  $S_n$ . A familiar example is provided by the product states of two particles with the spin 1/2,

Example  $D^{1/2} \otimes D^{1/2} = D^0 \oplus D^1$ :

$$V_{0} = \left\{ \frac{1}{\sqrt{2}} \left( |+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle \right) \right\},$$
$$V_{1} = \left\{ \frac{1}{\sqrt{2}} \left( |+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle \right), \quad |+\rangle \otimes |+\rangle, \quad |-\rangle \otimes |-\rangle \right\}.$$

Here the 1-dimensional antisymmetric subspace  $V_0$  corresponds to the irrep  $D^0$  with the spin 0, while 3-dimensional symmetric subspace  $V_1$  corresponds to the irrep  $D^1$  with the spin 1.

## 1. Irreducible representations of $S_n$

The basic idea behind the Young tableaux construction is to consider the regular representation  $D_{reg}$  of  $S_n$  and split it into different symmetry subspaces:

$$(1.1) D_{reg} = \bigoplus_{\lambda \in \mathcal{R}} r_{\lambda} D_{\lambda},$$

where  $\mathcal{R}$  is the set of all irreducible representations and  $r_{\lambda} = \dim D_{\lambda}$ . Each representation in this decomposition is then uniquely associated with some Young tableaux.

**1.1. Regular representation.** The vector space V on which  $D_{reg}$  acts is constructed by defining the basis  $\{\Psi_{\sigma} | \sigma \in S_n\}$  of dimension n!, such that any element v from V is given by a linear combination:

(1.2) 
$$v = \sum_{\sigma \in S_n} c_{\sigma} \Psi_{\sigma}$$

The action of  $D_{reg}(g), g \in S_n$  on V is then defined by the permutation of basis elements:

(1.3) 
$$g \cdot e_{\sigma} := \Psi_{g\sigma}.$$

As for any regular representation, we have dim  $D_{reg} = |S_n| = n!$ .

We are going to show now that the space V can be split into subspaces invariant under the action of  $D_{reg}$ . We first consider two special cases and then turn to a general one.

1.2. Symmetrization. Let us define the operator of full symmetrization

(1.4) 
$$\hat{S} = \sum_{\sigma \in S_n} \sigma,$$

and apply it to an arbitrary element of the basis e.g.,  $\Psi_e$ :

(1.5) 
$$\Psi_S = \hat{S} \Psi_e = \sum_{\sigma \in S_n} \Psi_{\sigma}.$$

Since  $g\hat{S} = \hat{S}$  for all  $g \in S_n$ , the vector  $\Psi_S$  is invariant under the action of any element from  $S_n$ . In other words  $D_{reg}$  acts on  $V_S = \{\Psi_S\}$  as one-dimensional trivial representation and  $\hat{S}$  is the corresponding projection operator (up to a normalization).

1.3. Antisymmetrization. Alternatively, we can define the antisymmetrization

(1.6) 
$$\hat{A} = \sum_{\sigma \in S_n} (-1)^{\varepsilon(\sigma)} \sigma,$$

where  $\varepsilon(\sigma)$  is parity of  $\sigma$ . After applying it to  $\Psi_e$  one gets

(1.7) 
$$\Psi_A = \hat{A}\Psi_e = \sum_{\sigma \in S_n} (-1)^{\varepsilon(\sigma)} \Psi_{\sigma}.$$

By  $g\hat{A} = (-1)^{\varepsilon(g)}\hat{A}$ , we have  $g\Psi_A = (-1)^{\varepsilon(g)}\Psi_A$ . This state defines the subspace  $V_A = \{\Psi_A\}$  on which  $D_{reg}$  acts as the one-dimensional alternating representation with  $\hat{A}$  being the corresponding projection operator (up to a normalization).

1.4. Projection operators for general irrep. So far we have constructed projection operators corresponding to two very special irreps. We give now a general construction providing any general irrep of  $S_n$ . Let  $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_k)$ ,  $\lambda_{i+1} \ge \lambda_i$  be partition of n into sum  $n = \sum_i \lambda_i$ . With each such partition we will associate a Young diagram. The k'th row of Young diagram is composed of  $\lambda_k$  empty boxes. Now fill these boxes by the numbers  $1, 2, \ldots n$  such that in each horizontal and each vertical line the numbers are ordered from lowest to largest. The resulting diagram Y with the filled numbers is called Young tableau. For the diagrams consisting of just one (vertical or horizontal) line there is only one way to place ordered numbers. In all other cases there exist several Young tableaux corresponding to one and the same Young diagram. For instance, if  $\lambda = (3, 1)$  there are three options:



## 1. IRREDUCIBLE REPRESENTATIONS OF $S_N$

Given a Young tableau Y one can construct the corresponding Young symmetrizer:

$$\hat{P}_Y = \hat{A}_Y \hat{S}_Y$$

Here  $\hat{S}_Y$  is symmetrization operation along each horizontal line (row) of Y, and  $\hat{A}_Y$  is antisymmetrization along each vertical line (column) of Y.

**Example.** The following example illustrates action of  $\hat{P}_Y$ ,  $Y = \frac{12}{3}$  on the state  $\Psi_e \equiv \Psi(1,2,3)$ .

$$\hat{P}_Y \Psi(1,2,3) = (e - (13))(e + (12))\Psi(1,2,3) = (e - (13))(\Psi(1,2,3) + \Psi(2,1,3)) = \Psi(1,2,3) + \Psi(2,1,3) - \Psi(3,2,1) + \Psi(2,3,1).$$

It can be shown then that (for a proof see Fulton & Harris [1]):

• The subspace  $V_Y := \hat{P}_Y V$  is invariant under the action of any element  $\sigma$  from  $S_n$ :

$$\sigma \cdot P_Y \Psi = P_Y \Psi'.$$

• With the proper normalization  $\hat{P}_Y$  are orthogonal projection operators:

$$P_Y P_{Y'} = \delta_{Y,Y'} P_Y, \quad \sum_Y P_Y = 1, \qquad P_Y = \frac{\dim V_Y}{n!} \hat{P}_Y.$$

• The dimensions of  $V_Y$  are the same for all Young tableaux corresponding to the same Young diagram.

Main result. From the above follows that  $\hat{P}_Y$  provide splitting of  $D_{reg}$  into irreps:

$$D_{reg} = \bigoplus_{\lambda} r_{\lambda} D_{\lambda},$$

where each copy of  $D_{\lambda}$  leaves invariant the subspace  $V_Y$  with Y being one of the Young diagrams corresponding to partition  $\lambda$ . Therefore the number of the irreps of  $S_n$  is the same as the number of different Young diagrams. Note that this is consistent with the fact that the number of irreps is the same as the number of conjugacy classes in  $S_n$ . The dimension of  $D_{\lambda}$  is the same as the number of times (i.e.,  $r_{\lambda}$ ) it appears in  $D_{reg}$  which in turn equals the number of Young tableaux for a given  $\lambda$ . These dimensions can be easily computed using a "hook" rule (easier to state than prove): Enter into each box of the Young diagram the number of boxes below and to the right of the box, including the box itself. Then dim  $D_{\lambda}$  for  $S_n$  is n! divided by the product of the numbers in all the boxes. For instance, if  $\lambda = (3, 1, 1)$ :

$$\begin{array}{c|c} 5 & 2 & 1 \\ \hline 2 \\ \hline 1 \end{array} \longrightarrow \qquad \dim D_{\lambda} = 5!/5 \cdot 2 \cdot 2 \cdot 1 \cdot 1 = 6$$

This result allows a construction of all irreps of  $S_n$  in a simple, systematic way.

Example: Irreps of  $S_3 \cong D_3$ .



Here the first two Young tableaux correspond to one and the same irrep of dimension 2. The second and the third one correspond to symmetric and antisymmetric irreps of the dimension 1, respectively. Note that  $1^2 + 1^2 + 2^2 = 3! = |S_3|$ , as it should be for a regular representation.

Example: Irreps of  $S_4 \cong T_d$ .



The upper tableaux correspond to the two three-dimensional representations, while the lower ones to the two two-dimensional and two one-dimensional irreps, respectively. As expected,  $1^2 + 1^2 + 2^2 + 3^2 + 3^2 = 4! = |S_4|$ .

**2.** Irreducible representations of SU(N)

FIGURE 1. Decomposition of product  $1/2 \otimes 1/2$  representation into symmetric and antisymmetric irreducible parts l = 1, l = 0 for SU(2).

Irreducible representations of SU(N) are constructed by applying Young symmetrizers  $P_Y$  to the vectors from the tensor product vector space:

$$\psi_{\sigma_1}(x_1) \otimes \psi_{\sigma_2}(x_2) \otimes \cdots \otimes \psi_{\sigma_n}(x_n).$$

Since the index  $\sigma_i$  runs here over values  $1, \ldots, N$ , the Young diagram cannot contain more the N rows (otherwise application of  $P_Y$  to the above vectors would give 0). Each diagram satisfying this condition, in turn, defines some irrep of SU(N). Its dimension is determined by the number of different ways the numbers  $1, \ldots, N$  can be placed in the boxes such that order is kept in each horizontal and vertical line. We show two examples of Young tableaux for SU(2), SU(3) in figures 1 and 2.



FIGURE 2. Tensor product of two fundamental representations SU(3) and its decomposition into irreducible representations.

### References

[1] W. Fulton and J. Harris, *Representation theory* (Springer, New York, 1991).

## LECTURE 13

# Classification of semi-simple Lie algebras

Among Lie algebras there is an important class of so-called semi-simple algebras which allows full classification. Not all Lie algebras appearing in physics are semisimple, the counterexamples include e.g., Poincaré algebra and Heisenberg algebra which contain elements (translations resp. unity operator) commuting with any other element of the group. However any algebra induced by a compact Lie group is indeed semisimple.

#### 1. Semisimple algebras

#### 1.1. Reminder. Adjoint representation. Killing form.

$$(L_i, L_j) = \operatorname{Tr}(\operatorname{Ad}(L_i)\operatorname{Ad}(L_j)) = g_{ij}$$

**1.2. Semisimple algebras.** A subalgebra I of an algebra g is called an **ideal** if it remains invariant under commutation operation:

$$[I, g] = \subset I.$$

Each ideal generates a normal subgroup of the corresponding Lie algebra G and vice-versa.

Lie algebra is called **simple** if it does not contain ideals and **semisimple** if it does not contain Abelian ideals. Any semisimple Lie algebra satisfies condition that it is non-degenerate: det  $\mathbf{g} \neq 0$ , i.e.,:

if 
$$(X, L) = 0$$
 for all  $L \in \mathbf{g} \Longrightarrow X = 0$ .

Simple algebras are building blocks of semisimple Lie algebras. Namely any semisimple algebra is a direct sum of simple Lie algebras:

$$g = g_1 \oplus g_2 \oplus \cdots \oplus g_k.$$

We will show this by using Killing form. Let I be an ideal of g. Consider its orthogonal complement P, (P, I) = 0. It is easy to see that, first P is also an ideal:

$$([P, L], I) = ([L, I], P) = 0$$
 for any  $L \implies [P, L] \in P$ ,

second  $\mathbf{g}$  is direct sum of P and I:

$$([P, I], L) = ([L, I], P) = 0$$
 for any  $L \implies [P, I] = 0$ .

If both P and I are simple then we found the decomposition, otherwise just continue the process.

# 2. Roots

#### 2.1. Weyl-Cartan basis.

2.1.1. Main properties.

$$2(\alpha,\beta)/|\alpha|^2 \in \mathbb{Z}$$
, for any  $\alpha,\beta \in \mathcal{R}$ 

If  $(\alpha, \beta) < 0$  then  $\beta + n\alpha \in \mathcal{R}$  for all  $n = 0, \dots - 2(\alpha, \beta)/|\alpha|^2$ . From this follows:

$$\sigma_{\alpha}(\beta) = \beta - \alpha \frac{2(\alpha, \beta)}{|\alpha|^2} \in \mathcal{R}$$
  
if  $(\alpha, \beta) < 0 \Longrightarrow \alpha + \beta \in \mathcal{R}$ ; if  $(\alpha, \beta) > 0 \Longrightarrow \alpha + \beta \in \mathcal{R}$ .

$$n_1 = 2(\alpha, \beta)/|\alpha|^2, \quad n_2 = 2(\alpha, \beta)/|\beta|^2, \quad n_1 n_2 \le 4.$$

Let  $\cos(\vartheta) = (\alpha, \beta)/|\alpha||\beta| = \frac{1}{2}\sqrt{n_1n_2}$ , where  $\vartheta$  is the angle between roots  $\alpha, \beta$ . Four different cases are possible:

- $n_1 = n_2 = 0, \ \theta = \pi/2$
- $n_1 = n_2 = 1, \ \theta = \pi/3, \ |\alpha| = |\beta|$
- $n_1 = 1, n_2 = 2, \theta = \pi/4, |\alpha| = \sqrt{2}|\beta|$
- $n_1 = 1, n_2 = 3, \theta = \pi/6, |\alpha| = \sqrt{3}|\beta|$



FIGURE 1. Root system for Lie algebras of rank 2.

For the algebra of rank 2 these possibilities lead to the root systems shown in figure 1.

2.1.2. Positive roots. Not all roots are independent, since they are *l*-dimensional vectors, where l is rank of the algebra. To construct an *l*-dimensional basis we introduce concept of **positive**  $\mathcal{R}_+$  and **negative**  $\mathcal{R}_-$  roots. Choose an arbitrary direction  $\vec{n}$  in the space spanned by all roots.  $\alpha \in \mathcal{R}_{\pm}$  if  $(\alpha, \vec{n}) \geq 0$  (resp.  $\leq 0$ ). The half of all roots are positive resp. negative, since both  $\pm \alpha \in \mathcal{R}$ . A simple root  $\alpha^{(i)}$  is a one which cannot be represented as sum of two other positive roots. We can immediately see that any positive root can be represented as sum over simple roots:

$$\alpha = \sum n_i \alpha^{(i)}.$$

Furthermore the number of simple roots is exactly l i,e., simple roots are independent and span the whole space. To show this first note that for two different simple roots  $\alpha^{(i)}\alpha^{(j)} \leq 0$ . If  $(\alpha^{(i)}\alpha^{(j)}) \geq 0$  then  $\alpha^{(i)} - \alpha^{(j)} \in \mathcal{R}_+$  or  $\alpha^{(j)} - \alpha^{(i)} \in \mathcal{R}_+$  and either  $\alpha^{(i)}$  can be represented as sum of two positive roots:  $(\alpha^{(i)} - \alpha^{(j)}) + \alpha^{(j)}$  or alternatively  $\alpha^{(j)}$ . This would contradict simplicity of either  $\alpha^{(i)}$  or  $\alpha^{(j)}$ . We need to show now that all  $\alpha^{(i)}$  are linearly independent. Suppose that

$$\sum c_i \alpha^{(i)} = 0.$$

#### 3. A B C D E F G CLASSIFICATION

Since all  $\alpha^{(i)}$  are positive we can divide the left side int two parts such that

$$\sum c_i \alpha^{(i)} = \sum c'_j \alpha^{(j)}$$

all coefficients are positive. From this follows:

$$(\sum c_i \alpha^{(i)})^2 = (\sum c_i \alpha^{(i)} \sum c'_j \alpha^{(j)}) = \sum c_i c'_j (\alpha^{(i)} \alpha^{(j)}) \le 0 \Rightarrow c_i = c'_j = 0.$$

Simple algebra of rank l has precisely l simple roots and

- they are linearly independent
- form a basis of  $\mathcal{R}_+$ .

# 3. A B C D E F G classification

Any semisimple Lie algebra is uniquely identified by its root system. In its own turn the root system can be described by the Cartan matrices:

$$K_{ij} = 2(\alpha^{(i)}, \alpha^{(j)}) / |\alpha^{(j)}|^2,$$

which is the matrix of scalar products between simple roots. To depict this information graphically one uses so-called **Dynkin diagrams**, where each root stands for a circle and the number of lines connecting roots  $\alpha^{(i)}, \alpha^{(j)}$  is given by  $|n_i n_j|$ ,

$$n_i = 2(\alpha^{(i)}, \alpha^{(j)})/|\alpha^{(i)}|^2, \qquad n_j = 2(\alpha^{(i)}, \alpha^{(j)})/|\alpha^{(j)}|^2.$$

In addition one puts arrow from  $\alpha^{(i)}$  to  $\alpha^{(j)}$  if the length of  $\alpha^{(j)}$  is smaller than the length of  $\alpha^{(i)}$ .

**3.1. Rank** 2 **algebras.** For algebras of rank two we have only few options for the root system. They are shown in figure 1). The corresponding Cartan matrices are given by:

 $SO(4) \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}; \quad SU(3) \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}; \quad SO(5) \begin{pmatrix} 2 & -1 \\ -2 & 2 \end{pmatrix}; \quad SO(4) \begin{pmatrix} 2 & -1 \\ -3 & 2 \end{pmatrix}$ 

and the Dynkin diagrams are shown in figure 2.



FIGURE 2. Dynkin diagrams for Lie algebras of rank 2.

**3.2. Explicit root system for** SU(N). For SU(N) the Cartan subalgebra is clearly spanned by all diagonal matrices:

$$H = \operatorname{diag} \left\{ x_1, x_2 \dots x_N \right\}, \qquad \sum_i x_i = 0.$$

The "raising-lowering" operators  $E_{ij}$  are just matrices with one non-zero element at i, j position:

$$E_{m,k}^{(a,b)} = \delta_{a,k} \delta_{b,m}, \qquad [H, E^{(a,b)}] = \underbrace{(x_a - x_b)}_{(\alpha^{(a,b)} \cdot x)} E^{(a,b)}.$$

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From this we conclude that the corresponding roots are given by N dimensional vectors:

$$\alpha^{(a,b)} = e_a - e_b, \qquad e_i = (0, \dots, 0, 1_i, 0, \dots, 0).$$

The scalar product between roots is 1 if roots have non-zero element at the same position and zero otherwise. Furthermore, N - 1 simple roots are given by:

$$\alpha^{(i)} = \alpha^{(i,i+1)}, \qquad i = 1, \dots N - 1.$$

It is straightforward to see that:

$$(\alpha^{(i)}\alpha^{(i+1)}) = -1, \qquad (\alpha^{(i)}\alpha^{(j)}) = 0, \qquad |i-j| \neq 0, 1,$$

implying that the Cartan matrix is:

$$K = \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & \dots & -1 & 2 \end{pmatrix}.$$

The corresponding Dynkin diagram  $A_{N-1}$  is shown in figure 3). Note that the same Lie algebra appears for non-compact groups: SU(p,q), SL(N) (all matrices with determinant one).

3.2.1. Other infinite series. Other infinite series  $B_l$ ,  $C_l D_l$  of simple Lie algebras come from the orthogonal and symplectic groups SO(2N + 1), Sp(2N), SO(2N).



FIGURE 3. Dynkin diagrams for simple Lie algebras. Regular series shown on the left. Exceptional on the right.

3.2.2. Exceptional algebras. The severe constraints on the possible angles between simple roots imply that there are only few options to construct a valid root system beyond four infinite series. This geometrical rigidity allows full classification of simple Lie algebras. The proof can be separated into few main steps.

• A) Dynkin diagram cannot contain any loop, i.e., it must be a tree.

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To prove this assume that such a loop consisting of V vertices exists and let  $e_1, e_2 \dots e_V$  be normalized roots forming this loop. By considering the following inequality:

$$|\sum_{i=1}^{n} \mathbf{e}_i|^2 \ge 0 \quad \Longrightarrow \quad k > -\sum_{i < j} 2(\mathbf{e}_i \mathbf{e}_j) > L,$$

where L is a number of bonds we come to the contradiction with an obvious fact that in the loops V = L.

• B) The number of lines emanating from any vertex is maximum 3.

# 4. REPRESENTATION

Suppose  $e_1, \ldots e_l$  are joined to  $e_{l+1}$ . By (A) all  $e_1, \ldots e_l$  are orthonormal to each other. Extend this basis by another orthogonal vector  $\tilde{e}_{l+1}$ . Then

$$\mathsf{e}_{l+1} = \sum_{i=1}^{\iota} (\mathsf{e}_i \mathsf{e}_{l+1}) \mathsf{e}_i + (\tilde{\mathsf{e}}_{l+1} \mathsf{e}_{l+1}) \tilde{\mathsf{e}}_{l+1} \Longrightarrow \sum (\mathsf{e}_i \mathsf{e}_{l+1})^2 = 1 - (\tilde{\mathsf{e}}_{l+1} \mathsf{e}_{l+1})^2 < 1.$$

But the left hand side of the last expression is the number of links divided by 4.

- C) By constructing a one-line bond from any admissible diagram one obtains another admissible diagram.
- D) If 3 bonds are connected to a vertex then the lengthes of their "legs" satisfy:

$$\frac{1}{p+1} + \frac{1}{q+1} + \frac{1}{r+1} > 1.$$

Under assumption  $p \ge q \ge r$  from the last inequality it follows that the only solutions are:

$$p = 2, q = 2, r = 1,$$
  $p = 3, q = 2, r = 1$   $p = 4, q = 2, r = 1,$ 

which correspond to  $E_6, E_7, E_8$ . Finally the inspection of "linear" diagrams gives one additional root system  $F_4$ .

**Remark:** It is actually a non-trivial problem to reconstruct the corresponding Lie algebra for each of the above root systems.

# 4. Representation

The representations of simple Lie algebras are constructed by introducing the set of fundamental weights and considering reciprocal lattice:

$$2(\lambda^{(i)}\alpha^{(j)})/|\alpha^{(j)}|^2 = \delta_{ij}, \qquad \Lambda = \{\sum_i n_i \lambda^{(i)} | n_i \in \mathbb{Z}\}.$$

Any representation  $D_{\lambda} = D(m_1, m_2, \dots, m_l)$  is uniquely determined by the highest weight  $\lambda = \sum_i m_i \lambda^{(i)}$ . The dimension of the representation is given by:

$$\dim D_{\lambda} = \frac{\prod_{\alpha \in \mathcal{R}_{+}} (\alpha, \lambda + \overline{\lambda})}{\prod_{\alpha \in \mathcal{R}_{+}} (\alpha, \overline{\lambda})}, \qquad \overline{\lambda} = \frac{1}{2} \sum_{\alpha \in \mathcal{R}_{+}} \alpha.$$

# LECTURE 14

# Infinite dimensional symmetries. String theory.

TBA