Lecture 21 — 11/20

c) (Discrete) Group Theory in AMO and in General

Questions related to symmetry that come up in AMO:

→ What are the possible single- and multi-particle states?

→ What degeneracies exist?

→ What couplings or selection rules are there?

Quantum Mechanics + Group Theory

What symmetries leave H invariant?

↳ Group of these symmetry operations → "group of the Schrödinger equation"

↳ The group can be represented in terms of matrices → "representations"

↳ These matrices act on the eigenstates / basis functions

↳ Dimension of degenerate eigenspaces = dimension of "irreducible representations"

Definitions

A group is a set $G = \{g_i\}$ with the following rules:

1) $g_i, g_j \in G \rightarrow g_i \cdot g_j \in G$, where $g_i \cdot g_j$ denotes the "product" or "addition" of the two elements

   ↳ for symmetry operations, $g_i \cdot g_j$ means that first g_j is applied, then g_i

2) $(g_i \cdot g_j) \cdot g_k = g_i \cdot (g_j \cdot g_k)$ → associative law

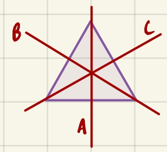
3) $\exists\, e \in G$ s.t. $g_i \cdot e = e \cdot g_i = g_i \quad \forall g_i \in G$ → existence of a unity element

4) $\exists\, g_i^{-1} \in G$ s.t. $g_i^{-1} \cdot g_i = g_i \cdot g_i^{-1} = e$

5) If $g_i \cdot g_j = g_j \cdot g_i \quad \forall\, g_i, g_j \in G$, then G is called "Abelian"

A subgroup S is a subset of G such that S is itself a group

Example: rotation & reflection symmetry of an equilateral triangle



E: do nothing
A, B, C: reflect about axis
D: rotate cw by $2\pi/3$ (120°)
F: rotate ccw by $2\pi/3$

→ $A^{-1} = A$, ..., $D^{-1} = F$, $F^{-1} = D$

Group multiplication table:

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

row · column

Representations

Let $\Gamma(g_i)$ be the (matrix) representation of $g_i \in G$

$$g_i \cdot g_j = g_k \rightarrow \Gamma(g_i)\cdot\Gamma(g_j) = \Gamma(g_k)$$

$$\Gamma(e) = \mathbb{1}$$ ← specifically when · is multiplication

We define the similarity transformation for any S as:

$$\Gamma'(g_i) = S^{-1}\Gamma(g_i)S$$

$$\Gamma'(g_i)\cdot\Gamma'(g_j) = \Gamma'(g_i\cdot g_j)$$

Γ is reducible if $\exists S$ s.t. for $\Gamma'(g_i) = S^{-1}\Gamma(g_i)S \;\forall g_i \in G$, Γ' is a "block matrix" with more than one block

$$\Gamma'_{red} = \begin{bmatrix} [\Gamma^{(1)}] & 0 \\ 0 & [\Gamma^{(2)}] \end{bmatrix}$$

Any Γ with $\det\Gamma \neq 0$ is similar to a unitary Γ.

Irreducible representations obey an orthogonality relation:

$$\sum_{g\in G} \Gamma^{(i)}(g)^*_{\mu\nu}\,\Gamma^{(j)}(g)_{\alpha\beta} = \frac{h}{l_i}\,\delta_{ij}\,\delta_{\mu\alpha}\,\delta_{\nu\beta}$$

↳ h: order of group G (number of group elements) — $h=6$ for the equilateral triangle!

↳ l_i: dimension of $\Gamma^{(i)}$

Dimensionality Theorem: $\sum_{i \in \text{irr. reps}} l_i^2 = h$

Classes

- → g_i and g_j are called "conjugate" if $g g_i g^{-1} = g_j$ for some $g \in G$
- → The set of all group elements conjugate to g_i = "class" of g_i
- → For an Abelian group, all elements are in their own class

$$g g_i g^{-1} = g g^{-1} g_i = e g_i = g_i$$

Equilatoral triangle example – non-Abelian, with 3 classes:

$C_1 = E, \quad C_2 = A, B, C, \quad C_3 = D, F$

Characters

The "character" is defined as: $\chi^{(i)}(g) = \text{Tr}\,\Gamma^{(i)}(g)$
for any representation $\Gamma^{(i)}$.

↳ invariant under similarity transformations:

$$\text{Tr}(S^{-1}\Gamma^{(i)}(g)S) = \text{Tr}(SS^{-1}\Gamma^{(i)}(g)) = \text{Tr}(\Gamma^{(i)}(g))$$

↳ all elements in a class have the same character.

The orthogonality relation in terms of characters:

$$\underbrace{\sum_{g \in G}}_{\text{sum over group elements}} \chi^{(i)}(g)^* \chi^{(i)}(g) = \underbrace{\sum_{k \in \text{classes}}}_{\text{sum over classes}} \chi^{(i)}(C_k)^* \chi^{(j)}(C_k) \underbrace{N_k}_{\substack{\text{size of} \\ \text{class } C_k}} = h\delta_{ij}$$

From this, we have: # irr. reps. = # classes ← so we know there are 3 irr. rep. for the Δ!

We can use this to help reduce representations Γ into their irreducible parts:

$$\Gamma = \sum a_i \Gamma^{(i)}$$

→ not exactly a sum; forms a larger block diagonal representation

$$\sum_{k \in \text{classes}} \chi^{(i)}(C_k)^* \, \chi(C_k) N_k$$

$$= \sum_k \chi^{(i)}(C_k)^* \sum_j a_j \, Tr(\Gamma^{(j)}) \; N_k$$

$$= h \, \delta_{ij}$$

$$\rightarrow \quad a_i = \frac{1}{h} \sum_{k \in \text{classes}} \chi^{(i)}(C_k)^* \, \chi(C_k) N_k$$

Often, the characters $\chi^{(i)}(C_k)$ are displayed in a "character table."

- rows: different irr. rep. $\Gamma^{(i)}$
- columns: different classes C_k
- entries: $\chi^{(i)} C_k$
- rows are orthogonal when weighted by N_k
- columns are orthogonal

For the triangle:

	C_1	$3C_2$	$2C_3$
$\Gamma^{(1)}$	1	1	1
$\Gamma^{(2)}$	1	-1	1
$\Gamma^{(3)}$	2	0	-1