Introduction to Group Theory

With Applications to Quantum Mechanics and Solid State Physics

Roland Winkler

rwinkler@niu.edu

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Please, let me know if you find misprints, errors or inaccuracies in these notes.
Thank you.

General Literature

- J. F. Cornwell, *Group Theory in Physics* (Academic, 1987)
  general introduction; discrete and continuous groups
- W. Ludwig and C. Falter, *Symmetries in Physics* (Springer, Berlin, 1988).
  general introduction; discrete and continuous groups
- W.-K. Tung, *Group Theory in Physics* (World Scientific, 1985).
  general introduction; main focus on continuous groups
- L. M. Falicov, *Group Theory and Its Physical Applications* (University of Chicago Press, Chicago, 1966).
  small paperback; compact introduction
- E. P. Wigner, *Group Theory* (Academic, 1959).
  classical textbook by the master
- Landau and Lifshitz, *Quantum Mechanics*, Ch. XII (Pergamon, 1977)
  brief introduction into the main aspects of group theory in physics
- R. McWeeny, *Symmetry* (Dover, 2002)
  elementary, self-contained introduction
- and many others

Specialized Literature

- G. L. Bir und G. E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors* (Wiley, New York, 1974)
  thorough discussion of group theory and its applications in solid state physics by two pioneers
- C. J. Bradley and A. P. Cracknell, *The Mathematical Theory of Symmetry in Solids* (Clarendon, 1972)
  comprehensive discussion of group theory in solid state physics
- G. F. Koster et al., *Properties of the Thirty-Two Point Groups* (MIT Press, 1963)
  small, but very helpful reference book tabulating the properties of the 32 crystallographic point groups (character tables, Clebsch-Gordan coefficients, compatibility relations, etc.)
- A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, 1960)
  comprehensive discussion of the (group) theory of angular momentum in quantum mechanics
- and many others

These notes are dedicated to

Prof. Dr. h.c. Ulrich Rössler

from whom I learned group theory

R.W.

Introduction and Overview

Definition: Group

A set $\mathcal{G} = \{a, b, c, \ldots\}$ is called a group, if there exists a group multiplication connecting the elements in $\mathcal{G}$ in the following way

(1)	$a, b \in \mathcal{G}: \quad c = a\,b \in \mathcal{G}$	(closure)
(2)	$a, b, c \in \mathcal{G}: \quad (ab)c = a(bc)$	(associativity)
(3)	$\exists\, e \in \mathcal{G}: \quad a\,e = a \quad \forall a \in \mathcal{G}$	(identity / neutral element)
(4)	$\forall a \in \mathcal{G} \quad \exists\, b \in \mathcal{G}: \quad a\,b = e, \quad \text{i.e., } b \equiv a^{-1}$	(inverse element)

Corollaries

(a)	$e^{-1} = e$	
(b)	$a^{-1}a = a\,a^{-1} = e \quad \forall a \in \mathcal{G}$	(left inverse = right inverse)
(c)	$e\,a = a\,e = a \quad \forall a \in \mathcal{G}$	(left neutral = right neutral)
(d)	$\forall a, b \in \mathcal{G}: \quad c = a\,b \;\Leftrightarrow\; c^{-1} = b^{-1}a^{-1}$	

Commutative (Abelian) Group

(5)	$\forall a, b \in \mathcal{G}: \quad a\,b = b\,a$	(commutatitivity)

Order of a Group = number of group elements

Examples

- integer numbers $\mathbb{Z}$ with addition
  (Abelian group, infinite order)
- rational numbers $\mathbb{Q}\backslash\{0\}$ with multiplication
  (Abelian group, infinite order)
- complex numbers $\{\exp(2\pi i\, m/n) : \; m = 1, \ldots, n\}$ with multiplication
  (Abelian group, finite order, example of *cyclic group*)
- invertible ($=$ nonsingular) $n \times n$ matrices with matrix multiplication
  (nonabelian group, infinite order, later important for representation theory!)
- permutations of n objects: $\mathcal{P}_n$
  (nonabelian group, $n!$ group elements)
- symmetry operations (rotations, reflections, etc.) of equilateral triangle
  $\equiv \mathcal{P}_3 \equiv$ permutations of numbered corners of triangle – more later!
- (continuous) translations in $\mathbb{R}^n$: (continuous) translation group
  $\equiv$ vector addition in $\mathbb{R}^n$
- symmetry operations of a sphere
  only rotations: $SO(3)$ $=$ special orthogonal group in $\mathbb{R}^3$
  $=$ real orthogonal 3×3 matrices

Group Theory in Physics

Group theory is the natural language to describe *symmetries* of a physical system

- symmetries correspond to conserved quantities
- symmetries allow us to classify quantum mechanical states
  - representation theory
  - degeneracies / level splittings
- evaluation of matrix elements $\Rightarrow$ Wigner-Eckart theorem
  e.g., selection rules: dipole matrix elements for optical transitions
- Hamiltonian $\hat{H}$ must be *invariant* under the symmetries of a quantum system

  $\Rightarrow$ construct $\hat{H}$ via symmetry arguments
- ...

Classical Mechanics

- Lagrange function $L(\mathbf{q}, \dot{\mathbf{q}})$,
- Lagrange equations $\displaystyle \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i} \qquad i = 1, \ldots, N$
- If for one j : $\displaystyle \frac{\partial L}{\partial q_j} = 0 \;\Rightarrow\; p_j \equiv \frac{\partial L}{\partial \dot{q}_j}$ is a conserved quantity

Examples

- q_j linear coordinate
  - translational invariance
  - linear momentum $p_j = \text{const.}$
  - translation group
- q_j angular coordinate
  - rotational invariance
  - angular momentum $p_j = \text{const.}$
  - rotation group

Quantum Mechanics

(1) Evaluation of matrix elements

- Consider particle in potential $V(x) = V(-x)$ even
- two possiblities for eigenfunctions $\psi(x)$

  $\psi_e(x)$ even: $\quad \psi_e(x) = \psi_e(-x)$

  $\psi_o(x)$ odd: $\quad \psi_o(x) = -\psi_o(-x)$

- overlapp $\quad \int \psi_i^*(x)\, \psi_j(x)\, \mathrm{d}x = \delta_{ij} \qquad i, j \in \{e, o\}$
- expectation value $\quad \langle i|x|i\rangle = \int \psi_i^*(x)\, x\, \psi_i(x)\, \mathrm{d}x = 0$

well-known explanation

- product of two even / two odd functions is even
- product of one even and one odd function is odd
- integral over an odd function vanishes

Quantum Mechanics

(1) Evaluation of matrix elements (cont'd)

Group theory provides systematic generalization of these statements

- representation theory
  $\equiv$ classification of how functions and operators transform under symmetry operations
- Wigner-Eckart theorem
  $\equiv$ statements on matrix elements if we know how the functions and operators transform under the symmetries of a system

Quantum Mechanics

(2) Degeneracies of Energy Eigenvalues

- Schrödinger equation $\hat{H}\psi = E\psi$ or $i\hbar\partial_t\psi = \hat{H}\psi$
- Let $\hat{O}$ with $i\hbar\partial_t\hat{O} = [\hat{O}, \hat{H}] = 0 \quad \Rightarrow$ $\hat{O}$ is conserved quantity

$\Rightarrow$ eigenvalue equations $\hat{H}\psi = E\psi$ and $\hat{O}\psi = \lambda_{\hat{O}}\,\psi$ can be solved simultaneously

$\Rightarrow$ eigenvalue $\lambda_{\hat{O}}$ of $\hat{O}$ is good quantum number for ψ

Example: H atom

- $\hat{H} = \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2mr^2} - \frac{e^2}{r} \quad \Rightarrow$ group $SO(3)$

$\Rightarrow$ $[\hat{L}^2, \hat{H}] = [\hat{L}_z, \hat{H}] = [\hat{L}^2, \hat{L}_z] = 0$

$\Rightarrow$ eigenstates $\psi_{nlm}(\mathbf{r})$: index $l \leftrightarrow \hat{L}^2$, $m \leftrightarrow \hat{L}_z$

- really another example for representation theory
- degeneracy for $0 \leq l \leq n-1$: dynamical symmetry (unique for H atom)

Quantum Mechanics

(3) Solid State Physics

in particular: crystalline solids, periodic assembly of atoms

$\Rightarrow$ discrete translation invariance

(i) Electrons in periodic potential $V(\mathbf{r})$

- $V(\mathbf{r}+\mathbf{R}) = V(\mathbf{r}) \quad \forall\, \mathbf{R} \in \{\text{lattice vectors}\}$

$\Rightarrow$ translation operator $\hat{T}_\mathbf{R}$:

$$\hat{T}_\mathbf{R}\, f(\mathbf{r}) = f(\mathbf{r}+\mathbf{R})$$

$$[\hat{T}_\mathbf{R}, \hat{H}] = 0$$

$\Rightarrow$ Bloch theorem $\psi_\mathbf{k}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\, u_\mathbf{k}(\mathbf{r})$ with $u_\mathbf{k}(\mathbf{r}+\mathbf{R}) = u_\mathbf{k}(\mathbf{r})$

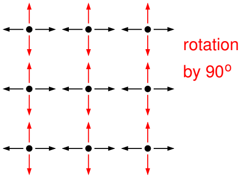
$\Rightarrow$ wave vector $\mathbf{k}$ is quantum number for the discrete translation invariance, $\mathbf{k} \in$ first Brillouin zone

Quantum Mechanics

(3) Solid State Physics

(ii) Phonons

- Consider square lattice



- frequencies of modes are equal
- degeneracies for particular propagation directions

(iii) Theory of Invariants

- How can we construct models for the dynamics of electrons or phonons that are compatible with given crystal symmetries?

Quantum Mechanics

(4) Nuclear and Particle Physics

Physics at small length scales: strong interaction

$$\left.\begin{array}{ll}\text{Proton} & m_p = 938.28\ \text{MeV} \\ \text{Neutron} & m_n = 939.57\ \text{MeV}\end{array}\right\} \quad \begin{array}{l}\text{rest mass of nucleons almost equal} \\ \sim \text{degeneracy}\end{array}$$

- Symmetry: isospin $\hat{I}$ with $[\hat{I}, \hat{H}_{\text{strong}}] = 0$
- SU(2): proton $|\frac{1}{2}\ \frac{1}{2}\rangle$, neutron $|\frac{1}{2}\ -\frac{1}{2}\rangle$

Mathematical Excursion: Groups

Basic Concepts

Group Axioms: see above

Definition: Subgroup Let $\mathcal{G}$ be a group. A subset $\mathcal{U} \subseteq \mathcal{G}$ that is itself a group with the same multiplication as $\mathcal{G}$ is called a subgroup of $\mathcal{G}$.

Group Multiplication Table: compilation of all products of group elements
$\Rightarrow$ complete information on mathematical structure of a (finite) group

Example: permutation group $\mathcal{P}_3$

$$e = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix} \quad a = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \quad b = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}$$

$$c = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} \quad d = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} \quad f = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}$$

$\mathcal{P}_3$	e	a	b	c	d	f
e	e	a	b	c	d	f
a	a	b	e	f	c	d
b	b	e	a	d	f	c
c	c	d	f	e	a	b
d	d	f	c	b	e	a
f	f	c	d	a	b	e

- $\{e\}$, $\{e, a, b\}$, $\{e, c\}$, $\{e, d\}$, $\{e, f\}$, $\mathcal{G}$ are subgroups of $\mathcal{G}$

Conclusions from Group Multiplication Table

$\mathcal{P}_3$	e	a	b	c	d	f
e	e	a	b	c	d	f
a	a	b	e	f	c	d
b	b	e	a	d	f	c
c	c	d	f	e	a	b
d	d	f	c	b	e	a
f	f	c	d	a	b	e

- Symmetry w.r.t. main diagonal
  $\Rightarrow$ group is Abelian
- order n of $g \in \mathcal{G}$: smallest $n > 0$ with $g^n = e$
- $\{g, g^2, \ldots, g^n = e\}$ with $g \in \mathcal{G}$ is Abelian subgroup (a cyclic group)
- in every row / column every element appears exactly once because:

  Rearrangement Lemma: for any fixed $g' \in \mathcal{G}$, we have

  $$\mathcal{G} = \{g'g : g \in \mathcal{G}\} = \{gg' : g \in \mathcal{G}\}$$

  i.e., the latter sets consist of the elements in $\mathcal{G}$ rearranged in order.

  proof: $g_1 \neq g_2 \;\Leftrightarrow\; g'g_1 \neq g'g_2 \quad \forall g_1, g_2, g' \in \mathcal{G}$

Goal: Classify elements in a group

(1) Conjugate Elements and Classes

- Let $a \in \mathcal{G}$. Then $b \in \mathcal{G}$ is called conjugate to a if $\exists\, x \in \mathcal{G}$ with $b = xax^{-1}$.

  Conjugation $b \sim a$ is equivalence relation:

  - $a \sim a$ — reflexive
  - $b \sim a \quad \Leftrightarrow \quad a \sim b$ — symmetric
  - $\left.\begin{array}{l} a \sim c \\ b \sim c \end{array}\right\} \Rightarrow a \sim b$ — transitive

    $a = xcx^{-1} \quad \Rightarrow \quad c = x^{-1}ax$

    $b = ycy^{-1} = (xy^{-1})^{-1}a(xy^{-1})$

- For fixed a, the set of all conjugate elements $\mathcal{C} = \{xax^{-1} : x \in \mathcal{G}\}$ is called a class.

  - identity e is its own class $\quad xex^{-1} = e \quad \forall x \in \mathcal{G}$
  - Abelian groups: each element is its own class

    $xax^{-1} = axx^{-1} = a \quad \forall a, x \in \mathcal{G}$
  - Each $b \in \mathcal{G}$ belongs to one and only one class

    $\Rightarrow$ decompose $\mathcal{G}$ into classes
  - in broad terms: "similar" elements form a class

Example: $\mathcal{P}_3$

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

$\Rightarrow$ classes $\{e\}$, $\{a, b\}$, $\{c, d, f\}$

(2) Subgroups and Cosets

- Let $\mathcal{U} \subset \mathcal{G}$ be a subgroup of $\mathcal{G}$ and $x \in \mathcal{G}$. The set $x\mathcal{U} \equiv \{xu : u \in \mathcal{U}\}$ (the set $\mathcal{U}x$) is called the left coset (right coset) of $\mathcal{U}$.
- In general, cosets are not groups.
  If $x \notin \mathcal{U}$, the coset $x\mathcal{U}$ lacks the identity element:
  suppose $\exists u \in \mathcal{U}$ with $xu = e \in x\mathcal{U} \;\Rightarrow\; x^{-1} = u \in \mathcal{U} \;\Rightarrow\; x = u^{-1} \in \mathcal{U}$ ↯
- If $x' \in x\mathcal{U}$, then $x'\mathcal{U} = x\mathcal{U}$ *any* $x' \in x\mathcal{U}$ can be used to define coset $x\mathcal{U}$
- If $\mathcal{U}$ contains s elements, then each coset also contains s elements (due to rearrangement lemma).
- Two left (right) cosets for a subgroup $\mathcal{U}$ are either equal or disjoint (due to rearrangement lemma).
- Thus: decompose $\mathcal{G}$ into cosets
  $\mathcal{G} = \mathcal{U} \cup x\mathcal{U} \cup y\mathcal{U} \cup \ldots \quad x, y, \ldots \notin \mathcal{U}$
- Thus Theorem 1: $\left.\begin{array}{l}\text{Let } h \text{ order of } \mathcal{G} \\ \text{Let } s \text{ order of } \mathcal{U} \subset \mathcal{G}\end{array}\right\} \Rightarrow \dfrac{h}{s} \in \mathbb{N}$
- Corollary: The order of a finite group is an integer multiple of the orders of its subgroups.
- Corollary: If h prime number $\Rightarrow$ $\{e\}, \mathcal{G}$ are the only subgroups
  $\Rightarrow$ $\mathcal{G}$ is isomorphic to cyclic group

(3) Invariant Subgroups and Factor Groups

connection: classes and cosets

- A subgroup $\mathcal{U} \subset \mathcal{G}$ containing only complete classes of $\mathcal{G}$ is called invariant subgroup (aka normal subgroup).
- Let $\mathcal{U}$ be an invariant subgroup of $\mathcal{G}$ and $x \in \mathcal{G}$
  $\Leftrightarrow \quad x\mathcal{U}x^{-1} = \mathcal{U}$
  $\Leftrightarrow \quad x\mathcal{U} = \mathcal{U}x$ (left coset = right coset)
- Multiplication of cosets of an invariant subgroup $\mathcal{U} \subset \mathcal{G}$:

  $x, y \in \mathcal{G}: \quad (x\mathcal{U})(y\mathcal{U}) = xy\mathcal{U} = z\mathcal{U} \qquad \text{where} \quad z = xy$

  well-defined: $(x\mathcal{U})(y\mathcal{U}) = x(\mathcal{U}y)\mathcal{U} = xy\mathcal{U}\mathcal{U} = z\mathcal{U}\mathcal{U} = z\mathcal{U}$
- An invariant subgroup $\mathcal{U} \subset \mathcal{G}$ and the distinct cosets $x\mathcal{U}$ form a group, called factor group $\mathcal{F} = \mathcal{G}/\mathcal{U}$
  - group multiplication: see above
  - $\mathcal{U}$ is identity element of factor group
  - $x^{-1}\mathcal{U}$ is inverse for $x\mathcal{U}$
- Every factor group $\mathcal{F} = \mathcal{G}/\mathcal{U}$ is homomorphic to $\mathcal{G}$ (see below).

Example: Permutation Group $\mathcal{P}_3$

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

invariant subgroup $\mathcal{U} = \{e, a, b\}$

$\Rightarrow$ one coset $c\mathcal{U} = d\mathcal{U} = f\mathcal{U} = \{c, d, f\}$

factor group $\mathcal{P}_3/\mathcal{U} = \{\mathcal{U}, c\mathcal{U}\}$

	$\mathcal{U}$	$c\mathcal{U}$
$\mathcal{U}$	$\mathcal{U}$	$c\mathcal{U}$
$c\mathcal{U}$	$c\mathcal{U}$	$\mathcal{U}$

- We can think of factor groups $\mathcal{G}/\mathcal{U}$ as coarse-grained versions of $\mathcal{G}$.
- Often, factor groups $\mathcal{G}/\mathcal{U}$ are a helpful intermediate step when working out the structure of more complicated groups $\mathcal{G}$.
- Thus: invariant subgroups are "more useful" subgroups than other subgroups.

Mappings of Groups

- Let $\mathcal{G}$ and $\mathcal{G}'$ be two groups. A mapping $\phi : \mathcal{G} \to \mathcal{G}'$ assigns to each $g \in \mathcal{G}$ an element $g' = \phi(g) \in \mathcal{G}'$, with every $g' \in \mathcal{G}'$ being the image of at least one $g \in \mathcal{G}$.

- If $\phi(g_1)\,\phi(g_2) = \phi(g_1\,g_2) \quad \forall g_1, g_2 \in \mathcal{G}$,
  then ϕ is a homomorphic mapping of $\mathcal{G}$ on $\mathcal{G}'$.
    - A homomorphic mapping is *consistent* with the group structures
    - A homomorphic mapping $\mathcal{G} \to \mathcal{G}'$ is always n-to-one ($n \geq 1$):
      The preimage of the unit element of $\mathcal{G}'$ is an invariant subgroup $\mathcal{U}$ of $\mathcal{G}$.
      $\mathcal{G}'$ is isomorphic to the factor group $\mathcal{G}/\mathcal{U}$.

- If the mapping ϕ is one-to-one, then it is an isomorphic mapping of $\mathcal{G}$ on $\mathcal{G}'$.
    - Short-hand: $\mathcal{G}$ isomorphic to $\mathcal{G}' \Rightarrow \mathcal{G} \simeq \mathcal{G}'$
    - Isomorphic groups have the *same* group structure.

- Examples:
    - trivial homomorphism $\quad \mathcal{G} = \mathcal{P}_3$ and $\mathcal{G}' = \{e\}$
    - isomorphism between permutation group $\mathcal{P}_3$ and symmetry group C_{3v} of equilateral triangle

Products of Groups

- Given two groups $\mathcal{G}_1 = \{a_i\}$ and $\mathcal{G}_2 = \{b_k\}$, their outer direct product is the group $\mathcal{G}_1 \times \mathcal{G}_2$ with elements (a_i, b_k) and multiplication
$$(a_i, b_k) \cdot (a_j, b_l) = (a_i a_j, b_k b_l) \in \mathcal{G}_1 \times \mathcal{G}_2$$
  - Check that the group axioms are satisfied for $\mathcal{G}_1 \times \mathcal{G}_2$.
  - Order of $\mathcal{G}_n$ is h_n $(n = 1, 2)$ $\Rightarrow$ order of $\mathcal{G}_1 \times \mathcal{G}_2$ is $h_1 h_2$
  - If $\mathcal{G} = \mathcal{G}_1 \times \mathcal{G}_2$, then both $\mathcal{G}_1$ and $\mathcal{G}_2$ are invariant subgroups of $\mathcal{G}$. Then we have isomorphisms $\mathcal{G}_2 \simeq \mathcal{G}/\mathcal{G}_1$ and $\mathcal{G}_1 \simeq \mathcal{G}/\mathcal{G}_2$.
  - Application: built more complex groups out of simpler groups

- If $\mathcal{G}_1 = \mathcal{G}_2 = \mathcal{G} = \{a_i\}$, the elements
$$(a_i, a_i) \in \mathcal{G} \otimes \mathcal{G}$$
define a group $\tilde{\mathcal{G}} \equiv \mathcal{G} \otimes \mathcal{G}$ called the inner product of $\mathcal{G}$.
  - The inner product $\mathcal{G} \otimes \mathcal{G}$ is isomorphic to $\mathcal{G}$ ($\Rightarrow$ same order as $\mathcal{G}$)
  - Compare: product representations (discussed below)

Matrix Representations of a Group

Motivation

- Consider symmetry group $\mathcal{C}_i = \{e, i\}$ $e =$ identity, $i =$ inversion

$\mathcal{C}_i$	e	i
e	e	i
i	i	e

- two "types" of basis functions: even and odd
- more abstract: reducible and irreducible representations

matrix representation (based on 1×1 and 2×2 matrices)

$$\left.\begin{array}{lcl} \Gamma_1 & = & \{\mathcal{D}_e = 1,\ \mathcal{D}_i = 1\} \\ \Gamma_2 & = & \{\mathcal{D}_e = 1,\ \mathcal{D}_i = -1\} \\ \Gamma_3 & = & \left\{\mathcal{D}_e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \mathcal{D}_i = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\} \end{array}\right\} \text{consistent with group multiplication table}$$

where Γ_1 : even function $f_e(x) = f_e(-x)$
Γ_2 : odd functions $f_o(x) = -f_o(-x)$
} irreducible representations

Γ_3 : reducible representation:
decompose any $f(x)$ into even and odd parts

$$f(x) = f_e(x) + f_o(x) \quad \text{with} \begin{cases} f_e(x) = \frac{1}{2}\left[f(x) + f(-x)\right] \\ f_o(x) = \frac{1}{2}\left[f(x) - f(-x)\right] \end{cases}$$

How to generalize these ideas for arbitrary groups?

Matrix Representations of a Group

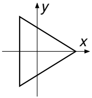
- Let group $\mathcal{G} = \{g_i : i = 1, \ldots, h\}$
- Associate with each $g_i \in \mathcal{G}$ a nonsingular square matrix $\mathcal{D}(g_i)$.
  If the resulting set $\{\mathcal{D}(g_i) : i = 1, \ldots, h\}$ is homomorphic to $\mathcal{G}$ it is called a matrix representation of $\mathcal{G}$.
  - $g_i \, g_j = g_k \Rightarrow \; \mathcal{D}(g_i) \, \mathcal{D}(g_j) = \mathcal{D}(g_k)$
  - $\mathcal{D}(e) = \mathbb{1}$ (identity matrix)
  - $\mathcal{D}(g_i^{-1}) = \mathcal{D}^{-1}(g_i)$
- dimension of representation = dimension of representation matrices

Example (1): $\mathcal{G} = C_\infty$ = rotations around a fixed axis (angle ϕ)

- C_∞ is isomorphic to group of orthogonal 2×2 matrices $SO(2)$
  $\mathcal{D}_2(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}$ $\Rightarrow$ two-dimensional (2D) representation
- C_∞ is homomorphic to group $\{\mathcal{D}_1(\phi) = 1\}$ $\Rightarrow$ trivial 1D representation
- C_∞ is isomorphic to group $\left\{ \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathcal{D}_2(\phi) \end{pmatrix} \right\}$ $\Rightarrow$ higher-dimensional representation
- Generally: given matrix representations of dimensions n_1 and n_2, we can construct $(n_1 + n_2)$ dimensional representations

Matrix Representations of a Group (cont'd)

Example (2): Symmetry group C_{3v} of equilateral triangle (isomorphic to permutation group $\mathcal{P}_3$)



	identity	rotation $\phi = 120°$	rotation $\phi = 240°$	reflection $y \leftrightarrow -y$	roto-reflection $\phi = 120°$	roto-reflection $\phi = 240°$
$\mathcal{P}_3$	e	a	$b = a^2$	$c = ec$	$d = ac$	$f = bc$
Koster	E	C_3	C_3^2	σ_v	σ_v	σ_v
Γ_1	(1)	(1)	(1)	(1)	(1)	(1)
Γ_2	(1)	(1)	(1)	(-1)	(-1)	(-1)
Γ_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$

multiplication table

$\mathcal{P}_3$	e	a	b	c	d	f
e	e	a	b	c	d	f
a	a	b	e	f	c	d
b	b	e	a	d	f	c
c	c	d	f	e	a	b
d	d	f	c	b	e	a
f	f	c	d	a	b	e

- mapping $\mathcal{G} \to \{\mathcal{D}(g_i)\}$ homomorphic, but in general not isomorphic (not faithful)
- *consistent* with group multiplication table
- Goal: characterize matrix representations of $\mathcal{G}$
- Will see: $\mathcal{G}$ fully characterized by its "distinct" matrix representations (only three for $\mathcal{G} = C_{3v}$!)

Goal: Identify and Classify Representations

- **Theorem 2:** If $\mathcal{U}$ is an invariant subgroup of $\mathcal{G}$, then every representation of the factor group $\mathcal{F} = \mathcal{G}/\mathcal{U}$ is likewise a representation of $\mathcal{G}$.

  Proof: $\mathcal{G}$ is homomorphic to $\mathcal{F}$, which is homomorphic to the representations of $\mathcal{F}$.

  Thus: To identify the representations of $\mathcal{G}$ it helps to identify the representations of $\mathcal{F}$.

- **Definition: Equivalent Representations**

  Let $\{\mathcal{D}(g_i)\}$ be a matrix representation for $\mathcal{G}$ with dimension n.
  Let X be a n-dimensional nonsingular matrix.

  The set $\{\mathcal{D}'(g_i) = X\,\mathcal{D}(g_i)\,X^{-1}\}$ forms a matrix representation called equivalent to $\{\mathcal{D}(g_i)\}$.

  Convince yourself: $\{\mathcal{D}'(g_i)\}$ is, indeed, another matrix representation.

Matrix representations are most convenient if matrices $\{\mathcal{D}\}$ are unitary. Thus

- **Theorem 3:** Every matrix representation $\{\mathcal{D}(g_i)\}$ is equivalent to a unitary representation $\{\mathcal{D}'(g_i)\}$ where $\mathcal{D}'^{\,\dagger}(g_i) = \mathcal{D}'^{\,-1}(g_i)$

- In the following, it is always assumed that matrix representations are unitary.

Proof of Theorem 3 (cf. Falicov)

Challenge: Matrix X has to be choosen such that it makes *all* matrices $\mathcal{D}'(g_i)$ unitary *simultaneously*.

- Let $\{\mathcal{D}(g_i) \equiv \mathcal{D}_i : i = 1, \ldots, h\}$ be a matrix representation for $\mathcal{G}$ (dimension h).
- Define $H = \sum_{i=1}^{h} \mathcal{D}_i \mathcal{D}_i^\dagger$ (Hermitean)
- Thus H can be diagonalized by means of a unitary matrix U.

$$\begin{aligned} d \;&\equiv\; U^{-1} H U = \sum_i U^{-1} \mathcal{D}_i \, \mathcal{D}_i^{-1} U = \sum_i \underbrace{U^{-1} \mathcal{D}_i \, U}_{=\tilde{\mathcal{D}}_i} \; \underbrace{U^{-1} \mathcal{D}_i^{-1} U}_{=\tilde{\mathcal{D}}_i^\dagger} \\ &= \sum_i \tilde{\mathcal{D}}_i \tilde{\mathcal{D}}_i^\dagger \quad \text{with } d_{\mu\nu} = d_\mu \delta_{\mu\nu} \text{ diagonal} \end{aligned}$$

- Diagonal entries d_μ are positive:

$$d_\mu = \sum_i \sum_\lambda (\tilde{\mathcal{D}}_i)_{\mu\lambda} (\tilde{\mathcal{D}}_i^\dagger)_{\lambda\mu} = \sum_{i\lambda} (\tilde{\mathcal{D}}_i)_{\mu\lambda} (\tilde{\mathcal{D}}_i^*)_{\mu\lambda} = \sum_{i\lambda} |(\tilde{\mathcal{D}}_i)_{\mu\lambda}|^2 > 0$$

- Take diagonal matrix $\tilde{d}_\pm$ with elements $(\tilde{d}_\pm)_{\mu\nu} \equiv d_\mu^{\pm 1/2} \, \delta_{\mu\nu}$
- Thus $\mathbb{1} = \tilde{d}_- \, d \, \tilde{d}_- = \tilde{d}_- \sum_i \tilde{\mathcal{D}}_i \tilde{\mathcal{D}}_i^\dagger \, \tilde{d}_-$ (identity matrix)

Proof of Theorem 3 (cont'd)

- Assertion: $\mathcal{D}'_i = \tilde{d}_- \, \tilde{D}_i \, \tilde{d}_+ = \tilde{d}_- \, U^{-1} \, \mathcal{D}_i \, U \, \tilde{d}_+$ are unitary matrices equivalent to $\mathcal{D}_i$
  - equivalent by construction: $X = \tilde{d}_- \, U^{-1}$
  - unitarity:

$$
\begin{aligned}
\mathcal{D}'_i \, \mathcal{D}'^{\dagger}_i &= \tilde{d}_- \tilde{\mathcal{D}}_i \tilde{d}_+ \overbrace{\left(\tilde{d}_- \sum_k \tilde{\mathcal{D}}_k \tilde{\mathcal{D}}_k^\dagger \, \tilde{d}_-\right)}^{=\mathbb{1}} \tilde{d}_+ \tilde{\mathcal{D}}_i^\dagger \tilde{d}_- \\
&= \tilde{d}_- \underbrace{\sum_k \underbrace{\tilde{\mathcal{D}}_i \, \tilde{\mathcal{D}}_k}_{=\tilde{\mathcal{D}}_j} \, \underbrace{\tilde{\mathcal{D}}_k^\dagger \, \tilde{\mathcal{D}}_i^\dagger}_{=\tilde{\mathcal{D}}_j^\dagger}}_{=d} \, \tilde{d}_- \qquad \text{(rearrangement lemma)} \\
&= \mathbb{1}
\end{aligned}
$$

qed

Reducible and Irreducible Representations
(RRs and IRs)

- If for a given representation $\{\mathcal{D}(g_i) : i = 1, \ldots, h\}$, an equivalent representation $\{\mathcal{D}'(g_i) : i = 1, \ldots, h\}$ can be found that is block diagonal

$$\mathcal{D}'(g_i) = \begin{pmatrix} \mathcal{D}'_1(g_i) & 0 \\ 0 & \mathcal{D}'_2(g_i) \end{pmatrix} \qquad \forall g_i \in \mathcal{G}$$

  then $\{\mathcal{D}(g_i) : i = 1, \ldots, h\}$ is called reducible, otherwise irreducible.

- Crucial: the same block diagonal form is obtained for all representation matrices $\mathcal{D}(g_i)$ simultaneously.

- Block-diagonal matrices do not mix, i.e., if $\mathcal{D}'(g_1)$ and $\mathcal{D}'(g_2)$ are block diagonal, then $\mathcal{D}'(g_3) = \mathcal{D}'(g_1)\,\mathcal{D}'(g_2)$ is likewise block diagonal.

  $\Rightarrow$ Decomposition of RRs into IRs decomposes the problem into the smallest subproblems possible.

- **Goal of Representation Theory**

  Identify and characterize the IRs of a group.

- **We will show**

  The number of inequivalent IRs equals the number of classes.

Schur's First Lemma

Schur's First Lemma: Suppose a matrix M commutes with all matrices $\mathcal{D}(g_i)$ of an *irreducible* representation of $\mathcal{G}$

$$\mathcal{D}(g_i)\, M = M\, \mathcal{D}(g_i) \qquad \forall g_i \in \mathcal{G} \tag{$\spadesuit$}$$

then M is a multiple of the identity matrix $M = c\mathbb{1}, \quad c \in \mathbb{C}$.

Corollaries

- If ($\spadesuit$) holds with $M \neq c\mathbb{1}$, $c \in \mathbb{C}$, then $\{\mathcal{D}(g_i)\}$ is reducible.
- All IRs of Abelian groups are one-dimensional

  Proof: Take $g_j \in \mathcal{G}$ arbitrary, but fixed.
  $\mathcal{G}$ Abelian $\;\Rightarrow\; \mathcal{D}(g_i)\,\mathcal{D}(g_j) = \mathcal{D}(g_j)\,\mathcal{D}(g_i) \quad \forall g_i \in \mathcal{G}$
  Lemma $\;\Rightarrow\; \mathcal{D}(g_j) = c_j \mathbb{1}$ with $c_j \in \mathbb{C}$, i.e., $\{\mathcal{D}(g_j) = c_j\}$ is an IR.

Proof of Schur's First Lemma (cf. Bir & Pikus)

- Take Hermitean conjugate of (♠): $M^\dagger\,\mathcal{D}^\dagger(g_i) = \mathcal{D}^\dagger(g_i)\,M^\dagger$
  Multiply with $\mathcal{D}^\dagger(g_i) = \mathcal{D}^{-1}(g_i)$: $\mathcal{D}(g_i)\,M^\dagger = M^\dagger\,\mathcal{D}(g_i)$
- Thus: (♠) holds for M and $M^\dagger$, and also the Hermitean matrices
  $$M' = \tfrac{1}{2}(M + M^\dagger) \qquad M'' = \tfrac{i}{2}(M - M^\dagger)$$
- It exists a unitary matrix U that diagonalizes M' (similar for M'')
  $$d = U^{-1}\,M'\,U \quad \text{with} \quad d_{\mu\nu} = d_\mu \delta_{\mu\nu}$$
- Thus (♠) implies $\mathcal{D}'(g_i)\,d = d\,\mathcal{D}'(g_i)$, where $\mathcal{D}'(g_i) = U^{-1}\,\mathcal{D}(g_i)\,U$
  more explicitly: $\mathcal{D}'_{\mu\nu}(g_i)\,(d_\mu - d_\nu) = 0 \quad \forall i, \mu, \nu$

Proof of Schur's First Lemma (cont'd)

Two possibilities:

- All d_μ are equal, i.e, $d = c\mathbb{1}$.

  So $M' = UdU^{-1}$ and M'' are likewise proportional to $\mathbb{1}$, and so is $M = M' - iM''$.

- Some d_μ are different:

  Say $\{d_\kappa : \kappa = 1, \ldots, r\}$ are different from $\{d_\lambda : \lambda = r+1, \ldots, h\}$.

  Thus: $\mathcal{D}'_{\kappa\lambda}(g_i) = 0 \quad \begin{array}{l} \forall\kappa = 1, \ldots, r; \\ \forall\lambda = r+1, \ldots, h \end{array}$

  Thus $\{\mathcal{D}'(g_i) : i = 1, \ldots, h\}$ is block-diagonal, contrary to the assumption that $\{\mathcal{D}(g_i)\}$ is irreducible qed

Schur's Second Lemma

Schur's Second Lemma: Suppose we have two IRs $\{\mathcal{D}_1(g_i), \text{dimension } n_1\}$ and $\{\mathcal{D}_2(g_i), \text{dimension } n_2\}$, as well as a $n_1 \times n_2$ matrix M such that

$$\mathcal{D}_1(g_i)\, M = M\, \mathcal{D}_2(g_i) \qquad \forall g_i \in \mathcal{G} \qquad (\clubsuit)$$

(1) If $\{\mathcal{D}_1(g_i)\}$ and $\{\mathcal{D}_2(g_i)\}$ are inequivalent, then $M = 0$.

(2) If $M \neq 0$ then $\{\mathcal{D}_1(g_i)\}$ and $\{\mathcal{D}_2(g_i)\}$ are equivalent.

Proof of Schur's Second Lemma (cf. Bir & Pikus)

- Take Hermitean conjugate of (♣); use $\mathcal{D}^\dagger(g_i) = \mathcal{D}^{-1}(g_i) = \mathcal{D}(g_i^{-1})$, so
$$M^\dagger \mathcal{D}_1(g_i^{-1}) = \mathcal{D}_2(g_i^{-1}) M^\dagger$$
- Multiply by M on the left; Eq. (♣) implies $M\,\mathcal{D}_2(g_i^{-1}) = \mathcal{D}_1(g_i^{-1})\,M$, so
$$MM^\dagger \mathcal{D}_1(g_i^{-1}) = \mathcal{D}_1(g_i^{-1}) MM^\dagger \qquad \forall g_i^{-1} \in \mathcal{G}$$
- Schur's first lemma implies that $MM^\dagger$ is square matrix with
$$MM^\dagger = c\mathbb{1} \qquad \text{with } c \in \mathbb{C} \qquad (*)$$
- Case a: $n_1 = n_2$
  - If $c \neq 0$ then $\det M \neq 0$ because of (*), i.e., M is invertible. So (♣) implies
$$M^{-1}\,\mathcal{D}_1(g_i)\,M = \mathcal{D}_2(g_i) \qquad \forall g_i \in \mathcal{G}$$
  thus $\{\mathcal{D}_1(g_i)\}$ and $\{\mathcal{D}_2(g_i)\}$ are equivalent.
  - If $c = 0$ then $MM^\dagger = 0$, i.e.,
$$\sum_\nu M_{\mu\nu} M^\dagger_{\nu\mu} = \sum_\nu M_{\mu\nu} M^*_{\mu\nu} = \sum_\nu |M_{\mu\nu}|^2 = 0 \qquad \forall \mu$$
  so that $M = 0$.

Proof of Schur's Second Lemma (cont'd)

- Case b: $n_1 \neq n_2$ $\quad$ ($n_1 < n_2$ to be specific)
  - Fill up M with $n_2 - n_1$ rows to get matrix $\tilde{M}$ with $\det \tilde{M} = 0$.
  - However $\tilde{M}\tilde{M}^\dagger = MM^\dagger$, so that
$$\det(MM^\dagger) = \det(\tilde{M}\tilde{M}^\dagger) = (\det \tilde{M})\,(\det \tilde{M}^\dagger) = 0$$
  - So $c = 0$, i.e., $MM^\dagger = 0$, and as before $M = 0$.

qed

Orthogonality Relations for IRs

Notation:

- Irreducible Representations (IR): $\Gamma_I = \{\mathcal{D}_I(g_i) : g_i \in \mathcal{G}\}$
- n_I = dimensionality of IR Γ_I
- h = order of group $\mathcal{G}$

Theorem 4: Orthogonality Relations for Irreducible Representations

(1) two inequivalent IRs $\Gamma_I \neq \Gamma_J$

$$\sum_{i=1}^{h} \mathcal{D}_I(g_i)^*_{\mu'\nu'}\, \mathcal{D}_J(g_i)_{\mu\nu} = 0 \qquad \begin{array}{l} \forall\ \mu', \nu' = 1, \ldots, n_I \\ \forall\ \mu, \nu = 1, \ldots, n_J \end{array}$$

(2) representation matrices of one IR Γ_I

$$\frac{n_I}{h} \sum_{i=1}^{h} \mathcal{D}_I(g_i)^*_{\mu'\nu'}\, \mathcal{D}_I(g_i)_{\mu\nu} = \delta_{\mu'\mu}\, \delta_{\nu'\nu} \qquad \forall\ \mu', \nu', \mu, \nu = 1, \ldots, n_I$$

Remarks

- $[\mathcal{D}_I(g_i)_{\mu\nu} : i = 1, \ldots, h]$ form vectors in a h-dim. vector space
- vectors are normalized to $\sqrt{h/n_I}$ (because Γ_I assumed to be unitary)
- vectors for different $I, \mu\nu$ are orthogonal
- in total, we have $\sum_I n_I^2$ such vectors; therefore $\sum_I n_I^2 \leq h$

Corollary: For finite groups the number of inequivalent IRs is finite.

Proof of Theorem 4: Orthogonality Relations for IRs

(1) two inequivalent IRs $\Gamma_I \neq \Gamma_J$

- Take arbitrary $n_J \times n_I$ matrix $X \neq 0$ (i.e., at least one $X_{\mu\nu} \neq 0$)
- Let $M \equiv \sum_i \mathcal{D}_J(g_i)\, X\, \mathcal{D}_I(g_i^{-1})$

$$\Rightarrow \quad \mathcal{D}_J(g_k)\, M = \sum_i \underbrace{\mathcal{D}_J(g_k)\overbrace{\mathcal{D}_J(g_i)}}\; \overbrace{X\; \underbrace{\mathcal{D}_I(g_i^{-1})}^{=M} \underbrace{\overbrace{\mathcal{D}_I^{-1}(g_k)}\, \mathcal{D}_I(g_k)}^{=\mathbb{1}}}$$

$$= \sum_i \quad \mathcal{D}_J(\underbrace{g_k\, g_i}_{=g_j}) \quad X \quad \mathcal{D}_I^{-1}(\underbrace{g_k\, g_i}_{=g_j}) \quad \mathcal{D}_I(g_k)$$

$$= \underbrace{\sum_j \mathcal{D}_J(g_j)\, X\, \mathcal{D}_I(g_j^{-1})}\; \mathcal{D}_I(g_k)$$

$$= \qquad M \qquad \mathcal{D}_I(g_k)$$

$\Rightarrow$ (Schur's Second Lemma)

$$0 = M_{\mu\mu'} \qquad \forall \mu, \mu'$$

$$= \sum_i \sum_{\kappa,\lambda} \mathcal{D}_J(g_i)_{\mu\kappa}\, X_{\kappa\lambda}\, \mathcal{D}_I(g_i^{-1})_{\lambda\mu'}$$

in particular correct for $X_{\kappa\lambda} = \delta_{\nu\kappa}\, \delta_{\lambda\nu'}$

$$= \sum_i \mathcal{D}_J(g_i)_{\mu\nu}\, \mathcal{D}_I(g_i^{-1})_{\nu'\mu'}$$

$$= \sum_i \mathcal{D}_I(g_i)^*_{\mu'\nu'}\, \mathcal{D}_J(g_i)_{\mu\nu}$$

qed

Proof of Theorem 4: Orthogonality Relations for IRs (cont'd)

(2) representation matrices of one IR Γ_I

First steps similar to case (1):

- Let $M \equiv \sum_i \mathcal{D}_I(g_i)\, X\, \mathcal{D}_I(g_i^{-1})$ with $n_I \times n_I$ matrix $X \neq 0$

$\Rightarrow$ $\mathcal{D}_I(g_k)\, M = M\, \mathcal{D}_I(g_k)$

$\Rightarrow$ (Schur's First Lemma): $M = c\,\mathbb{1}, \quad c \in \mathbb{C}$

- Thus $$c\,\delta_{\mu\mu'} = \sum_i \sum_{\kappa,\lambda} \mathcal{D}_I(g_i)_{\mu\kappa}\, X_{\kappa\lambda}\, \mathcal{D}_I(g_i^{-1})_{\lambda\mu'} \qquad \text{choose } X_{\kappa\lambda} = \delta_{\nu\kappa}\,\delta_{\lambda\nu'}$$ $$= \sum_i \mathcal{D}_I(g_i)_{\mu\nu}\, \mathcal{D}_I(g_i^{-1})_{\nu'\mu'} = M_{\mu\mu'}$$

- $$c = \frac{1}{n_I}\sum_\mu M_{\mu\mu} = \frac{1}{n_I}\sum_i \underbrace{\sum_\mu \mathcal{D}_I(g_i)_{\mu\nu}\, \mathcal{D}_I(g_i^{-1})_{\nu'\mu}}_{\mathcal{D}_I(g_i^{-1}g_i = e)_{\nu'\nu} = \delta_{\nu\nu'}} = \frac{h}{n_I}\delta_{\nu\nu'} \qquad \text{qed}$$

Characters

- The traces of the representation matrices are called characters

  $$\chi(g_i) \equiv \operatorname{tr} \mathcal{D}(g_i) = \sum_i \mathcal{D}(g_i)_{\mu\mu}$$

- Equivalent IRs are related via a similarity transformation

  $$\mathcal{D}'(g_i) = X\, \mathcal{D}(g_i) X^{-1} \qquad \text{with } X \text{ nonsingular}$$

  This transformation leaves the trace invariant: $\operatorname{tr} \mathcal{D}'(g_i) = \operatorname{tr} \mathcal{D}(g_i)$

  $\Rightarrow$ Equivalent representations have the same characters.

- **Theorem 5:** If $g_i, g_j \in \mathcal{G}$ belong to the same class $\mathcal{C}_k$ of $\mathcal{G}$, then for every representation Γ_I of $\mathcal{G}$ we have $\chi_I(g_i) = \chi_I(g_j)$

  Proof:
  - $g_i, g_j \in \mathcal{C} \;\Rightarrow\; \exists\, x \in \mathcal{G}$ with $g_i = x\, g_j\, x^{-1}$
  - Thus $\mathcal{D}_I(g_i) = \mathcal{D}_I(x)\, \mathcal{D}_I(g_j)\, \mathcal{D}_I(x^{-1})$
  - $$\begin{aligned} \chi_I(g_i) &= \operatorname{tr}\left[\mathcal{D}_I(x)\, \mathcal{D}_I(g_j)\, \mathcal{D}_I(x^{-1})\right] \\ &= \operatorname{tr}\left[\underbrace{\mathcal{D}_I(x^{-1})\, \mathcal{D}_I(x)}_{=\mathbb{1}}\, \mathcal{D}_I(g_j)\right] = \chi_I(g_k) \end{aligned}$$

    (trace invariant under cyclic permutation)

Characters (cont'd)

Notation

- $\chi_I(\mathcal{C}_k)$ denotes the character of group elements in class $\mathcal{C}_k$
- The array $[\chi_I(\mathcal{C}_k)]$ with $I = 1, \ldots, N$ $\quad$ (N = number of IRs)
  $k = 1, \ldots, \tilde{N}$ $\quad$ ($\tilde{N}$ = number of classes)
  is called character table.

Remark: For Abelian groups the character table is the table of the 1×1 representation matrices

Theorem 6: Orthogonality relations for characters

Let $\{\mathcal{D}_I(g_i)\}$ and $\{\mathcal{D}_J(g_i)\}$ be two IRs of $\mathcal{G}$. Let h_k be the number of elements in class $\mathcal{C}_k$ and $\tilde{N}$ the number of classes. Then

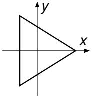
$$\sum_{k=1}^{\tilde{N}} \frac{h_k}{h} \chi_I^*(\mathcal{C}_k)\, \chi_J(\mathcal{C}_k) = \delta_{IJ} \qquad \forall\; I, J = 1, \ldots, N$$

Proof: Use orthogonality relation for IRs

- **Interpretation:** rows $[\chi_I(\mathcal{C}_k) : k = 1, \ldots \tilde{N}]$ of character table are like N orthonormal vectors in a $\tilde{N}$-dimensional vector space $\Rightarrow\; N \leq \tilde{N}$.
- If two IRs Γ_I and Γ_J have the same characters, this is necessary and sufficient for Γ_I and Γ_J to be equivalent.

Example: Symmetry group C_{3v} of equilateral triangle

(isomorphic to permutation group $\mathcal{P}_3$)

	identity	rotation $\phi = 120^\circ$	rotation $\phi = 240^\circ$	reflection $y \leftrightarrow -y$	roto-reflection $\phi = 120^\circ$	roto-reflection $\phi = 240^\circ$
$\mathcal{P}_3$	e	a	$b = a^2$	$c = ec$	$d = ac$	$f = bc$
Koster	E	C_3	C_3^2	σ_v	σ_v	σ_v
Γ_1	(1)	(1)	(1)	(1)	(1)	(1)
Γ_2	(1)	(1)	(1)	(-1)	(-1)	(-1)
Γ_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$

multiplication table

$\mathcal{P}_3$	e	a	b	c	d	f
e	e	a	b	c	d	f
a	a	b	e	f	c	d
b	b	e	a	d	f	c
c	c	d	f	e	a	b
d	d	f	c	b	e	a
f	f	c	d	a	b	e

Character table

$\mathcal{P}_3$	e	a, b	c, d, f
C_{3v}	E	$2C_3$	$3\sigma_v$
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	-1	0

Interpretation: Character Tables

- A character table is the uniquely defined signature of a group and its IRs Γ_I [independent of, e.g., phase conventions for representation matrices $\mathcal{D}_I(g_i)$ that are quite arbitrary].
- Isomorphic groups have the same character tables.
- Yet: the labeling of IRs Γ_I is a matter of convention. – Customary:
  - $\Gamma_1 =$ identity representation: all characters are 1
  - IRs are often numbered such that low-dimensional IRs come first; higher-dimensional IRs come later
  - If $\mathcal{G}$ contains the inversion, a superscript $\pm$ is added to Γ_I indicating the behavior of $\Gamma_I^\pm$ under inversion (even or odd)
  - other labeling schemes are inspired by compatibility relations (more later)
- Different authors use different conventions to label IRs. To compare such notations we need to compare the uniquely defined characters for each class of an IR.

  (See, e.g., Table 2.7 in Yu and Cardona: Fundamentals of Semiconductors; here we follow Koster *et al.*)

Decomposing Reducible Representations (RRs) Into Irreducible Representations (IRs)

Given an arbitrary RR $\{\mathcal{D}(g_i)\}$ the representation matrices $\{\mathcal{D}(g_i)\}$ can be brought into block-diagonal form by a suitable unitary transformation

$$\mathcal{D}(g_i) \quad \rightarrow \quad \mathcal{D}'(g_i) = \begin{pmatrix} \mathcal{D}_1(g_i) & & & & & \mathbf{0} \\ & \ddots & & & & \\ & & \mathcal{D}_1(g_i) & & & \\ & & & \ddots & & \\ & & & & \mathcal{D}_N(g_i) & \\ \mathbf{0} & & & & \ddots & \\ & & & & & \mathcal{D}_N(g_i) \end{pmatrix} \begin{matrix} \left.\vphantom{\begin{matrix}a\\b\\c\end{matrix}}\right\} a_1 \text{ times} \\ \vdots \\ \left.\vphantom{\begin{matrix}a\\b\\c\end{matrix}}\right\} a_N \text{ times} \end{matrix}$$

Theorem 7: Let a_I be the multiplicity, with which the IR $\Gamma_I \equiv \{\mathcal{D}_I(g_i)\}$ is contained in the representation $\{\mathcal{D}(g_i)\}$. Then

(1) $\chi(g_i) = \sum_{I=1}^{N} a_I \, \chi_I(g_i)$

(2) $a_I \;=\; \frac{1}{h} \sum_{i=1}^{h} \chi_I^*(g_i) \, \chi(g_i) \;=\; \sum_{k=1}^{\tilde{N}} \frac{h_k}{h} \, \chi_I^*(\mathcal{C}_k) \, \chi(\mathcal{C}_k)$

We say: $\{\mathcal{D}(g_i)\}$ contains the IR Γ_I a_I times.

Proof: Theorem 7

(1) due to invariance of trace under similarity transformations

(2) we have $\displaystyle\sum_{J=1}^{N} a_J\,\chi_J(g_i) = \chi(g_i) \qquad \Big|\; \frac{1}{h}\sum_{i=1}^{h} \chi_I^*(g_i)\times$

$$\Rightarrow \sum_{J=1}^{N} a_J \underbrace{\frac{1}{h}\sum_{i=1}^{h} \chi_I^*(g_i)\,\chi_J(g_i)}_{=\delta_{IJ}} = \frac{1}{h}\sum_{i=1}^{h} \chi_I^*(g_i)\,\chi(g_i) \qquad \text{qed}$$

Applications of Theorem 7:

- **Corollary:** The representation $\{\mathcal{D}(g_i)\}$ is irreducible if and only if

$$\sum_{i=1}^{h} |\chi(g_i)|^2 = h$$

Proof: Use Theorem 7 with $a_I = \begin{cases} 1 & \text{for one } I \\ 0 & \text{otherwise} \end{cases}$

- **Decomposition of Product Representations** (see later)

Where Are We?

We have discussed the orthogonality relations for

- irreducible representations
- characters

These can be complemented by matching completeness relations.

Proving those is a bit more cumbersome. It requires the introduction of the regular representation.

The Regular Representation

Finding the IRs of a group can be tricky. Yet for finite groups we can derive the *regular representation* which contains all IRs of the group.

- Interpret group elements g_ν as basis vectors $\{|g_\nu\rangle : \nu = 1, \dots h\}$ for a h-dim. representation

$\Rightarrow$ Regular representation:
νth column vector of $\mathcal{D}_R(g_i)$ gives image $|g_\mu\rangle = g_i|g_\nu\rangle \equiv |g_i g_\nu\rangle$ of basis vector $|g_\nu\rangle$

$$\Rightarrow \quad \mathcal{D}_R(g_i)_{\mu\nu} = \begin{cases} 1 & \text{if } g_\mu g_\nu^{-1} = g_i \\ 0 & \text{otherwise} \end{cases}$$

- **Strategy:**
  - Re-arrange the group multiplication table as shown on the right
  - For each $g_i \in \mathcal{G}$ we have $\mathcal{D}_R(g_i)_{\mu\nu} = 1$, if the entry (μ, ν) in the re-arranged group multiplication table equals g_i, otherwise $\mathcal{D}_R(g_i)_{\mu\nu} = 0$.

	g_1^{-1}	g_2^{-1}	g_3^{-1}	$\dots$
g_1	e		$\dots$	
g_2		e		
g_3	$\vdots$		e	
$\vdots$				e

Properties of the Regular Representation $\{\mathcal{D}_R(g_i)\}$

(1) $\{\mathcal{D}_R(g_i)\}$ is, indeed, a representation for the group $\mathcal{G}$

(2) It is a *faithful* representation, i.e., $\{\mathcal{D}_R(g_i)\}$ is isomorphic to $\mathcal{G} = \{g_i\}$.

(3) $\chi_R(g_i) = \begin{cases} h & \text{if } g_i = e \\ 0 & \text{otherwise} \end{cases}$

Proof:

(1) Matrices $\{\mathcal{D}_R(g_i)\}$ are nonsingular, as every row / every column contains "1" exactly once.

Show: if $g_i g_j = g_k$, then $\mathcal{D}_R(g_i)\mathcal{D}_R(g_j) = \mathcal{D}_R(g_k)$

Take i, j, μ, ν arbitrary, but fixed

$$\begin{cases} \mathcal{D}_R(g_i)_{\mu\lambda} = 1 & \text{only for} \quad g_\mu\, g_\lambda^{-1} = g_i \quad \Leftrightarrow \quad g_\lambda = g_i^{-1}\, g_\mu \\ \mathcal{D}_R(g_j)_{\lambda\nu} = 1 & \text{only for} \quad g_\lambda\, g_\nu^{-1} = g_j \quad \Leftrightarrow \quad g_\lambda = g_j\, g_\nu \end{cases}$$

$$\Leftrightarrow \quad \sum_\lambda \mathcal{D}_R(g_i)_{\mu\lambda}\, \mathcal{D}_R(g_j)_{\lambda\nu} = 1 \quad \text{only for } g_i^{-1}\, g_\mu = g_j\, g_\nu$$

$$\Leftrightarrow \quad g_\mu\, g_\nu^{-1} = g_i\, g_j = g_k \qquad [\text{definition of } \mathcal{D}_R(g_k)_{\mu\nu}]$$

(2) immediate consequence of definition of $\mathcal{D}_R(g_i)$

(3) $\mathcal{D}_R(g_i)_{\mu\mu} = \begin{cases} 1 & \text{if } g_i = g_\mu\, g_\mu^{-1} = e \\ 0 & \text{otherwise} \end{cases}$

$$\Rightarrow \quad \chi_R(g_i) = \sum_\mu \mathcal{D}_R(g_i)_{\mu\mu} = \begin{cases} h & \text{if } g_i = e \\ 0 & \text{otherwise} \end{cases}$$

Example: Regular Representation for $\mathcal{P}_3$

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

$\Rightarrow$

g^{-1}	e	b	a	c	d	f
e	e	b	a	c	d	f
a	a	e	b	f	c	d
b	b	a	e	d	f	c
c	c	f	d	e	a	b
d	d	c	f	b	e	a
f	f	d	c	a	b	e

Thus

$$e = \begin{pmatrix} 1 & 0 & 0 & & & \\ 0 & 1 & 0 & & & \\ 0 & 0 & 1 & & & \\ & & & 1 & 0 & 0 \\ & & & 0 & 1 & 0 \\ & & & 0 & 0 & 1 \end{pmatrix} \quad a = \begin{pmatrix} 0 & 0 & 1 & & & \\ 1 & 0 & 0 & & & \\ 0 & 1 & 0 & & & \\ & & & 0 & 1 & 0 \\ & & & 0 & 0 & 1 \\ & & & 1 & 0 & 0 \end{pmatrix} \quad b = \begin{pmatrix} 0 & 1 & 0 & & & \\ 0 & 0 & 1 & & & \\ 1 & 0 & 0 & & & \\ & & & 0 & 0 & 1 \\ & & & 1 & 0 & 0 \\ & & & 0 & 1 & 0 \end{pmatrix}$$

$$c = \begin{pmatrix} & & & 1 & 0 & 0 \\ & & & 0 & 1 & 0 \\ & & & 0 & 0 & 1 \\ 1 & 0 & 0 & & & \\ 0 & 1 & 0 & & & \\ 0 & 0 & 1 & & & \end{pmatrix} \quad d = \begin{pmatrix} & & & 0 & 1 & 0 \\ & & & 0 & 0 & 1 \\ & & & 1 & 0 & 0 \\ 0 & 0 & 1 & & & \\ 1 & 0 & 0 & & & \\ 0 & 1 & 0 & & & \end{pmatrix} \quad f = \begin{pmatrix} & & & 0 & 0 & 1 \\ & & & 1 & 0 & 0 \\ & & & 0 & 1 & 0 \\ 0 & 1 & 0 & & & \\ 0 & 0 & 1 & & & \\ 1 & 0 & 0 & & & \end{pmatrix}$$

Completeness of Irreducible Representations

Lemma: The regular representation contains every IR n_I times, where n_I = dimensionality of IR Γ_I.

Proof: Use Theorem 7: $\chi_R(g_i) = \sum_i a_I \, \chi_I(g_i)$ where

$$a_I = \tfrac{1}{h} \sum_i \chi_I^*(g_i) \, \chi_R(g_i) = \tfrac{1}{h} \underbrace{\chi_I^*(e)}_{=n_I} \underbrace{\chi_R(e)}_{=h} = n_I$$

Corollary (Burnside's Theorem): For a group $\mathcal{G}$ of order h, the dimensionalities n_I of the IRs Γ_I obey

$$\sum_I n_I^2 = h$$

Proof: $h = \chi_R(e) = \sum_I a_I \, \chi_I(e) = \sum_I n_I^2$
serious constraint for dimensionalities of IRs

Theorem 8: The representation matrices $\mathcal{D}_I(g_i)$ of a group $\mathcal{G}$ of order h obey the completeness relation

$$\sum_I \sum_{\mu,\nu} \frac{n_I}{h} \, \mathcal{D}_I^*(g_i)_{\mu\nu} \, \mathcal{D}_I(g_j)_{\mu\nu} = \delta_{ij} \qquad \forall \, i,j = 1, \ldots, h \qquad (*)$$

Proof:

- Theorem 4: Interpret $[\mathcal{D}_I(g_i)_{\mu\nu} : i = 1, \ldots, h]$ as orthonormal row vectors of a matrix $\mathcal{M}$
- Corollary: $\mathcal{M}$ has h columns

$\Big\}$ $\Rightarrow$ $\mathcal{M}$ is square matrix: unitary
$\Rightarrow$ column vectors also orthonormal
= completeness (*)

Completeness Relation for Characters

Theorem 9: Completeness Relation for Characters

If $\chi_I(\mathcal{C}_k)$ is the character for class $\mathcal{C}_k$ and irreducible representation I, then

$$\frac{h_k}{h} \sum_I \chi_I^*(\mathcal{C}_k)\chi_I(\mathcal{C}_{k'}) = \delta_{kk'} \qquad \forall\, k, k' = 1, \ldots, \tilde{N}$$

- **Interpretation:** columns $\begin{pmatrix} \chi_1(\mathcal{C}_k) \\ \vdots \\ \chi_N(\mathcal{C}_k) \end{pmatrix}$ of character table $[k = 1, \ldots, \tilde{N}]$

  are like $\tilde{N}$ orthonormal vectors in a N-dimensional vector space

- Thus $\tilde{N} \leq N$. (from completeness)
- Also $N \leq \tilde{N}$ (from orthogonality)

Number N of irreducible representations

$=$ Number $\tilde{N}$ of classes

- **Character table**
  - square table
  - rows and column form orthogonal vectors

Proof of Theorem 9: Completeness Relation for Characters

Lemma: Let $\{\mathcal{D}_I(g_i)\}$ be an n_I-dimensional IR of $\mathcal{G}$. Let $\mathcal{C}_k$ be a class of $\mathcal{G}$ with h_k elements. Then

$$\sum_{i \in \mathcal{C}_k} \mathcal{D}_I(g_i) = \frac{h_k}{n_I} \chi_I(\mathcal{C}_k) \, \mathbb{1}$$

The sum over all representation matrices in a class of an IR is proportional to the identity matrix.

Proof of Lemma:

- For arbitrary $g_j \in \mathcal{G}$

$$\mathcal{D}_I(g_j) \left[\sum_{i \in \mathcal{C}_k} \mathcal{D}_I(g_i) \right] \mathcal{D}_I(g_j^{-1}) = \sum_{i \in \mathcal{C}_k} \underbrace{\mathcal{D}_I(g_j)\, \mathcal{D}_I(g_i)\, \mathcal{D}_I(g_j^{-1})}_{= \mathcal{D}_I(g_{i'}) \text{ with } i' \in \mathcal{C}_k} \underset{\uparrow}{=} \sum_{i' \in \mathcal{C}_k} \mathcal{D}_I(g_{i'})$$

because g_j maps $g_{i_1} \neq g_{i_2}$ onto $g_{i'_1} \neq g_{i'_2}$

$\Rightarrow$ (Schur's First Lemma): $\sum_{i \in \mathcal{C}_k} \mathcal{D}_I(g_i) = c_k \, \mathbb{1}$

- $c_k = \dfrac{1}{n_I} \operatorname{tr} \left[\sum_{i \in \mathcal{C}_k} \mathcal{D}_I(g_i) \right] = \dfrac{h_k}{n_I} \chi_I(\mathcal{C}_k)$ qed

Proof of Theorem 9: Completeness Relation for Characters

- Use Theorem 8 (Completeness Relations for Irreducible Representations)

$$\sum_{l=1}^{N} \sum_{\mu,\nu} \frac{n_l}{h} \mathcal{D}_l^*(g_i)_{\mu\nu} \, \mathcal{D}_l(g_j)_{\mu\nu} = \delta_{ij} \qquad \Big| \sum_{i \in \mathcal{C}_k} \sum_{j \in \mathcal{C}_{k'}}$$

$$\Rightarrow \sum_{l} \frac{n_l}{h} \sum_{\mu,\nu} \underbrace{\underbrace{\Big[\sum_{i \in \mathcal{C}_k} \mathcal{D}_l^*(g_i)\Big]_{\mu\nu}}_{\frac{h_k}{n_l}\chi_l^*(\mathcal{C}_k)\,\delta_{\mu\nu}} \underbrace{\Big[\sum_{j \in \mathcal{C}_{k'}} \mathcal{D}_l(g_j)\Big]_{\mu\nu}}_{\frac{h_{k'}}{n_l}\chi_l(\mathcal{C}_{k'})\,\delta_{\mu\nu}}}_{\frac{h_k\, h_{k'}}{n_l^2}\chi_l^*(\mathcal{C}_k)\;\chi_l(\mathcal{C}_{k'})\;\underbrace{\sum_{\mu,\nu}\delta_{\mu\nu}}_{=n_l}} = h_k \delta_{kk'}$$

(Lemma)

qed

Summary: Orthogonality and Completeness Relations

Theorem 4: Orthogonality Relations for Irreducible Representations

$$\frac{n_I}{h} \sum_{i=1}^{h} \mathcal{D}_I(g_i)^*_{\mu'\nu'}\, \mathcal{D}_J(g_i)_{\mu\nu} = \delta_{IJ}\, \delta_{\mu\mu'}\, \delta_{\nu\nu'} \qquad \begin{aligned} I, J &= 1, \ldots, N \\ \mu', \nu' &= 1, \ldots, n_I \\ \mu, \nu &= 1, \ldots, n_J \end{aligned}$$

Theorem 8: Completeness Relations for Irreducible Representations

$$\sum_{I=1}^{N} \sum_{\mu,\nu} \frac{n_I}{h}\, \mathcal{D}_I^*(g_i)_{\mu\nu}\, \mathcal{D}_I(g_j)_{\mu\nu} = \delta_{ij} \qquad \forall\, i, j = 1, \ldots, h$$

Theorem 6: Orthogonality Relations for Characters

$$\sum_{k=1}^{\tilde{N}} \frac{h_k}{h}\, \chi_I^*(\mathcal{C}_k)\, \chi_J(\mathcal{C}_k) = \delta_{IJ} \qquad \forall\, I, J = 1, \ldots, N$$

Theorem 9: Completeness Relation for Characters

$$\frac{h_k}{h} \sum_{I=1}^{N} \chi_I^*(\mathcal{C}_k) \chi_I(\mathcal{C}_{k'}) = \delta_{kk'} \qquad \forall\, k, k' = 1, \ldots, \tilde{N}$$

Unreducible

More on ~~Irreducible~~ Problems

Group Theory in Quantum Mechanics

Topics:

- Behavior of quantum mechanical states and operators under symmetry operations
- Relation between irreducible representations and invariant subspaces of the Hilbert space
- Connection between eigenvalue spectrum of quantum mechanical operators and irreducible representations
- Selection rules: symmetry-induced vanishing of matrix elements and Wigner-Eckart theorem

Note:

Operator formalism of QM convenient to discuss group theory.

Yet: many results also applicable in other areas of physics.

Symmetry Operations in Quantum Mechanics (QM)

- Let $\mathcal{G} = \{g_i\}$ be a group of symmetry operations of a qm system

  e.g., translations, rotations, permutation of particles

- Translated into the language of group theory:

  In the Hilbert space of the qm system we have a group of unitary operators $\mathcal{G}' = \{\hat{P}(g_i)\}$ such that $\mathcal{G}'$ is isomorphic to $\mathcal{G}$.

Examples

- translations $T_\mathbf{a}$

  $\rightarrow$ unitary operator $\hat{P}(T_\mathbf{a}) = \exp\left(i\hat{\mathbf{p}} \cdot \mathbf{a}/\hbar\right)$ ($\hat{\mathbf{p}}$ = momentum)

  $$\hat{P}(T_\mathbf{a})\,\psi(\mathbf{r}) = \left[1 + \nabla \cdot \mathbf{a} + \tfrac{1}{2}(\nabla \cdot \mathbf{a})^2 + \ldots\right]\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{a})$$

- rotations R_ϕ

  $\rightarrow$ unitary operator $\hat{P}(\mathbf{n}, \phi) = \exp\left(i\hat{\mathbf{L}} \cdot \mathbf{n}\phi/\hbar\right)$ ($\hat{\mathbf{L}}$ = angular momentum, ϕ = angle of rotation, $\mathbf{n}$ = axis of rotation)

Transformation of QM States

- Let $\{|\nu\rangle\}$ be an orthonormal basis
- Let $\hat{P}(g_i)$ be the symmetry operator for the symmetry transformation g_i with symmetry group $\mathcal{G} = \{g_i\}$.
- Then $$\hat{P}(g_i)\,|\nu\rangle \underset{\uparrow \atop \mathbb{1}=\sum_\mu |\mu\rangle\langle\mu|}{=} \sum_\mu |\mu\rangle \underbrace{\langle\mu|\,\hat{P}(g_i)\,|\nu\rangle}_{\mathcal{D}(g_i)_{\mu\nu}}$$
- So $$\hat{P}(g_i)\,|\nu\rangle = \sum_\mu \mathcal{D}(g_i)_{\mu\nu}\,|\mu\rangle$$ where $\mathcal{D}(g_i)_{\mu\nu} =$ matrix of a unitary representation of $\mathcal{G}$ because $\hat{P}(g_i)$ unitary
- Note: bras and kets transform according to complex conjugate representations $$\langle\nu|\hat{P}(g_i)^\dagger = \sum_\mu \langle\mu|\,\mathcal{D}(g_i)^*_{\mu\nu}$$
- Let $g_i, g_j \in \mathcal{G}$ with $g_i\, g_j = g_k \in \mathcal{G}$. Then (consistent with matrix multiplication)

$$\hat{P}(g_i)\,\hat{P}(g_j)\,|\nu\rangle = \begin{cases} \sum_{\kappa\mu} |\kappa\rangle \overbrace{\langle\kappa|\,\hat{P}(g_i)\,|\mu\rangle}^{\mathcal{D}(g_i)_{\kappa\mu}} \overbrace{\langle\mu|\,\hat{P}(g_j)\,|\nu\rangle}^{\mathcal{D}(g_j)_{\mu\nu}} = \sum_{\kappa\mu} \mathcal{D}(g_i)_{\kappa\mu}\mathcal{D}(g_j)_{\mu\nu}|\kappa\rangle \\ \hat{P}(g_k)\,|\nu\rangle = \sum_\kappa \mathcal{D}(g_k)_{\kappa\nu}|\kappa\rangle \end{cases}$$

Transformation of (Wave) Functions $\psi(\mathbf{r})$

- $\hat{P}(g_i)|\mathbf{r}\rangle = |\mathbf{r}'{=}g_i\,\mathbf{r}\rangle \;\Leftrightarrow\; \langle\mathbf{r}|\hat{P}(g_i) = \langle\mathbf{r}'{=}g_i^{-1}\,\mathbf{r}|$ b/c $\hat{P}(g)^\dagger = \hat{P}(g^{-1})$
- Let $\psi(\mathbf{r}) \equiv \langle\mathbf{r}|\psi\rangle$

  $\Rightarrow\; \hat{P}(g_i)\,\psi(\mathbf{r}) \equiv \langle\mathbf{r}|\hat{P}(g_i)|\psi\rangle = \psi(g_i^{-1}\mathbf{r}) \equiv \psi_i(\mathbf{r})$
- In general, the functions $V = \{\psi_i(\mathbf{r}) : i = 1, \ldots, h\}$ are linear dependent

  $\Rightarrow$ Choose instead linear independent functions $\psi_\nu(\mathbf{r}) \equiv \langle\mathbf{r}|\nu\rangle$ spanning V

  $\Rightarrow$ Expand images $\hat{P}(g_i)\,\psi_\nu(\mathbf{r})$ in terms of $\{\psi_\nu(\mathbf{r})\}$:

  $$\hat{P}(g_i)\,\psi(\mathbf{r}) = \langle\mathbf{r}|\hat{P}(g_i)|\psi\rangle = \sum_\mu \langle\mathbf{r}|\mu\rangle\langle\mu|\hat{P}(g_i)|\nu\rangle = \sum_\mu \mathcal{D}(g_i)_{\mu\nu}\,\psi_\mu(\mathbf{r})$$

  $$\Rightarrow \quad \boxed{\hat{P}(g_i)\,\psi_\nu(\mathbf{r}) = \psi_\nu(g_i^{-1}\mathbf{r}) = \sum_\mu \mathcal{D}(g_i)_{\mu\nu}\,\psi_\mu(\mathbf{r})}$$
- Thus: every function $\psi(\mathbf{r})$ induces a matrix representation $\Gamma = \{\mathcal{D}(g_i)\}$
- Also: every representation $\Gamma = \{\mathcal{D}(g_i)\}$ is completely characterized by a (nonunique) set of basis functions $\{\psi_\nu(\mathbf{r})\}$ transforming according to Γ.
- Dirac bra-ket notation convenient for formulating group theory of functions. Yet: results applicable in many areas of physics beyond QM.

Important Representations in Physics (usually reducible)

(1) Representations for polar and axial (cartesian) vectors

- generally: two types of point group symmetry operations
  - proper rotations $g_{\text{pr}} = (\mathbf{n}, \theta)$ about axis $\mathbf{n}$, angle θ

$\mathcal{D}[g_{\text{pr}} = (\mathbf{n}, \theta)] =$ Rodrigues' rotation formula

$$\begin{pmatrix} n_x^2(1-\cos\theta)+\cos\theta & n_x n_y(1-\cos\theta)-n_z\sin\theta & n_x n_z(1-\cos\theta)+n_y\sin\theta \\ n_y n_x(1-\cos\theta)+n_z\sin\theta & n_y^2(1-\cos\theta)+\cos\theta & n_y n_z(1-\cos\theta)-n_x\sin\theta \\ n_z n_x(1-\cos\theta)-n_y\sin\theta & n_z n_y(1-\cos\theta)+n_x\sin\theta & n_z^2(1-\cos\theta)+\cos\theta \end{pmatrix}$$

    - $\det \mathcal{D}(g_{\text{pr}}) = +1$
    - $\chi(g_{\text{pr}}) = \operatorname{tr}\mathcal{D}(g_{\text{pr}}) = 1 + 2\cos\theta$ independent of $\mathbf{n}$
  - improper rotations $g_{\text{im}} \equiv i\, g_{\text{pr}} = g_{\text{pr}}\, i$ where i = inversion

- **polar vectors**
  - proper rotations g_{pr}:
    - $\det \mathcal{D}_{\text{pol}}(g_{\text{pr}}) = +1$
    - $\operatorname{tr}\mathcal{D}_{\text{pol}}(g_{\text{pr}}) = 1 + 2\cos\theta$
  - inversion i: $\mathcal{D}_{\text{pol}}(i) = -\mathbb{1}_{3\times 3}$
  - improper rotations $g_{\text{im}} = i\, g_{\text{pr}}$:
    - $\mathcal{D}_{\text{pol}}(g_{\text{im}}) = -\mathcal{D}_{\text{pol}}(g_{\text{pr}})$
    - $\det \mathcal{D}_{\text{pol}}(g_{\text{im}}) = -1$
    - $\operatorname{tr}\mathcal{D}_{\text{pol}}(g_{\text{im}}) = -(1 + 2\cos\theta)$
  - $\Gamma_{\text{pol}} = \{\mathcal{D}_{\text{pol}}(g)\} \subseteq O(3)$ always a faithful representation (i.e., isomorphic to $\mathcal{G}$)
  - examples: position $\mathbf{r}$, linear momentum $\mathbf{p}$, electric field $\boldsymbol{\mathcal{E}}$

Important Representations in Physics

(1) Representations for polar and axial (cartesian) vectors (cont'd)

- **axial vectors**
  - proper rotations $g_{\rm pr}$:
    - $\mathcal{D}_{\rm ax}(g_{\rm pr}) = \mathcal{D}_{\rm pol}(g_{\rm pr})$
    - $\det \mathcal{D}_{\rm ax}(g_{\rm pr}) = +1$
    - $\mathrm{tr}\, \mathcal{D}_{\rm ax}(g_{\rm pr}) = 1 + 2\cos\theta$
  - inversion i: $\mathcal{D}_{\rm ax}(i) = +\mathbb{1}_{3\times 3}$
  - improper rotations $g_{\rm im} = i\, g_{\rm pr}$:
    - $\mathcal{D}_{\rm ax}(g_{\rm im}) = \mathcal{D}_{\rm ax}(g_{\rm pr}) = -\mathcal{D}_{\rm pol}(g_{\rm pr})$
    - $\det \mathcal{D}_{\rm ax}(g_{\rm im}) = +1$
    - $\mathrm{tr}\, \mathcal{D}_{\rm ax}(g_{\rm im}) = 1 + 2\cos\theta$
  - $\Gamma_{\rm ax} = \{\mathcal{D}_{\rm ax}(g)\} \subseteq SO(3)$
  - examples: angular momentum $\mathbf{L}$, magnetic field $\mathbf{B}$

- systems with discrete symmetry group $\mathcal{G} = \{g_i : i = 1, \ldots, h\}$:

$$\begin{aligned}\Gamma_{\rm pol} &= \{\mathcal{D}_{\rm pol}(g_i) : i = 1, \ldots, h\} \\ \Gamma_{\rm ax} &= \{\mathcal{D}_{\rm ax}(g_i) : i = 1, \ldots, h\}\end{aligned}$$

We have a "universal recipe" to construct the 3×3 matrices $\mathcal{D}_{\rm pol}(g)$ and $\mathcal{D}_{\rm ax}(g)$ for each group element $g_{\rm pr} = (\mathbf{n}, \theta)$ and $g_{\rm im} = i\,(\mathbf{n}, \theta)$

Important Representations in Physics (cont'd)

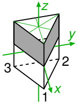
(2) Equivalence Representations Γ_{eq}

- Consider symmetric object (symmetry group $\mathcal{G}$)
  - vertices, edges, and faces of platonic solids are *equivalent* by symmetry
  - atoms / atomic orbitals $|\mu\rangle$ in a molecule may be *equivalent* by symmetry
- Equivalence representation Γ_{eq} describes mapping of equivalent objects
- Generally: $\hat{P}(g)\,|\mu\rangle = \sum_{\nu} \mathcal{D}_{\text{eq}}(g)_{\nu\mu}\,|\nu\rangle$
- **Example:** orbitals of equivalent H atoms in NH_3 molecule (group C_{3v})

  Equivalent to: permutations of corners of triangle (group $\mathcal{P}_3$)

Example: Symmetry group C_{3v} of equilateral triangle

(isomorphic to permutation group $\mathcal{P}_3$)

	identity	rotation $\phi = 120^\circ$	rotation $\phi = 240^\circ$	reflection $y \leftrightarrow -y$	roto-reflection $\phi = 120^\circ$	roto-reflection $\phi = 240^\circ$
$\mathcal{P}_3$	e	a	$b = a^2$	$c = ec$	$d = ac$	$f = bc$
Koster	E	C_3	C_3^2	σ_v	σ_v	σ_v
Γ_1	(1)	(1)	(1)	(1)	(1)	(1)
Γ_2	(1)	(1)	(1)	(-1)	(-1)	(-1)
Γ_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbf{n}, \theta$	$(0,0,1),\ 0$	$(0,0,1),\ 2\pi/3$	$(0,0,1),\ 4\pi/3$	$(0,1,0),\ \pi$	$(-\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0),\ \pi$	$(-\frac{\sqrt{3}}{2}, \frac{1}{2}, 0),\ \pi$
$\Gamma_{pol} = \Gamma_1 + \Gamma_3$	$\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & \\ & & 1 \end{pmatrix}$
$\Gamma_{ax} = \Gamma_2 + \Gamma_3$	$\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & \\ & & -1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \\ & & -1 \end{pmatrix}$
$\Gamma_{eq} = \Gamma_1 + \Gamma_3$	$\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} & & 1 \\ 1 & & \\ & 1 & \end{pmatrix}$	$\begin{pmatrix} & 1 & \\ & & 1 \\ 1 & & \end{pmatrix}$	$\begin{pmatrix} 1 & & \\ & & 1 \\ & 1 & \end{pmatrix}$	$\begin{pmatrix} & & 1 \\ & 1 & \\ 1 & & \end{pmatrix}$	$\begin{pmatrix} & 1 & \\ 1 & & \\ & & 1 \end{pmatrix}$

Transformation of QM States (cont'd)

- in general: representation $\{\mathcal{D}(g_i)\}$ of states $\{|\nu\rangle\}$ is reducible
- We have $\mathcal{D}'(g_i) = U^{-1}\,\mathcal{D}(g_i)\,U$
- More explicitly:

$$\begin{aligned}\mathcal{D}'(g_i)_{\mu'\nu'} &= \sum_{\mu\nu} U^{-1}_{\mu'\mu} \underbrace{\mathcal{D}(g_i)_{\mu\nu}}_{\langle\mu|\,\hat{P}(g_i)\,|\nu\rangle} U_{\nu\nu'} \\ &= \sum_{\mu\nu} \left(\langle\mu|U^{-1}_{\mu'\mu}\right)\,\hat{P}(g_i)\,\left(U_{\nu\nu'}|\nu\rangle\right) \\ &= \langle\mu'|\,\hat{P}(g_i)\,|\nu'\rangle\end{aligned}$$

with $|\nu'\rangle = \sum_\nu U_{\nu\nu'}|\nu\rangle$

- **Thus:** block diagonalization

$$\{\mathcal{D}(g_i)\} \;\to\; \{\mathcal{D}'(g_i) = U^{-1}\,\mathcal{D}(g_i)\,U\}$$

corresponds to change of basis

$$\{|\nu\rangle\} \;\to\; \{|\nu'\rangle = \sum_\nu U_{\nu\nu'}|\nu\rangle\}$$

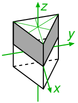
Basis Functions for Irreducible Representations

- matrices $\{\mathcal{D}_I(g_i)\}$ are fully characterized by basis functions $\{\psi_\nu^I(\mathbf{r}) : \nu = 1, \ldots n_I\}$ transforming according to IR Γ_I

$$\hat{P}(g_i)\,\psi_\nu^I(\mathbf{r}) = \psi_\nu(g_i^{-1}\mathbf{r}) = \sum_\mu \mathcal{D}_I(g_i)_{\mu\nu}\,\psi_\mu^I(\mathbf{r})$$

- convenient if we need to spell out phase conventions for $\{\mathcal{D}_I(g_i)\}$ ($\rightarrow$ Koster)
- identify IRs for (components of) polar and axial vectors

Example: Symmetry group C_{3v}



	identity	rotation $\phi = 120°$	rotation $\phi = 240°$	reflection $y \leftrightarrow -y$	roto-reflection $\phi = 120°$	roto-reflection $\phi = 240°$	basis functions
Γ_1	(1)	(1)	(1)	(1)	(1)	(1)	$x^2 + y^2$; z; $L_x^2 + L_y^2$
Γ_2	(1)	(1)	(1)	(-1)	(-1)	(-1)	L_z
Γ_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	x, y
	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	L_x, L_y

$\mathbf{r} = (x, y, z) =$ polar vector, $\mathbf{L} = (L_x, L_y, L_z) =$ axial vector

Invariant Subspaces

Definition:

- Let $\mathcal{G} = \{g_i\}$ be a group of symmetry transformations.
  Let $\mathcal{H} = \{|\mu\rangle\}$ be a Hilbert space with states $|\mu\rangle$.

  A subspace $\mathcal{S} \subset \mathcal{H}$ is called invariant subspace (with respect to $\mathcal{G}$) if

  $$\hat{P}(g_i)\,|\mu\rangle \in \mathcal{S} \qquad \forall\, g_i \in \mathcal{G}, \quad \forall\,|\mu\rangle \in \mathcal{S}$$

- If an invariant subspace can be decomposed into smaller invariant subspaces, it is called reducible, otherwise it is called irreducible.

Theorem 10:

An invariant subspace $\mathcal{S}$ is irreducible if and only if the states in $\mathcal{S}$ transform according to an irreducible representation.

Proof:

- Suppose $\{\mathcal{D}(g_i)\}$ is reducible.
- $\exists$ unitary transformation U with $\{\mathcal{D}'(g_i) = U^{-1}\,\mathcal{D}(g_i)\,U\}$ block diagonal
- For $\{\mathcal{D}'(g_i)\}$ we have the basis $\{|\mu'\rangle = \sum_\mu U_{\mu\mu'}|\mu\rangle\}$
- The block diagonal form of $\{\mathcal{D}'(g_i)\}$ implies that $\{|\mu'\rangle$ is reducible

Invariant Subspaces (cont'd)

Corollary: Every Hilbert space $\mathcal{H}$ can be decomposed into irreducible invariant subspaces $\mathcal{S}_I$ transforming according to the IR Γ_I

Remark: Given a Hilbert space $\mathcal{H}$ we can generally have multiple (possibly orthogonal) irreducible invariant subspaces $\mathcal{S}_I^\alpha$

$$\mathcal{S}_I^\alpha = \big\{ |I\,\nu\,\alpha\rangle : \nu = 1, \ldots, n_I \big\}$$

transforming according to the same IR Γ_I

$$\hat{P}(g_i)\,|I\,\nu\,\alpha\rangle = \sum_\mu \mathcal{D}_I(g_i)_{\mu\nu} |I\,\mu\,\alpha\rangle$$

Theorem 11:

(1) States transforming according to different IRs are orthogonal

(2) For states $|I\,\mu\alpha\rangle$ and $|I\,\nu\,\beta\rangle$ transforming according to the same IR Γ_I we have

$$\langle I\,\mu\alpha\,|\,I\,\nu\,\beta\rangle = \delta_{\mu\nu}\langle I\,\alpha||\,I\,\beta\rangle$$

where the reduced matrix element $\langle I\,\alpha||\,I\,\beta\rangle$ is independent of μ, ν.

Remark: This theorem lets us anticipate the Wigner-Eckart theorem

Invariant Subspaces (cont'd)

Proof of Theorem 11

- Use unitarity of $\hat{P}(g_j)$: $\quad \mathbb{1} = \hat{P}(g_j)^\dagger \, \hat{P}(g_j) = \frac{1}{h}\sum_i \hat{P}(g_i)^\dagger \, \hat{P}(g_i)$
- Then

$$\langle I \, \mu\alpha \, | J \nu \, \beta \rangle = \frac{1}{h}\sum_i \underbrace{\langle I \, \mu\alpha | \, \hat{P}(g_i)^\dagger}_{\sum_{\mu'} \langle I \, \mu' \, \alpha | \mathcal{D}_I(g_i)^*_{\mu' \mu}} \; \underbrace{\hat{P}(g_i) \, | J \nu \, \beta \rangle}_{\sum_{\nu'} \mathcal{D}_J(g_i)_{\nu' \nu} | J \nu' \, \beta \rangle}$$

$$= \sum_{\mu' \nu'} \langle I \, \mu' \, \alpha \, | J \nu' \, \beta \rangle \, \underbrace{\frac{1}{h}\sum_i \mathcal{D}_I(g_i)^*_{\mu' \mu} \, \mathcal{D}_J(g_i)_{\nu' \nu}}_{(1/n_I) \, \delta_{IJ} \, \delta_{\mu\nu} \, \delta_{\mu' \nu'}}$$

$$= \delta_{IJ} \, \delta_{\mu\nu} \; \underbrace{\frac{1}{n_I} \sum_{\mu'} \langle I \, \mu' \, \alpha \, | I \, \mu' \, \beta \rangle}_{\equiv \langle I \, \alpha || I \, \beta \rangle}$$

qed

Discussion Theorem 11

- $\Gamma_J \times \Gamma_I$ contains the identity representation Γ_1 if and only if the IR Γ_J is the complex conjugate of Γ_I, i.e., $\Gamma_J^* = \Gamma_I \Leftrightarrow \mathcal{D}_J(g)^* = \mathcal{D}_I(g) \, \forall g$.
- If the ket $|J\mu\alpha\rangle$ transforms according to the IR Γ_J, the bra $\langle J\mu\alpha|$ transforms according to the complex conjugate representation Γ_J^*.
- Thus: $\langle J\mu\alpha|I\nu\beta\rangle \neq 0$ equivalent to
  - bra and ket transform according to complex conjugate representations
  - $\langle J\mu\alpha|I\nu\beta\rangle$ contains the identity representation
- Indeed, common theme of representation theory applied to physics:

  Terms are only nonzero if they transform according to a representation that contains the identity representation.

- Variant of Theorem 11 (Bir & Pikus):

  If $f_I(x)$ transforms according to some IR Γ_I, then $\int f_I(x)\, dx \neq 0$ only if Γ_I is the identity representation.

- Applications
  - Wigner-Eckart Theorem
  - Nonzero elements of material tensors
  - *Our universe would be zero "by symmetry" if the apparently trivial identity representation did not exist.*

Decomposition into Irreducible Invariant Subspaces

- **Goal:** Decompose general state $|\psi\rangle \in \mathcal{H}$ into components from irreducible invariant subspaces $\mathcal{S}_I$
- **Generalized projection operator** $\hat{\Pi}^I_{\mu\mu'} := \frac{n_I}{h} \sum_i \mathcal{D}_I(g_i)^*_{\mu\mu'} \, \hat{P}(g_i)$
- **Theorem 12:** (i) $\hat{\Pi}^I_{\mu\mu'} |J\nu\alpha\rangle = \delta_{IJ}\, \delta_{\mu'\nu} |I\mu\alpha\rangle$

  (ii) $\hat{\Pi}^I_{\mu\mu'} \, \hat{\Pi}^J_{\nu\nu'} = \delta_{IJ}\, \delta_{\mu'\nu} \hat{\Pi}^J_{\mu\nu'}$

  (iii) $\sum_{I\mu} \hat{\Pi}^I_{\mu\mu} = \mathbb{1}$

Proof:

(i) $$\hat{\Pi}^I_{\mu\mu'} |J\nu\alpha\rangle = \frac{n_I}{h} \sum_i \mathcal{D}_I(g_i)^*_{\mu\mu'} \underbrace{\hat{P}(g_i)\, |J\nu\alpha\rangle}_{\sum_{\nu'} \mathcal{D}_J(g_i)_{\nu'\nu}\, |J\nu'\alpha\rangle} = \sum_{\nu'} \underbrace{\frac{n_I}{h} \sum_i \mathcal{D}_I(g_i)^*_{\mu\mu'}\, \mathcal{D}_J(g_i)_{\nu'\nu}}_{\delta_{IJ}\, \delta_{\mu\nu'}\, \delta_{\mu'\nu}} |J\nu'\alpha\rangle$$

(ii) $$\begin{aligned} \hat{\Pi}^I_{\mu\mu'} \, \hat{\Pi}^J_{\nu\nu'} &= \frac{n_I}{h} \sum_i \frac{n_J}{h} \sum_j \mathcal{D}_I(g_i)^*_{\mu\mu'} \mathcal{D}_J(g_j)^*_{\nu\nu'} \, \hat{P}(g_i)\, \hat{P}(g_j) \qquad \text{subst. } g_i g_j = g_k \\ &= \frac{n_I}{h} \sum_i \frac{n_J}{h} \sum_k \mathcal{D}_I(g_i)^*_{\mu\mu'} \mathcal{D}_J(g_i^{-1} g_k)^*_{\nu\nu'} \, \hat{P}(g_k) \\ &= \frac{n_J}{h} \sum_{k\lambda} \underbrace{\frac{n_I}{h} \sum_i \mathcal{D}_I(g_i)^*_{\mu\mu'} \underbrace{\mathcal{D}_J(g_i^{-1})^*_{\nu\lambda}}_{\mathcal{D}_J(g_i)_{\lambda\nu}}}_{\delta_{IJ}\delta_{\mu\lambda}\delta_{\mu'\nu}} \mathcal{D}_J(g_k)^*_{\lambda\nu'} \, \hat{P}(g_k) \end{aligned}$$

[or use (i)]

(iii) $$\sum_{I\mu} \hat{\Pi}^I_{\mu\mu} = \sum_i \frac{1}{h} \sum_I \underbrace{\sum_\mu \mathcal{D}_I(g_i)^*_{\mu\mu'}}_{\chi_I^*(g_i)} \underbrace{n_I}_{\chi_I(e)} \, \hat{P}(g_i) = \sum_i \delta_{g_i e}\, \hat{P}(g_i) = \hat{P}(e) \equiv \mathbb{1}$$

Decomposition into Invariant Subspaces (cont'd)

Discussion

- Let $|\psi\rangle = \sum_{J\nu\alpha} c_{J\nu\alpha} \, |J\nu\alpha\rangle$ general state with coefficients $c_{J\mu\alpha}$ (*)
- Diagonal operator $\hat{\Pi}^I_{\mu\mu}$ projects $|\psi\rangle$ on components $|I\mu\alpha\rangle$:
  - $(\hat{\Pi}^I_{\mu\mu})^2|\psi\rangle = \hat{\Pi}^I_{\mu\mu}|\psi\rangle = \sum_{\alpha} c_{I\mu\alpha} \, |I\mu\alpha\rangle$
  - $\sum_{I\,\mu} \hat{\Pi}^I_{\mu\mu} = \mathbb{1}$
- Let $\hat{\Pi}^I \equiv \sum_{\mu} \hat{\Pi}^I_{\mu\mu} = \frac{n_I}{h} \sum_i \chi^*_I(g_i) \, \hat{P}(g_i)$:
  - $\hat{\Pi}^I|\psi\rangle = \sum_{\nu\alpha} c_{I\nu\alpha} \, |I\nu\alpha\rangle$
  - $\hat{\Pi}^I$ projects $|\psi\rangle$ on the invariant subspace $\mathcal{S}_I$ (IR Γ_I)
- For functions $\psi(\mathbf{r}) \equiv \langle \mathbf{r}|\psi\rangle$:

$$\hat{\Pi}^I_{\mu\mu'} \, \psi(\mathbf{r}) = \frac{n_I}{h} \sum_i \mathcal{D}_I(g_i)^*_{\mu\mu'} \, \psi(g_i^{-1}\mathbf{r})$$

we need not know the expansion (*)

Irreducible Invariant Subspaces (cont'd)

Example:

- Group $\mathcal{C}_i = \{e, i\}$ $\quad e =$ identity, $i =$ inversion

$\mathcal{C}_i$	e	i
e	e	i
i	i	e

- character table

$\mathcal{C}_i$	e	i
Γ_1	1	1
Γ_2	1	-1

- $\hat{P}(e)\,\psi(x) = \psi(x), \quad \hat{P}(i)\,\psi(x) = \psi(-x)$

- **Projection operator** $\hat{\Pi}^I = \frac{n_I}{h} \sum_i \chi_I^*(g_i)\,\hat{P}(g_i)$ $\quad$ with $n_I = 1,\ h = 2$

- $\hat{\Pi}^1 = \frac{1}{2}\,[\hat{P}(e) + \hat{P}(i)] \quad \Rightarrow \quad \hat{\Pi}^1\,\psi(x) = \frac{1}{2}\,[\psi(x) + \psi(-x)]$ even part

  $\hat{\Pi}^2 = \frac{1}{2}\,[\hat{P}(e) - \hat{P}(i)] \quad \Rightarrow \quad \hat{\Pi}^2\,\psi(x) = \frac{1}{2}\,[\psi(x) - \psi(-x)]$ odd part

Product Representations

- Let $\{|I\mu\rangle : \mu = 1, \dots n_I\}$ and $\{|J\nu\rangle : \nu = 1, \dots n_J\}$ denote basis functions for invariant subspaces $\mathcal{S}_I$ and $\mathcal{S}_J$ (need not be irreducible)

  Consider the product functions

  $$\{|I\mu\rangle\,|J\nu\rangle : \mu = 1, \dots, n_I;\ \nu = 1, \dots, n_J\}.$$

  How do these functions transform under $\mathcal{G}$?

- **Definition:** Let $\mathcal{D}_I(g)$ and $\mathcal{D}_J(g)$ be representation matrices for $g \in \mathcal{G}$.

  The direct product (Kronecker product) $\mathcal{D}_I(g) \otimes \mathcal{D}_J(g)$ denotes the matrix whose elements in row $(\mu\nu)$ and column $(\mu'\nu')$ are given by

  $$[\mathcal{D}_I(g) \otimes \mathcal{D}_J(g)]_{\mu\nu,\mu'\nu'} = \mathcal{D}_I(g)_{\mu\mu'}\,\mathcal{D}_J(g)_{\nu\nu'} \qquad \begin{matrix} \mu, \mu' = 1, \dots, n_I \\ \nu, \nu' = 1, \dots, n_J \end{matrix}$$

- **Example:** Let $\mathcal{D}_I(g) = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}$ and $\mathcal{D}_J(g) = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix}$

  $$\mathcal{D}_I(g) \otimes \mathcal{D}_J(g) = \begin{pmatrix} x_{11}\,\mathcal{D}_J(g) & x_{12}\,\mathcal{D}_J(g) \\ x_{21}\,\mathcal{D}_J(g) & x_{22}\,\mathcal{D}_J(g) \end{pmatrix} = \begin{pmatrix} x_{11}y_{11} & x_{11}y_{12} & x_{12}y_{11} & x_{12}y_{12} \\ x_{11}y_{21} & x_{11}y_{22} & x_{12}y_{21} & x_{12}y_{22} \\ x_{21}y_{11} & x_{21}y_{12} & x_{22}y_{11} & x_{22}y_{12} \\ x_{21}y_{21} & x_{21}y_{22} & x_{22}y_{21} & x_{22}y_{22} \end{pmatrix}$$

- Details of the arrangement in the following not relevant

Product Representations (cont'd)

- Dimension of product matrix

$$\dim\,[\mathcal{D}_I(g) \otimes \mathcal{D}_J(g)] = \dim\,\mathcal{D}_I(g)\ \dim\,\mathcal{D}_J(g)$$

- Let $\Gamma_I = \{\mathcal{D}_I(g_i)\}$ and $\Gamma_J = \{\mathcal{D}_J(g_i)\}$ be representations of $\mathcal{G}$. Then

$$\Gamma_I \times \Gamma_J \equiv \{\mathcal{D}_I(g) \otimes \mathcal{D}_J(g)\}$$

  is a representation of $\mathcal{G}$ called product representation.

- $\Gamma_I \times \Gamma_J$ is, indeed, a representation:

  Let $\mathcal{D}_I(g_i)\,\mathcal{D}_I(g_j) = \mathcal{D}_I(g_k)$ and $\mathcal{D}_J(g_i)\,\mathcal{D}_J(g_j) = \mathcal{D}_J(g_k)$

$$\Rightarrow \left([\mathcal{D}_I(g_i) \otimes \mathcal{D}_J(g_i)]\,[\mathcal{D}_I(g_j) \otimes \mathcal{D}_J(g_j)]\right)_{\mu\nu,\mu'\nu'}$$

$$= \sum_{\kappa\lambda} \mathcal{D}_I(g_i)_{\mu\kappa}\,\mathcal{D}_J(g_i)_{\nu\lambda}\,\mathcal{D}_I(g_j)_{\kappa\mu'}\,\mathcal{D}_J(g_j)_{\lambda\nu'}$$

$$\to \mathcal{D}_I(g_k)_{\mu\mu'} \qquad \to \mathcal{D}_J(g_k)_{\nu\nu'}$$

$$= [\mathcal{D}_I(g_k) \otimes \mathcal{D}_J(g_k)]_{\mu\nu,\mu'\nu'}$$

- Let $\hat{P}(g)\,|I\mu\rangle = \sum_{\mu'} \mathcal{D}_I(g)_{\mu'\mu}\,|I\mu'\rangle$

$$\hat{P}(g)\,|J\nu\rangle = \sum_{\nu'} \mathcal{D}_J(g)_{\nu'\nu}\,|J\nu'\rangle$$

  Then $\hat{P}(g)\,|I\mu\rangle|J\nu\rangle = \sum_{\mu'\nu'} [\mathcal{D}_I(g) \otimes \mathcal{D}_J(g)]_{\mu'\nu',\mu\nu}\,|I\mu'\rangle|J\nu'\rangle$

Product Representations (cont'd)

- The characters of the product representation are
  $$\chi_{I \times J}(g_i) = \chi_I(g_i)\,\chi_J(g_i)$$

Decomposing Product Representations

- Let $\Gamma_I = \{\mathcal{D}_I(g_i)\}$ and $\Gamma_J = \{\mathcal{D}_J(g_i)\}$ be irreducible representations of $\mathcal{G}$

  The product representation $\Gamma_I \times \Gamma_J = \{\mathcal{D}_{I\times J}(g_i)\}$ is generally reducible

- According to Theorem 7, we have

$$\Gamma_I \times \Gamma_J = \sum_K a_K^{IJ}\,\Gamma_K \qquad \text{where} \quad a_K^{IJ} = \sum_{k=1}^{\tilde{N}} \frac{h_k}{h}\,\chi_K^*(\mathcal{C}_k)\,\underbrace{\chi_{I\times J}(\mathcal{C}_k)}_{=\chi_I(\mathcal{C}_k)\,\chi_J(\mathcal{C}_k)}$$

- The multiplication table for the irreducible representations Γ_I of $\mathcal{G}$ lists $\sum_k a_K^{IJ}\,\Gamma_K$

$\Gamma_I \times \Gamma_J$	Γ_1	Γ_2	$\ldots$
Γ_1			
Γ_2			
$\vdots$			

- **Example:** Permutation group $\mathcal{P}_3$

$\chi(\mathcal{C})$	e	a, b	c, d, f
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	-1	0

$\Gamma_I \times \Gamma_J$	Γ_1	Γ_2	Γ_3
Γ_1	Γ_1	Γ_2	Γ_3
Γ_2		Γ_1	Γ_3
Γ_3			$\Gamma_1 + \Gamma_2 + \Gamma_3$

(Anti-) Symmetrized Product Representations

Let $\{|\sigma_\mu\rangle\}$ and $\{|\tau_\nu\rangle\}$ be two sets of basis functions for the *same* n-dim. representation $\Gamma = \{\mathcal{D}(g)\}$ with characters $\{\chi(g)\}$. (again: need not be irreducible)

(1) "Simple" Product: (discussed previously)

- $|\psi_{\mu\nu}\rangle = |\sigma_\mu\rangle|\tau_\nu\rangle$, $\left.\begin{array}{l}\mu = 1, \ldots, n \\ \nu = 1, \ldots n\end{array}\right\}$ total: n^2
- $$\begin{aligned}\hat{P}(g)|\psi_{\mu\nu}\rangle &= \sum_{\mu'=1}^{n}\sum_{\nu'=1}^{n}\mathcal{D}(g)_{\mu'\mu}\mathcal{D}(g)_{\nu'\nu}\,|\sigma_{\mu'}\rangle|\tau_{\nu'}\rangle \\ &\equiv \sum_{\mu'=1}^{n}\sum_{\nu'=1}^{n}[\mathcal{D}(g)\otimes\mathcal{D}(g)]_{\mu'\nu',\mu\nu}\,|\psi_{\mu'\nu'}\rangle\end{aligned}$$
- Character $\mathrm{tr}[\mathcal{D}(g)\otimes\mathcal{D}(g)] = \chi^2(g)$

(Anti-) Symmetrized Product Representations (cont'd)

(2) Symmetrized Product:

- $|\psi^s_{\mu\nu}\rangle = \frac{1}{2}(|\sigma_\mu\rangle|\tau_\nu\rangle + |\sigma_\nu\rangle|\tau_\mu\rangle), \qquad \left.\begin{array}{l}\mu = 1,\ldots,n \\ \nu = 1,\ldots\mu\end{array}\right\}$ total: $\frac{1}{2}n(n+1)$
- $$\begin{aligned}\hat{P}(g)|\psi^s_{\mu\nu}\rangle &= \frac{1}{2}\sum_{\mu'=1}^{n}\sum_{\nu'=1}^{n}\mathcal{D}_{\mu'\mu}\mathcal{D}_{\nu'\nu}\left(|\sigma_\mu\rangle|\tau_\nu\rangle + |\sigma_\nu\rangle|\tau_\mu\rangle\right) \\ &= \sum_{\mu'=1}^{n}\left[\sum_{\nu'=1}^{\mu'-1}(\mathcal{D}_{\mu'\mu}\mathcal{D}_{\nu'\nu} + \mathcal{D}_{\mu'\nu}\mathcal{D}_{\nu'\mu})|\psi^s_{\mu'\nu'}\rangle + \mathcal{D}_{\mu'\mu}\mathcal{D}_{\mu'\nu}|\psi^s_{\mu'\mu'}\rangle\right] \\ &\equiv \sum_{\mu'=1}^{n}\sum_{\nu'=1}^{\mu'}[\mathcal{D}(g)\otimes\mathcal{D}(g)]^{(s)}_{\mu'\nu',\mu\nu}\,|\psi^s_{\mu'\nu'}\rangle\end{aligned}$$
- $$\begin{aligned}\mathrm{tr}[\mathcal{D}(g)\otimes\mathcal{D}(g)]^{(s)} &= \sum_{\mu=1}^{n}\left[\sum_{\nu=1}^{\mu-1}(\mathcal{D}_{\mu\mu}\mathcal{D}_{\nu\nu} + \mathcal{D}_{\mu\nu}\mathcal{D}_{\nu\mu}) + \mathcal{D}_{\mu\mu}\mathcal{D}_{\mu\mu}\right] \\ &= \frac{1}{2}\sum_{\mu=1}^{n}\sum_{\nu=1}^{n}[\mathcal{D}_{\mu\mu}(g)\mathcal{D}_{\nu\nu}(g) + \mathcal{D}_{\mu\nu}(g)\mathcal{D}_{\nu\mu}(g)] \\ &= \frac{1}{2}\sum_{\mu=1}^{n}\left[\mathcal{D}_{\mu\mu}(g)\sum_{\nu=1}^{n}\mathcal{D}_{\nu\nu}(g) + \mathcal{D}_{\mu\mu}(g^2)\right] \\ &= \frac{1}{2}[\chi(g)^2 + \chi(g^2)]\end{aligned}$$

(Anti-) Symmetrized Product Representations (cont'd)

(3) Antisymmetrized Product:

- $|\psi^a_{\mu\nu}\rangle = \frac{1}{2}(|\sigma_\mu\rangle|\tau_\nu\rangle - |\sigma_\nu\rangle|\tau_\mu\rangle), \qquad \left.\begin{array}{l}\mu = 1, \ldots, n \\ \nu = 1, \ldots \mu - 1\end{array}\right\}$ total: $\frac{1}{2}n(n-1)$
- $$\begin{aligned} \hat{P}(g)|\psi^a_{\mu\nu}\rangle &= \frac{1}{2}\sum_{\mu'=1}^{n}\sum_{\nu'=1}^{n}\mathcal{D}_{\mu'\mu}\mathcal{D}_{\nu'\nu}\left(|\sigma_\mu\rangle|\tau_\nu\rangle - |\sigma_\nu\rangle|\tau_\mu\rangle\right) \\ &= \sum_{\mu'=1}^{n}\sum_{\nu'=1}^{\mu'-1}(\mathcal{D}_{\mu'\mu}\mathcal{D}_{\nu'\nu} - \mathcal{D}_{\mu'\nu}\mathcal{D}_{\nu'\mu})|\psi^a_{\mu'\nu'}\rangle \\ &\equiv \sum_{\mu'=1}^{n}\sum_{\nu'=1}^{\mu'-1}[\mathcal{D}(g)\otimes\mathcal{D}(g)]^{(a)}_{\mu'\nu',\mu\nu}\,|\psi^a_{\mu'\nu'}\rangle \end{aligned}$$
- $$\begin{aligned} \mathrm{tr}[\mathcal{D}(g)\otimes\mathcal{D}(g)]^{(a)} &= \sum_{\mu=1}^{n}\sum_{\nu=1}^{\mu-1}(\mathcal{D}_{\mu\mu}\mathcal{D}_{\nu\nu} - \mathcal{D}_{\mu\nu}\mathcal{D}_{\nu\mu}) \\ &= \frac{1}{2}\sum_{\mu=1}^{n}\sum_{\nu=1}^{n}[\mathcal{D}_{\mu\mu}(g)\mathcal{D}_{\nu\nu}(g) - \mathcal{D}_{\mu\nu}(g)\mathcal{D}_{\nu\mu}(g)] \\ &= \frac{1}{2}\sum_{\mu=1}^{n}\left[\mathcal{D}_{\mu\mu}(g)\sum_{\nu=1}^{n}\mathcal{D}_{\nu\nu}(g) - \mathcal{D}_{\mu\mu}(g^2)\right] \\ &= \frac{1}{2}[\chi(g)^2 - \chi(g^2)] \end{aligned}$$

Intermezzo: Material Tensors

to be added . . .

Discussion

- **Representation – Vector Space**
  The matrices $\{\mathcal{D}(g_i)\}$ of an n-dimensional (reducible or irreducible) representation describe a linear mapping of a vector space $\mathcal{V}$ onto itself.
  $$\mathbf{u} = (u_1, \ldots, u_n) \in \mathcal{V} : \quad \mathbf{u} \xrightarrow{\mathcal{D}(g_i)} \mathbf{u}' \in \mathcal{V} \quad \text{with} \quad u'_\mu = \sum_\nu \mathcal{D}(g_i)_{\mu\nu}\, u_\nu$$
- **Irreducible Representation (IR) – Invariant Subspace**
  The decomposition of a reducible representation into IRs Γ_I corresponds to a decomposition of the vector space $\mathcal{V}$ into invariant subspaces $\mathcal{S}_I$ such that
  $$\mathcal{S}_I \xrightarrow{\mathcal{D}_I(g_i)} \mathcal{S}_I \quad \forall g_i \in \mathcal{G} \qquad \text{(i.e., no mixing)}$$

  This decomposition of $\mathcal{V}$ lets us break down a big physical problem into smaller, more tractable problems
- **Product Representation – Product Space**
  A product representation $\Gamma_I \times \Gamma_J$ describes a linear mapping of the product space $\mathcal{S}_I \times \mathcal{S}_J$ onto itself
  $$\mathcal{S}_I \times \mathcal{S}_J \xrightarrow{\mathcal{D}_{I\times J}(g_i)} \mathcal{S}_I \times \mathcal{S}_J \quad \forall g_i \in \mathcal{G}$$
- The block diagonalization $\Gamma_I \times \Gamma_J = \sum_K a_K^{IJ}\, \Gamma_K$ corresponds to a decomposition of $\mathcal{S}_I \times \mathcal{S}_J$ into invariant subspaces $\mathcal{S}_K$

Clebsch-Gordan Coefficients (CGC)

- The block diagonalization $\Gamma_I \times \Gamma_J = \sum_K a_K^{IJ} \Gamma_K$ corresponds to a decomposition of $\mathcal{S}_I \times \mathcal{S}_J$ into invariant subspaces $\mathcal{S}_K$

$\Rightarrow$ **Change of Basis:** unitary transformation

$$\begin{cases} \mathcal{S}_I \times \mathcal{S}_J & \longrightarrow & \displaystyle\sum_K \sum_{\ell=1}^{a_K^{IJ}} \mathcal{S}_K^\ell \\ \text{old basis } \{\mathbf{e}_\mu^I \mathbf{e}_\nu^J\} & \longrightarrow & \text{new basis } \{\mathbf{e}_\kappa^{K\ell}\} \end{cases}$$

Thus
$$\mathbf{e}_\kappa^{K\ell} = \sum_{\mu\nu} \left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu & \nu & \kappa \end{array} \right) \mathbf{e}_\mu^I \, \mathbf{e}_\nu^J$$

index ℓ not needed if often $a_K^{IJ} \leq 1$

where $\left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu & \nu & \kappa \end{array} \right)$ = Clebsch-Gordan coefficients (CGC)

Clebsch-Gordan coefficients describe the unitary transformation for the decomposition of the product space $\mathcal{S}_I \times \mathcal{S}_J$ into invariant subspaces $\mathcal{S}_K^\ell$

Clebsch-Gordan Coefficients (cont'd)

Remarks

- CGC are independent of the group elements g_i
- CGC are tabulated for all important groups (e.g., Koster, Edmonds)
- **Note:** Tabulated CGC refer to a particular definition (phase convention) for the basis vectors $\{\mathbf{e}_\mu^I\}$ and representation matrices $\{\mathcal{D}_I(g_i)\}$
- Clebsch-Gordan coefficients $\underline{\underline{\mathcal{C}}}$ describe a *unitary* basis transformation

  $$\underline{\underline{\mathcal{C}}}^\dagger \, \underline{\underline{\mathcal{C}}} = \underline{\underline{\mathcal{C}}} \, \underline{\underline{\mathcal{C}}}^\dagger = \mathbb{1}$$

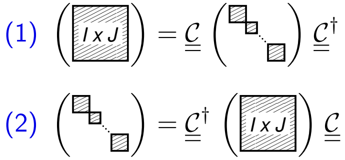
- Thus **Theorem 13:** Orthogonality and completeness of CGC

  $$\sum_{\mu\nu} \left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu & \nu & \kappa \end{array} \right)^* \left(\begin{array}{cc|c} I & J & K'\,\ell' \\ \mu & \nu & \kappa' \end{array} \right) = \delta_{KK'}\,\delta_{\kappa\kappa'}\,\delta_{\ell\ell'}$$

  $$\sum_{K\ell\kappa} \left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu & \nu & \kappa \end{array} \right)^* \left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu' & \nu' & \kappa \end{array} \right) = \delta_{\mu\mu'}\,\delta_{\nu\nu'}$$

Clebsch-Gordan Coefficients (cont'd)

Clebsch-Gordan coefficients block-diagonalize the representation matrices (unitary transformation)



More explicitly:

Theorem 14: Reduction of Product Representation $\Gamma_I \times \Gamma_J$

(1) $$\mathcal{D}_I(g_i)_{\mu\mu'}\, \mathcal{D}_J(g_i)_{\nu\nu'} = \sum_{K\ell} \sum_{\kappa\kappa'} \left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu & \nu & \kappa \end{array} \right) \mathcal{D}_K(g_i)_{\kappa\kappa'} \left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu' & \nu' & \kappa' \end{array} \right)^*$$

(2) $$\mathcal{D}_K(g_i)_{\kappa\kappa'}\, \delta_{KK'}\, \delta_{\ell\ell'} = \sum_{\mu\mu'} \sum_{\nu\nu'} \left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu & \nu & \kappa \end{array} \right)^* \mathcal{D}_I(g_i)_{\mu\mu'}\, \mathcal{D}_J(g_i)_{\nu\nu'} \left(\begin{array}{cc|c} I & J & K'\,\ell' \\ \mu' & \nu' & \kappa' \end{array} \right)$$

Evaluating Clebsch-Gordan Coefficients

- A group $\mathcal{G}$ is called simply reducible if its product representations $\Gamma_I \times \Gamma_J$ contain the IRs Γ_K only with multiplicities $a_K^{IJ} = 0$ or 1.
- For simply reducible groups ($\Rightarrow$ no index ℓ) according to Theorem 14 (1):

$$\frac{n_K}{h} \sum_i \mathcal{D}_I(g_i)_{\mu\mu'}\, \mathcal{D}_J(g_i)_{\nu\nu'} \mathcal{D}_K^*(g_i)_{\tilde\kappa\tilde\kappa'}$$
$$= \sum_{K'} \sum_{\kappa\kappa'} \left(\begin{array}{cc|c} I & J & K' \\ \mu & \nu & \kappa \end{array}\right) \left(\begin{array}{cc|c} I & J & K' \\ \mu' & \nu' & \kappa' \end{array}\right)^* \underbrace{\frac{n_K}{h} \sum_i \mathcal{D}_{K'}(g_i)_{\kappa\kappa'} \mathcal{D}_K^*(g_i)_{\tilde\kappa\tilde\kappa'}}_{= \delta_{K'K}\,\delta_{\tilde\kappa\kappa}\,\delta_{\tilde\kappa'\kappa'} \quad \text{(Theorem 4)}}$$
$$= \left(\begin{array}{cc|c} I & J & K \\ \mu & \nu & \tilde\kappa \end{array}\right) \left(\begin{array}{cc|c} I & J & K \\ \mu' & \nu' & \tilde\kappa' \end{array}\right)^*$$

- Choose triple $\mu = \mu' = \mu_0$, $\nu = \nu' = \nu_0$, and $\tilde\kappa = \tilde\kappa' = \kappa_0$ such that LHS $\neq 0$

$$\Rightarrow \left(\begin{array}{cc|c} I & J & K \\ \mu_0 & \nu_0 & \kappa_0 \end{array}\right) = \sqrt{\frac{n_K}{h} \sum_i \mathcal{D}_I(g_i)_{\mu_0\mu_0}\, \mathcal{D}_J(g_i)_{\nu_0\nu_0} \mathcal{D}_K^*(g_i)_{\kappa_0\kappa_0}} \quad > 0$$

Given the representation matrices $\{\mathcal{D}_I(g)\}$, the CGCs are unique for each triple I, J, K up to an overall phase that we choose such that $\left(\begin{array}{cc|c} I & J & K \\ \mu_0 & \nu_0 & \kappa_0 \end{array}\right) > 0$

$$\Rightarrow \left(\begin{array}{cc|c} I & J & K \\ \mu & \nu & \kappa \end{array}\right) = \frac{1}{\left(\begin{array}{cc|c} I & J & K \\ \mu_0 & \nu_0 & \kappa_0 \end{array}\right)} \frac{n_K}{h} \sum_i \mathcal{D}_I(g_i)_{\mu\mu_0}\, \mathcal{D}_J(g_i)_{\nu\nu_0} \mathcal{D}_K^*(g_i)_{\kappa\kappa_0} \qquad \forall \mu, \nu, \kappa$$

- If $a_K^{IJ} > 1$: CGCs not unique $\Rightarrow$ trickier!

Example: CGC for group $\mathcal{P}_3 \simeq C_{3v}$

This group is simply reducible, $a_K^{IJ} \leq 1$, so we may drop the index ℓ.

Here: For Γ_3 use the representation matrices $\{\mathcal{D}_3(g)\}$ corresponding to the basis functions x, y.

$$\begin{pmatrix} 1\;1 & 1 \\ 1\;1 & 1 \end{pmatrix} = \begin{pmatrix} 1\;2 & 2 \\ 1\;1 & 1 \end{pmatrix} = \begin{pmatrix} 2\;2 & 1 \\ 1\;1 & 1 \end{pmatrix} = 1$$

$$\begin{pmatrix} 1\;3 & 3 \\ 1\;\mu & \nu \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_{\mu\nu} \qquad \begin{pmatrix} 2\;3 & 3 \\ 1\;\mu & \nu \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}_{\mu\nu}$$

$$\begin{pmatrix} 3\;3 & 1 \\ \mu\;\nu & 1 \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} \end{pmatrix}_{\mu\nu} \qquad \begin{pmatrix} 3\;3 & 2 \\ \mu\;\nu & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{pmatrix}_{\mu\nu}$$

$$\begin{pmatrix} 3\;3 & 3 \\ \mu\;\nu & 1 \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & 0 \\ 0 & -1/\sqrt{2} \end{pmatrix}_{\mu\nu} \qquad \begin{pmatrix} 3\;3 & 3 \\ \mu\;\nu & 2 \end{pmatrix} = \begin{pmatrix} 0 & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{pmatrix}_{\mu\nu}$$

Comparison: Rotation Group

- Angular momentum $j = 0, 1/2, 1, 3/2, \ldots$ corresponds to the irreducible representations of the rotation group
- For each j, these IRs are $(2j+1)$-dimensional, i.e., the z component of angular momentum labels the basis states for the IR Γ_j.
- $\Gamma_{j=0}$ is the identity representation of the rotation group
- The product representation $\Gamma_{j_1} \times \Gamma_{j_2}$ corresponds to the addition of angular momenta j_1 and j_2;

  $$\Gamma_{j_1} \times \Gamma_{j_2} = \Gamma_{|j_1 - j_2|} + \ldots + \Gamma_{j_1 + j_2}$$

  Here all multiplicities $a_{j_3}^{j_1 j_2}$ are one.
- In our lecture, Clebsch-Gordan coefficients have the same meaning as in the context of the rotation group:

  They describe the unitary transformation from the reducible product space to irreducible invariant subspaces.

  This unitary transformation depends only on (the representation matrices of) the IRs of the symmetry group of the problem so that the CGC can be tabulated.

Symmetry of Observables

- Consider Hermitian operator (observable) $\hat{\mathcal{O}}$.

  Let $\mathcal{G} = \{g_i\}$ be a group of symmetry transformations with $\{\hat{P}(g_i)\}$ the group of unitary operators isomorphic to $\mathcal{G}$.

  - For arbitrary $|\phi\rangle$ we have $|\psi\rangle = \hat{\mathcal{O}}|\phi\rangle$.
  - Application of g_i gives $|\psi'\rangle = \hat{P}(g_i)|\psi\rangle$ and $|\phi'\rangle = \hat{P}(g_i)|\phi\rangle$.
  - Thus $|\psi'\rangle = \hat{\mathcal{O}}'|\phi'\rangle$ requires $\hat{\mathcal{O}}' = \hat{P}(g_i)\,\hat{\mathcal{O}}\,\hat{P}(g_i)^{-1}$

  If $\hat{\mathcal{O}}' = \hat{P}(g_i)\,\hat{\mathcal{O}}\,\hat{P}(g_i)^{-1} = \hat{\mathcal{O}} \;\Leftrightarrow\; [\hat{P}(g_i), \hat{\mathcal{O}}] = 0 \qquad \forall g_i \in \mathcal{G}$

  we call $\mathcal{G}$ the symmetry group of $\hat{\mathcal{O}}$ which leaves $\hat{\mathcal{O}}$ invariant.

  Of course, we want the largest $\mathcal{G}$ possible.

- **Lemma:** If $|n\rangle$ is an eigenstate of $\hat{\mathcal{O}}$, i.e., $\hat{\mathcal{O}}\,|n\rangle = \lambda_n\,|n\rangle$, and $[\hat{P}(g_i), \hat{\mathcal{O}}] = 0$, then $\hat{P}(g_i)\,|n\rangle$ is likewise an eigenstate of $\hat{\mathcal{O}}$ for the same eigenvalue λ_n.

  As always $\hat{P}(g_i)\,|n\rangle$ need not be orthogonal to $|n\rangle$.

  Proof: $\hat{\mathcal{O}}\,[\hat{P}(g_i)\,|n\rangle] = \hat{P}(g_i)\,\hat{\mathcal{O}}\,|n\rangle = \lambda_n\,[\hat{P}(g_i)\,|n\rangle]$

Symmetry of Observables (cont'd)

- **Theorem 15:**
  Let $\mathcal{G} = \{\hat{P}(g_i)\}$ be the symmetry group of the observable $\hat{\mathcal{O}}$.
  Then the eigenstates of a d-fold degenerate eigenvalue λ_n of $\hat{\mathcal{O}}$ form a d-dimensional invariant subspace $\mathcal{S}_n$.

  The proof follows immediately from the preceding lemma.

- Most often: $\mathcal{S}_n$ is irreducible
  - central property of nature for applying group theory to physics problems
  - unless noted otherwise, always assumed in the following
  - Identify d-fold degeneracy of λ_n with d-dimensional IR of $\mathcal{G}$.

- Under which cirumstances can $\mathcal{S}_n$ be reducible?
  - $\mathcal{G}$ does not include all symmetries realized in the system, i.e., $\mathcal{G} \subsetneqq \mathcal{G}'$ ("hidden symmetry"). Then $\mathcal{S}_n$ is an irreducible invariant subspace of $\mathcal{G}'$.

    Examples: hydrogen atom, m-dimensional harmonic oscillator ($m > 1$).
  - A variant of the preceding case: The extra degeneracy is caused by the antiunitary time reversal symmetry (more later).
  - The degeneracy cannot be explained by symmetry: rare!
    (Usually such "accidental degeneracies" correspond to singular points in the parameter space of a system.)

Symmetry of Observables (cont'd)

Remarks:

- IRs of $\mathcal{G}$ give the degeneracies that may occur in the spectrum of observable $\hat{\mathcal{O}}$.
- Usually, all IRs of $\mathcal{G}$ are realized in the spectrum of observable $\hat{\mathcal{O}}$

  (reasonable if eigenfunctions of $\hat{\mathcal{O}}$ form complete set)

Application 1: Symmetry-Adapted Basis

Let $\hat{\mathcal{O}} = \hat{H} =$ Hamiltonian

- Classify the eigenvalues and eigenstates of $\hat{H}$ according to the IRs Γ_I of the symmetry group $\mathcal{G}$ of $\hat{H}$.

  Notation: $\hat{H}\,|I\mu,\alpha\rangle = E_{I\alpha}\,|I\mu,\alpha\rangle \quad \mu = 1,\ldots,n_I$

  α: distinguish different levels transforming according to same Γ_I

  If Γ_I is n_I-dimensional, then eigenvalues $E_{I\alpha}$ are n_I-fold degenerate.

  Note: In general, the "quantum number" I cannot be associated directly with an observable.

- For given $E_{I\alpha}$, it suffices to calculate one eigenstate $|I\mu_0,\alpha\rangle$. Then

  $$\{|I\mu,\alpha\rangle : \mu = 1,\ldots,n_I\} = \{\hat{P}(g_i)\,|I\mu_0,\alpha\rangle : g_i \in \mathcal{G}\}$$

  (i.e., both sets span the same subspace of $\mathcal{H}$)

- Expand eigenstates $|I\mu,\alpha\rangle$ in a symmetry-adapted basis $\left\{|J\nu,\beta\rangle : \begin{array}{l} J = 1,\ldots,N; \\ \nu = 1,\ldots,n_J; \\ \beta = 1,2,\ldots \end{array}\right\}$

  $$|I\mu,\alpha\rangle = \sum_{J\nu,\beta} \underbrace{\langle J\nu,\beta|I\mu,\alpha\rangle}_{=\delta_{IJ}\,\delta_{\mu\nu}\,\langle I\,\alpha||I\,\beta\rangle} |J\nu,\beta\rangle = \sum_{\beta}\langle I\,\alpha||I\,\beta\rangle\,|I\mu,\beta\rangle$$

  see Theorem 11

  $\Rightarrow$ partial diagonalization of $\hat{H}$ independent of specific details

Application 2: Effect of Perturbations

- Let $\hat{H} = \hat{H}_0 + \hat{H}_1$, $\quad \hat{H}_0$ = unperturbed Hamiltonian: $\hat{H}_0 |n\rangle = E_n^{(0)} |n\rangle$
  $\hat{H}_1$ = perturbation
- Perturbation expansion $E_n = E_n^{(0)} + \langle n|\hat{H}_1|n\rangle + \sum_{n' \neq n} \frac{|\langle n|\hat{H}_1|n'\rangle|^2}{E_n^{(0)} - E_{n'}^{(0)}} + \ldots$

  $\Rightarrow$ need matrix elements $\langle n|\hat{H}|n'\rangle = E_n^{(0)}\,\delta_{nn'} + \langle n|\hat{H}_1|n'\rangle$
- Let $\mathcal{G}_0$ = symmetry group of $\hat{H}_0$
  $\mathcal{G}$ = symmetry group of $\hat{H}$ $\Big\}$ usually $\mathcal{G} \subsetneqq \mathcal{G}_0$
- The unperturbed eigenkets $\{|n\rangle\}$ transform according to IRs Γ_I^0 of $\mathcal{G}_0$
- $\{\Gamma_I^0\}$ are also representations of $\mathcal{G}$, yet then *reducible*
- Every IR Γ_I^0 of $\mathcal{G}_0$ breaks down into (usually multiple) IRs $\{\Gamma_J\}$ of $\mathcal{G}$

  $$\Gamma_I^0 = \sum_J a_J \Gamma_J \qquad \text{(see Theorem 7)}$$

  $\Rightarrow$ **compatibility relations** for irreducible representations
- **Theorem 16:** $\langle n = J\mu\alpha|\hat{H}|n' = J'\mu'\alpha'\rangle = \delta_{JJ'}\,\delta_{\mu\mu'}\langle J\alpha||\hat{H}||J'\alpha'\rangle$

  Proof: Similar to Theorem 11 with $\hat{H} = \hat{P}(g_j)^\dagger\,\hat{H}\,\hat{P}(g_j) = \frac{1}{h}\sum_i \hat{P}(g_i)^\dagger\,\hat{H}\,\hat{P}(g_i)$

Example: Compatibility Relations for $C_{3v} \simeq \mathcal{P}_3$

- Character table $C_{3v} \simeq \mathcal{P}_3$

C_{3v}	E	$2C_3$	$3\sigma_v$
$\mathcal{P}_3$	e	a, b	c, d, f
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	-1	0

- $C_{3v} \simeq \mathcal{P}_3$ has two subgroups $C_3 = \{E, C_3, C_3^2 = C_3^{-1}\} \simeq G_1 = \{e, a, b\}$

$$C_s = \{E, \sigma_v\} \simeq G_2 = \{e, c\} = \{e, d\} = \{e, f\}$$

- Both subgroups are Abelian, so they have only 1-dim. IRs

C_3	E	C_3	C_3^2
E	E	C_3	C_3^2
C_3	C_3	C_3^2	E
C_3^2	C_3^2	E	C_3

C_3	E	C_3	C_3^2
Γ_1	1	1	1
Γ_2	1	ω	ω^*
Γ_3	1	ω^*	ω

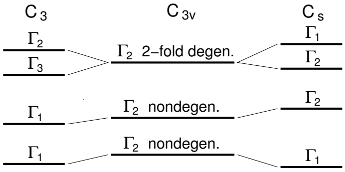
$\omega \equiv e^{2\pi i/3}$

C_s	E	σ_i
E	E	σ_i
σ_i	σ_i	E

C_s	E	σ_i
Γ_1	1	1
Γ_2	1	-1

- **compatibility relations**

C_{3v}	$\mathcal{P}_3$	Γ_1	Γ_2	Γ_3
C_3	G_1	Γ_1	Γ_1	$\Gamma_2 + \Gamma_3$
C_s	G_2	Γ_1	Γ_2	$\Gamma_1 + \Gamma_2$



Discussion: Compatibility Relations

Compatibility relations and Theorem 16 tell us how a degenerate level transforming according to the IR Γ_I^0 of $\mathcal{G}_0$ splits into multiple levels transforming according to certain IRs $\{\Gamma_J\}$ of $\mathcal{G}$ when the perturbation $\hat{H}_1$ reduces the symmetry from $\mathcal{G}_0$ to $\mathcal{G} \subsetneq \mathcal{G}_0$.

Thus qualitative statements:

- Which degenerate levels split because of $\hat{H}_1$?
- Which degeneracies remain unaffected by $\hat{H}_1$?
- These statements do not require any perturbation theory in the conventional sense.
  (For every pair $\mathcal{G}_0$ and $\mathcal{G}$, they can be tabulated once and forever!)
- These statements do not require some kind of "smallness" of $\hat{H}_1$.
- But no statement whether (or how much) a level will be raised or lowered by $\hat{H}_1$.

(Ir)Reducible Operators

- Up to now: symmetry group of operator $\hat{\mathcal{O}}$ requires
  $$\hat{P}(g_i)\,\hat{\mathcal{O}}\,\hat{P}(g_i)^{-1} = \hat{\mathcal{O}} \qquad \forall g_i \in \mathcal{G}$$

- **More general:** A set of operators $\{\hat{\mathcal{Q}}_\nu : \nu = 1, \ldots, n\}$ with
  $$\hat{P}(g_i)\,\hat{\mathcal{Q}}_\nu\,\hat{P}(g_i)^{-1} = \sum_{\mu=1}^{n} \mathcal{D}(g_i)_{\mu\nu}\,\hat{\mathcal{Q}}_\mu \qquad \begin{array}{l} \forall\ \nu = 1, \ldots, n \\ \forall\ g_i \in \mathcal{G} \end{array}$$
  is called reducible (irreducible), if $\Gamma = \{\mathcal{D}(g_i) : g_i \in \mathcal{G}\}$
  is a reducible (irreducible) representation of $\mathcal{G}$.

  Often a shorthand notation is used: $g_i\,\hat{\mathcal{Q}}_\nu \equiv \hat{P}(g_i)\,\hat{\mathcal{Q}}_\nu\,\hat{P}(g_i)^{-1}$

- **We say:** The operators $\{\hat{\mathcal{Q}}_\nu\}$ transform according to Γ.

- **Note:** In general, the eigenstates of $\{\hat{\mathcal{Q}}_\nu\}$ will <u>not</u> transform according to Γ.

(Ir)Reducible Operators (cont'd)

Examples:

- $\Gamma_1 =$ "identity representation"; $\mathcal{D}(g_i) = 1 \quad \forall g_i \in \mathcal{G}; \quad n_I = 1$

  $$\Rightarrow \quad \hat{P}(g_i)\, \hat{\mathcal{Q}}\, \hat{P}(g_i)^{-1} = \hat{\mathcal{Q}} \qquad \forall g_i \in \mathcal{G}$$

  We say: $\hat{\mathcal{Q}}$ is a scalar operator or invariant.

- most important scalar operator: the Hamiltonian $\hat{H}$
  i.e., $\hat{H}$ always transforms according to Γ_1

  The symmetry group of $\hat{H}$ is the largest symmetry group that leaves $\hat{H}$ invariant.

- position operator $\hat{x}_\nu$
  momentum operator $\hat{p}_\nu = -i\hbar\, \partial_{x_\nu}$ $\qquad \nu = 1, 2, 3 \qquad$ (polar vectors)

  $\Rightarrow \quad \{\hat{x}_\nu\}$ and $\{\hat{p}_\nu\}$ transform according to 3-dim. representation Γ_{pol} (possibly reducible!)

- composite operators (= tensor operators)

  e.g., angular momentum $\hat{l}_\nu = \sum_{\lambda,\mu} \varepsilon_{\lambda\mu\nu}\, \hat{x}_\lambda \hat{p}_\mu \qquad \nu = 1, 2, 3 \qquad$ (axial vector)

Tensor Operators

- Let $\hat{\boldsymbol{\mathcal{Q}}}^I \equiv \{\hat{\mathcal{Q}}^I_\mu : \mu = 1, \ldots, n_I\}$ transform according to $\Gamma_I = \{\mathcal{D}_I(g_i)\}$
  $\hat{\boldsymbol{\mathcal{Q}}}^J \equiv \{\hat{\mathcal{Q}}^J_\nu : \nu = 1, \ldots, n_J\}$ transform according to $\Gamma_J = \{\mathcal{D}_J(g_i)\}$
- Then $\left\{\hat{\mathcal{Q}}^I_\mu \, \hat{\mathcal{Q}}^J_\nu : {\scriptstyle \mu = 1, \ldots, n_I \atop \nu = 1, \ldots, n_J}\right\}$ transforms according to the product representation $\Gamma_I \times \Gamma_J$
- $\Gamma_I \times \Gamma_J$ is, in general, reducible

  $\Rightarrow$ The set of tensor operators $\left\{\hat{\mathcal{Q}}^I_\mu \, \hat{\mathcal{Q}}^J_\nu\right\}$ is likewise reducible
- A unitary transformation brings $\Gamma_I \times \Gamma_J = \{\mathcal{D}_I(g_i) \otimes \mathcal{D}_J(g_i)\}$ into block-diagonal form

  $\Rightarrow$ The same transformation decomposes $\left\{\hat{\mathcal{Q}}^I_\mu \, \hat{\mathcal{Q}}^J_\nu\right\}$ into irreducible tensor operators (use CGC)

Where Are We?

We have discussed

- the transformational properties of states
- the transformational properties of operators

Now:

- the transformational properties of matrix elements

$\Rightarrow$ Wigner-Eckart Theorem

Wigner-Eckart Theorem

Let $\{|I\mu,\alpha\rangle \quad : \mu = 1,\ldots,n_I\}$ transform according to $\Gamma_I = \{\mathcal{D}_I(g_i)\}$

$\{|I'\mu',\alpha'\rangle : \mu' = 1,\ldots,n_{I'}\}$ transform according to $\Gamma_{I'} = \{\mathcal{D}_{I'}(g_i)\}$

$\hat{\boldsymbol{\mathcal{Q}}}^J = \{\hat{\mathcal{Q}}^J_\nu : \nu = 1,\ldots,n_J\}$ transform according to $\Gamma_J = \{\mathcal{D}_J(g_i)\}$

Then $\langle I'\mu',\alpha' \,|\, \hat{\mathcal{Q}}^J_\nu \,|\, I\mu,\alpha\rangle = \sum_\ell \left(\begin{array}{cc|c} J & I & I'\,\ell \\ \nu & \mu & \mu' \end{array}\right) \langle I'\alpha' \,||\, \hat{\mathcal{Q}}^J \,||\, I\alpha\rangle_\ell$

where the reduced matrix element $\langle I'\alpha' \,||\, \hat{\mathcal{Q}}^J \,||\, I\alpha\rangle_\ell$ is independent of μ, μ' and ν.

Proof:

- $\left\{\hat{\mathcal{Q}}^J_\nu \,|I\mu,\alpha\rangle : \begin{smallmatrix}\mu = 1,\ldots,n_I \\ \nu = 1,\ldots,n_J\end{smallmatrix}\right\}$ transforms according to $\Gamma_I \times \Gamma_J$
- Thus CGC expansion $\hat{\mathcal{Q}}^J_\nu \,|I\mu,\alpha\rangle = \sum_{K\kappa,\ell} \left(\begin{array}{cc|c} J & I & K\,\ell \\ \nu & \mu & \kappa \end{array}\right) |K\kappa,\ell\rangle$
- $\langle I'\mu',\alpha' \,|\, \hat{\mathcal{Q}}^J_\nu \,|\, I\mu,\alpha\rangle = \sum_{K\kappa,\ell} \left(\begin{array}{cc|c} J & I & K\,\ell \\ \nu & \mu & \kappa \end{array}\right) \underbrace{\langle I'\mu',\alpha' \,|\, K\kappa,\ell\rangle}_{\equiv\, \delta_{I'K}\,\delta_{\mu'\kappa}\,\langle I'\alpha' \,||\, \hat{\mathcal{Q}}^J \,||\, I\alpha\rangle_\ell}$ Theorem 11

Discussion: Wigner-Eckart Theorem

- Matrix elements factorize into two terms
  - the reduced matrix element independent of μ, μ' and ν
  - CGC indexing the elements μ, μ' and ν of Γ_I, $\Gamma_{I'}$ and Γ_J.
    (CGC are tabulated, independent of $\hat{\mathcal{Q}}^J$)

- Thus:

$$\begin{aligned} \text{reduced matrix element} &= \text{“physics”} \\ \text{Clebsch-Gordan coefficients} &= \text{“geometry”} \end{aligned}$$

- Matrix elements for different values of μ, μ' and ν have a fixed ratio independent of $\hat{\mathcal{Q}}^J$

- If $\Gamma_{I'}$ is not contained in $\Gamma_I \times \Gamma_J$

  Equivalent to: If $\Gamma^*_{I'} \times \Gamma_J \times \Gamma_I$ does not contain the identity representation

  $$\Rightarrow \left(\begin{array}{cc|c} J & I & I' \ell \\ \nu & \mu & \mu' \end{array} \right) = 0 \quad \forall\, \nu, \mu, \mu'$$

  $$\Rightarrow \langle I' \mu', \alpha' \,|\, \hat{\mathcal{Q}}^J_\nu \,|\, I \mu, \alpha \rangle = 0 \quad \forall\, \nu, \mu, \mu'$$

  Many important selection rules are some variation of this result.

- Theorems 11 and 16 are special cases of the WE theorem for $\hat{\mathcal{Q}}^1 = \mathbb{1}$ and $\hat{\mathcal{Q}}^1 = \hat{H}$ (yet we proved the WE theorem via Theorem 11)

Discussion: Wigner-Eckart Theorem (cont'd)

Application: Perturbation theory

- Compatibility relations and Theorem 16 describe splitting of degenerate levels using the symmetry group $\mathcal{G}$ of perturbed problem
- Alternative approach
  Splitting of levels using the symmetry group $\mathcal{G}_0$ of unperturbed problem
  (i.e., no need to know group $\mathcal{G}$ of perturbed problem)
  - Let $\hat{\boldsymbol{\mathcal{Q}}}^J$ be tensor operator transforming according to IR Γ_J of $\mathcal{G}_0$
  - Often: perturbation $\hat{H}_1 = \boldsymbol{\mathcal{F}}^J \cdot \hat{\boldsymbol{\mathcal{Q}}}^J = \mathcal{F}_\nu^J \, \hat{\mathcal{Q}}_\nu^J$ i.e., $\hat{H}_1$ is proportional to only νth component of tensor operator $\hat{\boldsymbol{\mathcal{Q}}}^J$
    $\hat{\boldsymbol{\mathcal{Q}}}^J$ projected on component $\hat{\mathcal{Q}}_\nu^J$ via suitable orientation of field $\boldsymbol{\mathcal{F}}^J$
  - Symmetry group of $\hat{H} = \hat{H}_0 + \hat{H}_1$ is subgroup $\mathcal{G} \subset \mathcal{G}_0$ which leaves $\hat{\mathcal{Q}}_\nu^J$ invariant.
  - WE Theorem:
    $$\langle n|\hat{H}_1|n'\rangle = \mathcal{F}_\nu^J \, \langle n{=}I\mu\alpha|\hat{\mathcal{Q}}_\nu^J|n'{=}I'\mu'\alpha'\rangle = \sum_\ell \left(\begin{array}{cc|c} J & I' & I\,\ell \\ \nu & \mu' & \mu \end{array}\right) \langle I\alpha \,||\, \hat{\mathcal{Q}}^J \,||\, I'\alpha'\rangle_\ell \qquad (*)$$
  - Changing the orientation of $\boldsymbol{\mathcal{F}}^J$ changes only the CGCs in $(*)$
    The reduced matrix elements $\langle I\alpha \,||\, \hat{\mathcal{Q}}^J \,||\, I'\alpha'\rangle_\ell$ are "universal"

Example: Optical Selection Rules

Example: Optical transitions for a system with symmetry group C_{3v} (e.g., NH_3 molecule)

- Optical matrix elements $\langle i_I | \mathbf{e} \cdot \hat{\mathbf{r}} | f_J \rangle$ (dipole approximation)

  where $|i_I\rangle$ = initial state (with IR Γ_I); $|f_J\rangle$ = final state (IR Γ_J)
  $\mathbf{e} = (e_x, e_y, e_z)$ = polarization vector
  $\hat{\mathbf{r}} = (\hat{x}, \hat{y}, \hat{z})$ = dipole operator ($\equiv$ position operator)

- $\hat{x}, \hat{y}$ transform according to Γ_3
  $\hat{z}$ transforms according to Γ_1

- e.g., light xy polarized: $\langle i_1 | e_x \hat{x} + e_y \hat{y} | f_3 \rangle$
  - transition allowed because $\Gamma_3 \times \Gamma_3 = \Gamma_1 + \Gamma_2 + \Gamma_3$
  - in total 4 different matrix elements, but only one reduced matrix element

- z polarized: $\langle i_1 | e_z \hat{z} | f_3 \rangle$
  - transition forbidden because $\Gamma_1 \times \Gamma_3 = \Gamma_3$

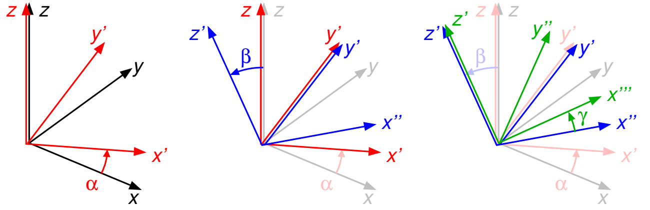
- These results are independent of any microscopic models for the NH_3 molecule!

Rotations and Euler Angles

- So far: transformation of functions and operators dependent on position
- Now: systems with spin degree of freedom
  $\Rightarrow$ wave functions are two-component Pauli spinors

$$\Psi(\mathbf{r}) = \psi_\uparrow(\mathbf{r})\,|\!\uparrow\rangle + \psi_\downarrow(\mathbf{r})\,|\!\downarrow\rangle \equiv \begin{pmatrix} \psi_\uparrow(\mathbf{r}) \\ \psi_\downarrow(\mathbf{r}) \end{pmatrix}$$

- How do Pauli spinors transform under symmetry operations?
- Parameterize rotations via Euler angles α, β, γ



axis z, angle α   axis y', angle β   axis z', angle γ

- Thus general rotation $\quad R(\alpha,\beta,\gamma) = R_{z'}(\gamma)\, R_{y'}(\beta)\, R_z(\alpha)$

Rotations and Euler Angles (cont'd)

- General rotation $R(\alpha,\beta,\gamma) = R_{z'}(\gamma)\, R_{y'}(\beta)\, R_z(\alpha)$
- Difficulty: axes y' and z' refer to rotated body axes (not fixed in space)
- Use
$$\begin{aligned} R_{z'}(\gamma) &= R_{y'}(\beta)\, R_z(\gamma)\, R_{y'}^{-1}(\beta) \\ R_{y'}(\beta) &= R_z(\alpha)\, R_y(\beta)\, R_z^{-1}(\alpha) \end{aligned}$$
preceding rotations are temporarily undone
- Thus $R(\alpha,\beta,\gamma) = \underbrace{R_{y'}(\beta)}_{R_z(\alpha)\, R_y(\beta)\, R_z^{-1}(\alpha)}\, R_z(\gamma)\, \underbrace{R_{y'}^{-1}(\beta)\, R_{y'}(\beta)}_{=\mathbb{1}}\, R_z(\alpha)$

  rotations about z axis commute
- Thus $R(\alpha,\beta,\gamma) = R_z(\alpha)\, R_y(\beta)\, R_z(\gamma)$

  rotations about space-fixed axes!
- More explicitly: rotations of vectors $\mathbf{r} = (x,y,z) \in \mathbb{R}^3$
$$R_z(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad R_y(\beta) = \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \quad \text{etc.}$$
- $SO(3)$ = set of all rotation matrices $R(\alpha,\beta,\gamma)$

  = set of all orthogonal 3×3 matrices R with $\det R = +1$.
- $R(2\pi,0,0) = R(0,2\pi,0) = R(0,0,2\pi) = \mathbb{1} \equiv e$

Rotations: Spin 1/2 Systems

- Rotation matrices for spin-1/2 spinors (axis $\mathbf{n}$)

$$\mathcal{R}_{\mathbf{n}}(\phi) = \exp\left(-\tfrac{i}{2}\boldsymbol{\sigma}\cdot\mathbf{n}\,\phi\right) = \mathbb{1}\cos(\phi/2) - i\mathbf{n}\cdot\boldsymbol{\sigma}\sin(\phi/2)$$

- $$\begin{aligned} \mathcal{R}(\alpha,\beta,\gamma) &= \mathcal{R}_z(\alpha)\,\mathcal{R}_y(\beta)\,\mathcal{R}_z(\gamma) \\ &= \begin{pmatrix} e^{-i(\alpha+\gamma)/2}\cos(\beta/2) & -e^{-i(\alpha-\gamma)/2}\sin(\beta/2) \\ e^{-i(\alpha-\gamma)/2}\sin(\beta/2) & e^{i(\alpha+\gamma)/2}\cos(\beta/2) \end{pmatrix} \end{aligned}$$

transformation matrix for spin 1/2 states

- $SU(2)$ = set of all matrices $\mathcal{R}(\alpha,\beta,\gamma)$
  = set of all unitary 2×2 matrices $\mathcal{R}$ with $\det\mathcal{R} = +1$.

- $\mathcal{R}(2\pi,0,0) = \mathcal{R}(0,2\pi,0) = \mathcal{R}(0,0,2\pi) = -\mathbb{1} \equiv \bar{e}$ — rotation by 2π is not identity

- $\mathcal{R}(4\pi,0,0) = \mathcal{R}(0,4\pi,0) = \mathcal{R}(0,0,4\pi) = \mathbb{1} = e$ — rotation by 4π is identity

- Every $SO(3)$ matrix $R(\alpha,\beta,\gamma)$ corresponds to two $SU(2)$ matrices $\mathcal{R}(\alpha,\beta,\gamma)$ and $\mathcal{R}(\alpha+2\pi,\beta,\gamma) = \mathcal{R}(\alpha,\beta+2\pi,\gamma) = \mathcal{R}(\alpha,\beta,\gamma+2\pi)$
  $= \bar{e}\,\mathcal{R}(\alpha,\beta,\gamma) = \mathcal{R}(\alpha,\beta,\gamma)\,\bar{e}$

$\Rightarrow$ $SU(2)$ is called **double group** for $SO(3)$

Double Groups

- **Definition: Double Group**
  Let the group of spatial symmetry transformations of a system be
  $$\mathcal{G} = \{g_i = R(\alpha_i, \beta_i, \gamma_i) : i = 1, \ldots, h\} \subset SO(3)$$
  Then the corresponding double group is
  $$\begin{aligned} \mathcal{G}_d = & \quad \{g_i = \mathcal{R}(\alpha_i, \beta_i, \gamma_i) : i = 1, \ldots, h\} \\ & \cup \{g_i = \mathcal{R}(\alpha_i + 2\pi, \beta_i, \gamma_i) : i = 1, \ldots, h\} \subset SU(2) \end{aligned}$$
- Thus with every element $g_i \in \mathcal{G}$ we associate two elements g_i and $\bar{g}_i \equiv \bar{e}\, g_i = g_i\, \bar{e} \in \mathcal{G}_d$
- If the order of $\mathcal{G}$ is h, then the order of $\mathcal{G}_d$ is $2h$.
- **Note:** $\mathcal{G}$ is not a subgroup of $\mathcal{G}_d$ because the elements of $\mathcal{G}$ are not a closed subset of $\mathcal{G}_d$.

  Example: Let g = rotation by π
  - in $\mathcal{G}$: $g^2 = e$
  - in $\mathcal{G}_d$: $g^2 = \bar{e}$

  the same group element g is thus interpreted differently in $\mathcal{G}$ and $\mathcal{G}_d$
- **Yet:** $\{e, \bar{e}\}$ is invariant subgroup of $\mathcal{G}_d$
  and the factor group $\mathcal{G}_d/\{e, \bar{e}\}$ is isomorphic to $\mathcal{G}$.

  $\Rightarrow$ The IRs of $\mathcal{G}$ are also IRs of $\mathcal{G}_d$

Example: Double Group C_{3v}

C_{3v}	E	$\bar{E}$	$2C_3$	$2\bar{C}_3$	$3\sigma_v$	$3\bar{\sigma}_v$
Γ_1	1	1	1	1	1	1
Γ_2	1	1	1	1	-1	-1
Γ_3	2	2	-1	-1	0	0
Γ_4	2	-2	1	-1	0	0
Γ_5	1	-1	-1	1	i	$-i$
Γ_6	1	-1	-1	1	$-i$	i

- For Γ_1, Γ_2, and Γ_3 the "barred" group elements have the same characters as the "unbarred" elements.
  Here the double group gives us the same IRs as the "single group"

- For other groups a class may contain both "barred" and "unbarred" group elements.
  $\Rightarrow$ the number of classes and IRs in the double group need not be twice the number of classes and IRs of the "single group"

Time Reversal (Reversal of Motion)

- Time reversal operator $\hat{\theta}$: $t \to -t$
- Action of $\hat{\theta}$:

$$\hat{\theta}\,\hat{\mathbf{r}}\,\hat{\theta}^{-1} = \hat{\mathbf{r}} \quad \Big\} \quad \text{independent of } t$$

$$\left.\begin{aligned} \hat{\theta}\,\hat{\mathbf{p}}\,\hat{\theta}^{-1} &= -\hat{\mathbf{p}} \\ \hat{\theta}\,\hat{\mathbf{L}}\,\hat{\theta}^{-1} &= -\hat{\mathbf{L}} \\ \hat{\theta}\,\hat{\mathbf{S}}\,\hat{\theta}^{-1} &= -\hat{\mathbf{S}} \end{aligned}\right\} \quad \text{linear in } t$$

- Consider time evolution: $\hat{\mathcal{U}}(\delta t) = 1 - i\hat{H}\,\delta t/\hbar$

$$\Rightarrow \quad \hat{\mathcal{U}}(\delta t)\,\hat{\theta}\,|\psi\rangle = \hat{\theta}\,\hat{\mathcal{U}}(-\delta t)\,|\psi\rangle$$

$$\Leftrightarrow \quad -i\hat{H}\,\hat{\theta}\,|\psi\rangle = \hat{\theta}\,i\hat{H}\,|\psi\rangle$$

but need also $[\hat{\theta}, \hat{H}] = 0$

$\Rightarrow$ Need $\hat{\theta} = UK$

U = unitary operator
K = complex conjugation

Properties of $\hat{\theta} = UK$:

- $K\big(c_1|\alpha\rangle + c_2|\beta\rangle\big) = c_1^*|\alpha\rangle + c_2^*|\beta\rangle$ (antilinear)
- Let $|\tilde{\alpha}\rangle = \hat{\theta}\,|\alpha\rangle$ and $|\tilde{\beta}\rangle = \hat{\theta}\,|\beta\rangle$

$$\Rightarrow \langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle$$

} $\hat{\theta} = UK$ is antiunitary operator

Time Reversal (cont'd)

The explicit form of $\hat{\theta}$ depends on the representation

- position representation: $\hat{\theta}\,\hat{\mathbf{r}}\,\hat{\theta}^{-1} = \hat{\mathbf{r}} \quad \Rightarrow \quad \hat{\theta}\,\psi(\mathbf{r}) = \psi^*(\mathbf{r})$
- momentum representation: $\hat{\theta}\,\hat{\mathbf{p}}\,\hat{\theta}^{-1} = -\hat{\mathbf{p}} \quad \Rightarrow \quad \hat{\theta}\,\psi(\mathbf{p}) = \psi^*(-\mathbf{p})$
- spin $1/2$ systems:
  - $\hat{\theta} = i\sigma_y\,K \quad \Rightarrow \quad \hat{\theta}^2 = -\mathbb{1}$
  - all eigenstates $|n\rangle$ of $\hat{H}$ are at least two-fold degenerate (Kramers degeneracy)

Time Reversal and Group Theory

- Consider a system with Hamiltonian $\hat{H}$.

- Let $\mathcal{G} = \{g_i\}$ be the symmetry group of spatial symmetries of $\hat{H}$

$$[\hat{P}(g_i), \hat{H}] = 0 \quad \forall g_i \in \mathcal{G}$$

- Let $\{|I\nu\rangle : \nu = 1, \ldots, n_I\}$ be an n_I-fold degenerate eigenspace of $\hat{H}$ which transforms according to IR $\Gamma_I = \{\mathcal{D}_I(g_i)\}$

$$\begin{aligned} \hat{H}\,|I\nu\rangle &= E_I\,|I\nu\rangle \quad \forall\nu \\ \hat{P}(g_i)\,|I\nu\rangle &= \sum_\mu \mathcal{D}_I(g_i)_{\mu\nu}|I\mu\rangle \end{aligned}$$

- Let $\hat{H}$ be time-reversal invariant: $[\hat{H}, \hat{\theta}] = 0$
  $\Rightarrow$ $\hat{\theta}$ is additional symmetry operator (beyond $\{\hat{P}(g_i)\}$) with

$$[\hat{\theta}, \hat{P}(g_i)] = 0$$

- $\hat{P}(g_i)\,\hat{\theta}\,|I\nu\rangle = \hat{\theta}\,\hat{P}(g_i)|I\nu\rangle = \hat{\theta}\sum_\mu \mathcal{D}_I(g_i)_{\mu\nu}\,|I\mu\rangle = \sum_\mu \mathcal{D}_I^*(g_i)_{\mu\nu}\,\hat{\theta}\,|I\mu\rangle$

- Thus: time-reversed states $\{\hat{\theta}\,|I\nu\rangle\}$ transform according to complex conjugate IR $\Gamma_I^* = \{\mathcal{D}_I^*(g_i)\}$

Time Reversal and Group Theory (cont'd)

- time-reversed states $\{\hat{\theta}\,|I\nu\rangle\}$ transform according to complex conjugate IR $\Gamma_I^* = \{\mathcal{D}_I^*(g_i)\}$

Three possiblities (known as "cases a, b, and c")

(a) $\{|I\nu\rangle\}$ and $\{\hat{\theta}\,|I\nu\rangle\}$ are linear dependent

(b) $\{|I\nu\rangle\}$ and $\{\hat{\theta}\,|I\nu\rangle\}$ are linear independent
The IRs Γ_I and Γ_I^* are distinct, i.e., $\chi_I(g_i) \neq \chi_I^*(g_i)$

(c) $\{|I\nu\rangle\}$ and $\{\hat{\theta}\,|I\nu\rangle\}$ are linear independent
$\Gamma_I = \Gamma_I^*$, i.e., $\chi_I(g_i) = \chi_I^*(g_i) \quad \forall\, g_i$

Discussion

- Case (a): time reversal is additional constraint for $\{|I\nu\rangle\}$
  e.g., $n_I = 1 \;\Rightarrow\; |\nu\rangle$ reell
- Cases (b) and (c): time reversal results in additional degeneracies
- Our definition of cases (a)–(c) follows Bir & Pikus. Often (e.g., Koster) a different classification is used which agrees with Bir & Pikus for spinless systems. But cases (a) and (c) are reversed for spin-1/2 systems.

Time Reversal and Group Theory (cont'd)

- When do we have case (a), (b), or (c)?

Criterion by Frobenius & Schur

$$\frac{1}{h}\sum_i \chi_I(g_i^2) = \begin{cases} \eta & \text{case (a)} \\ 0 & \text{case (b)} \\ -\eta & \text{case (c)} \end{cases}$$

where $\eta = \begin{cases} +1 & \text{systems with integer spin} \\ -1 & \text{systems with half-integer spin} \end{cases}$

Proof: Tricky! (See, e.g., Bir & Pikus)

Example: Cyclic Group $\mathcal{C}_3$

- $\mathcal{C}_3$ is Abelian group with 3 elements: $\mathcal{C}_3 = \{q, q^2, q^3 \equiv e\}$

- **Multiplication table**

$\mathcal{C}_3$	e	q	q^2
e	e	q	q^2
q	q	q^2	e
q^2	q^2	e	q

Character table

$\mathcal{C}_3$	e	q	q^2	time reversal
Γ_1	1	1	1	a
Γ_2	1	ω	ω^*	b
Γ_3	1	ω^*	ω	b

$\omega \equiv e^{2\pi i/3}$

- IR Γ_1: no additional degeneracies because of time reversal

- IRs Γ_2 and Γ_3: these complex IRs need to be combined

  $\Rightarrow$ two-fold degeneracy because of time reversal symmetry (though here no spin!)

Group Theory in Solid State Physics

First: Some terminology

- **Lattice:** periodic array of atoms (or groups of atoms)
- **Bravais lattice:**

  $\mathbf{R}_\mathbf{n} = n_x \mathbf{a}_x + n_y \mathbf{a}_y + n_z \mathbf{a}_z$ $\qquad$ $\mathbf{n} = (n_1, n_2, n_3) \in \mathbb{Z}^3$, $\mathbf{a}_i$ linearly independent

  Every lattice site $\mathbf{R}_\mathbf{n}$ is occupied with one atom

  Example: 2D honeycomb lattice is not a Bravais lattice

- **Lattice with basis:**
  - Every lattice site $\mathbf{R}_\mathbf{n}$ is occupied with z atoms
  - Position of atoms relative to $\mathbf{R}_\mathbf{n}$: $\quad \boldsymbol{\tau}_i, \quad i = 1, \ldots, q$
  - These q atoms with relative positions $\boldsymbol{\tau}_i$ form a basis.
  - **Example:** two neighboring atoms in 2D honeycomb lattice

Symmetry Operations of Lattice

- Translation $\mathbf{t}$ (not necessarily by lattice vectors $\mathbf{R_n}$)
- Rotation, inversion $\rightarrow$ 3×3 matrices α
- Combinations of translation, rotation, and inversion

  $\Rightarrow$ general transformation for position vector $\mathbf{r} \in \mathbb{R}^3$:

$$\mathbf{r}' = \alpha \mathbf{r} + \mathbf{t} \equiv \{\alpha | \mathbf{t}\}\, \mathbf{r}$$

- Notation $\{\alpha|\mathbf{t}\}$ includes also
  - Mirror reflection = rotation by π about axis perpendicular to mirror plane followed by inversion
  - Glide reflection = translation followed by reflection
  - Screw axis = translation followed by rotation

Symmetry operations $\{\alpha|\mathbf{t}\}$ form a group

- Multiplication $\{\alpha'|\mathbf{t}'\} \underbrace{\{\alpha|\mathbf{t}\}\,\mathbf{r}}_{\mathbf{r}'=\alpha\mathbf{r}+\mathbf{t}} = \alpha'\mathbf{r}' + \mathbf{t}' = \alpha'\alpha\mathbf{r} + \alpha'\mathbf{t} + \mathbf{t}'$

  $= \{\alpha'\alpha | \alpha'\mathbf{t} + \mathbf{t}'\}\,\mathbf{r}$
- Inverse Element $\{\alpha|\mathbf{t}\}^{-1} = \{-\alpha^{-1}| -\alpha^{-1}\mathbf{t}\}$

  because $\{\alpha|\mathbf{t}\}^{-1}\{\alpha|\mathbf{t}\} = \{\alpha^{-1}\alpha|\alpha^{-1}\mathbf{t} - \alpha^{-1}\mathbf{t}\} = \{\mathbb{1}|\mathbf{0}\}$

Classification

Symmetry Groups of Crystals

to be added ...

Translation Group

Translation group = set of operations $\{\mathbb{1}|\mathbf{R_n}\}$

- $\{\mathbb{1}|\mathbf{R_{n'}}\}\,\{\mathbb{1}|\mathbf{R_n}\} = \{\mathbb{1}|\mathbf{R_{n'}} + \mathbb{1}\,\mathbf{R_n}\} = \{\mathbb{1}|\mathbf{R_{n'+n}}\}$
  $\Rightarrow$ Abelian group
- associativity (trivial)
- identity element $\{\mathbb{1}|\mathbf{0}\} = \{\mathbb{1}|\mathbf{R_0}\}$
- inverse element $\{\mathbb{1}|\mathbf{R_n}\}^{-1} = \{\mathbb{1}|-\mathbf{R_n}\}$

Translation group Abelian $\Rightarrow$ only one-dimensional IRs

Irreducible Representations of Translation Group

(for clarity in one spatial dimension)

- Consider translations $\{\mathbb{1}|a\}$
- Translation operator $\hat{T}_a = \hat{T}_{\{\mathbb{1}|a\}}$ is unitary operator
  $\Rightarrow$ eigenvalues have modulus 1
- eigenvalue equation $\quad \hat{T}_a \, |\phi\rangle \; = \; e^{-i\phi} \, |\phi\rangle \qquad -\pi < \phi \leq \pi$
  more generally $\qquad \hat{T}_{na} \, |\phi\rangle = e^{-in\phi} \, |\phi\rangle \qquad n \in \mathbb{Z}$
- $\Rightarrow$ representations $\mathcal{D}(\{\mathbb{1}|R_{na}\}) = e^{-in\phi} \qquad -\pi < \phi \leq \pi$

Physical Interpretation of ϕ

Consider $\overbrace{\langle r \,|\, \hat{T}_a}^{\langle r-a|} \underbrace{\,|\, \phi\rangle}_{e^{-i\phi}|\phi\rangle}$ $\qquad \Rightarrow \qquad \langle r - a|\phi\rangle = e^{-i\phi} \, \langle r|\phi\rangle$

Thus: **Bloch Theorem** $\qquad$ (for $\phi = ka$)

- The wave vector k (or $\phi = ka$) labels the IRs of the translation group
- The wave functions transforming according to the IR Γ_k are Bloch functions $\quad \langle r|\phi\rangle = e^{ikr} u_k(r) \quad$ with

$$e^{ik(r-a)} u_k(r-a) = e^{ikr} u_k(r) e^{-ika} \qquad \text{or} \qquad u_k(r-a) = u_k(r)$$

Irreducible Representations of Space Groups

to be added . . .

Theory of Invariants

Luttinger (1956)
Bir & Pikus

Idea:

- Hamiltonian must be invariant under all symmetry transformations of the system

- Example: free particle

$$\hat{H} = E_{\text{kin}} = \underbrace{\frac{\hat{p}^2}{2m}}_{\text{scalar}} + \underbrace{\cancel{c_1\, \hat{\mathbf{p}}}}_{\text{not inversion symmetric}} + \underbrace{\cancel{c_2\, \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}}}_{\text{breaks time reversal}} + \underbrace{c_4\, \hat{p}^4}_{\text{scalar}} + \; . \; . \; .$$

- Crystalline solids:

$$E_{\text{kin}} = E(\mathbf{k}) = \text{kinetic energy of Bloch electron with crystal momentum } \mathbf{p} = \hbar\mathbf{k}$$

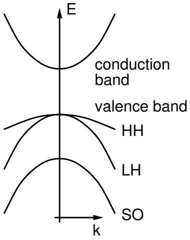
$\Rightarrow$ dispersion $E(\mathbf{k})$ must reflect crystal symmetry

$$E(\mathbf{k}) = a_0 + \underbrace{a_1\, k}_{} + a_2\, k^2 + \underbrace{a_3\, k^3}_{} + \ldots$$

only in crystals without inversion symmetry

Theory of Invariants (cont'd)

More generally:



- Bands $E(\mathbf{k})$ at expansion point $\mathbf{k}_0$ n-fold degenerate
- Bands split for $\mathbf{k} \neq \mathbf{k}_0$
- Example: GaAs ($\mathbf{k}_0 = 0$)
- Band structure $E(\mathbf{k})$ for small $\mathbf{k}$ via diagonalization of $n \times n$ matrix Hamiltonian $\mathcal{H}(\mathbf{k})$.
- **Goal:** Set up matrix Hamiltonian $\mathcal{H}(\mathbf{k})$ by exploiting the symmetry at expansion point $\mathbf{k}_0$
- Incorporate also perturbations such as
  - spin-orbit coupling (spin $\mathbf{S}$)
  - electric field $\boldsymbol{\mathcal{E}}$, magnetic field $\mathbf{B}$
  - strain ε
  - etc.

Invariance Condition

- Consider $n \times n$ matrix Hamiltonian $\mathcal{H}(\mathcal{K})$
- $\mathcal{K} = \mathcal{K}\,(\mathbf{k}, \mathbf{S}, \boldsymbol{\mathcal{E}}, \mathbf{B}, \varepsilon, \ldots) =$ general tensor operator

  where $\mathbf{k}$ = wave vector $\quad \boldsymbol{\mathcal{E}}$ = electric field $\quad \varepsilon$ = strain field
  $\mathbf{S}$ = spin $\quad \mathbf{B}$ = magnetic field $\quad$ etc.

- Basis functions $\{\psi_\nu(\mathbf{r}) : \nu = 1, \ldots, n\}$ transform according to representation $\Gamma_\psi = \{\mathcal{D}_\psi(g_i)\}$ of group $\mathcal{G}$. (Γ_ψ does not have to be IR)
- Symmetry transformation $g_i \in \mathcal{G}$ applied to tensor $\mathcal{K}$

$$\mathcal{K} \;\rightarrow\; g_i\,\mathcal{K} \equiv \hat{P}(g_i)\,\mathcal{K}\,\hat{P}(g_i)^{-1}$$

$$\Rightarrow \quad \mathcal{H}(\mathcal{K}) \;\rightarrow\; \mathcal{H}(g_i\,\mathcal{K})$$

- Equivalent to *inverse* transformation g_i^{-1} applied to $\psi_\nu(\mathbf{r})$:

$$\psi_\nu(\mathbf{r}) \;\rightarrow\; \psi_\nu(g_i\mathbf{r}) = \sum_\mu \mathcal{D}_\psi(g_i^{-1})_{\mu\nu}\,\psi_\mu(\mathbf{r})$$

$$\Rightarrow \quad \mathcal{H}(\mathcal{K}) \;\rightarrow\; \mathcal{D}_\psi(g_i)\,\mathcal{H}(\mathcal{K})\,\mathcal{D}_\psi(g_i^{-1})$$

- Thus $\quad \mathcal{D}_\psi(g_i^{-1})\,\mathcal{H}(g_i\,\mathcal{K})\,\mathcal{D}_\psi(g_i) = \mathcal{H}(\mathcal{K}) \qquad \forall\, g_i \in \mathcal{G}$

  really n^2 equations!

Invariance Condition (cont'd)

Remarks

- If $-\mathbf{k}_0$ is in the same star as the expansion point $\mathbf{k}_0$, additional constraints arise from time reversal symmetry.

  in particular: $-\mathbf{k}_0 = \mathbf{k}_0 = 0$

- If Γ_ψ is reducible, the invariance condition can be applied to each "irreducible block" of $\mathcal{H}(\mathcal{K})$ (see below).

Invariant Expansion

Expand $\mathcal{H}(\mathcal{K})$ in terms of irreducible tensor operators and basis matrices

- Decompose tensors $\mathcal{K}$ into irreducible tensors $\mathcal{K}^J$ transforming according to IR Γ_J of $\mathcal{G}$

$$\mathcal{K}_\nu^J \;\rightarrow\; g_i\, \mathcal{K}_\nu^J \;\equiv \sum_\mu \mathcal{D}_J(g_i)_{\mu\nu}\, \mathcal{K}_\mu^J$$

- n^2 linearly independent basis matrices $\{X_q : q = 1, \ldots, n^2\}$ transforming as

$$X_q \;\rightarrow\; g_i\, X_q \equiv \mathcal{D}_\psi(g_i^{-1})\, X_q\, \mathcal{D}_\psi(g_i) = \sum_p \mathcal{D}_X(g_i)_{pq}\, X_p$$

  with "expansion coefficents" $\mathcal{D}_X(g_i)_{pq}$

- Representation $\Gamma_X \simeq \Gamma_\psi^* \times \Gamma_\psi$ is usually reducible.

  We have IR Γ_ψ for the ket basis functions of $\mathcal{H}$ and
  IR Γ_ψ^* (i.e., the complex conjugate IR) for the bras

  $\Rightarrow$ from $\{X_q : q = 1, \ldots, n^2\}$ form linear combinations $X_\nu^{I^*}$ transforming according to the IRs Γ_I^* occuring in $\Gamma_\psi^* \times \Gamma_\psi$

$$X_\mu^{I^*} \;\rightarrow\; g_i\, X_\mu^{I^*} = \sum_\nu \mathcal{D}_I^*(g_i)_{\mu\nu}\, X_\mu^{I^*}$$

Invariant Expansion (cont'd)

- Consider most general expansion

$$\mathcal{H}(\boldsymbol{\mathcal{K}}) = \sum_{IJ} \sum_{\mu\nu} b_{\mu\nu}^{IJ} \, X_\mu^{I^*} \mathcal{K}_\nu^J \qquad b_{\mu\nu}^{IJ} = \text{expansion coefficients}$$

- Transformations $g_i \in \mathcal{G}$:

$$X_\mu^{I^*} \to \sum_{\mu'} \mathcal{D}_I^*(g_i)_{\mu'\mu} \, X_{\mu'}^{I^*}, \qquad \mathcal{K}_\nu^J \to \sum_{\nu'} \mathcal{D}_J(g_i)_{\nu'\nu} \, \mathcal{K}_{\nu'}^J$$

- Use invariance condition (must hold $\forall \, g_i \in \mathcal{G}$)

$$\sum_{\mu\nu} b_{\mu\nu}^{IJ} X_\mu^{I^*} \mathcal{K}_\nu^J = \sum_{\mu\nu} b_{\mu\nu}^{IJ} \sum_{\mu'\nu'} \underbrace{\frac{1}{h} \sum_i \mathcal{D}_I^*(g_i)_{\mu'\mu} \, \mathcal{D}_J(g_i)_{\nu'\nu}}_{\delta_{IJ} \, \delta_{\mu'\nu'} \, \delta_{\mu\nu}} X_{\mu'}^{I^*} \, \mathcal{K}_{\nu'}^J$$

$$= \delta_{IJ} \underbrace{\sum_\mu b_{\mu\mu}^{II}}_{\equiv a_I} \sum_{\mu'} X_{\mu'}^{I^*} \, \mathcal{K}_{\mu'}^I$$

- Then $\mathcal{H}(\boldsymbol{\mathcal{K}}) = \sum_I a_I \sum_\nu X_\nu^{I^*} \mathcal{K}_\nu^I$

Irreducible Tensor Operators

Construction of irreducible tensor operators $\mathcal{K} = \mathcal{K}(\mathbf{k}, \mathbf{S}, \mathcal{E}, \mathbf{B}, \varepsilon)$

- Components k_i, S_i, $\mathcal{E}_i$, B_i, ε_{ij} transform according to some IRs Γ_I of $\mathcal{G}$.
  $\Rightarrow$ "elementary" irreducible tensor operators $\mathcal{K}^I$

- Construct higher-order irreducible tensor operators with CGC:

$$\mathcal{K}^K_\kappa = \sum_{\mu\nu} \left(\begin{array}{cc|c} I & J & K\,\ell \\ \mu & \nu & \kappa \end{array} \right) \mathcal{K}^I_\mu \, \mathcal{K}^J_\nu$$

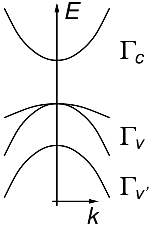
  If we have multiplicities $a^{IJ}_K > 1$ we get different tensor operators for each value ℓ

- Irreducible tensor operators $\mathcal{K}^I$ are "universally valid" for any matrix Hamiltonian transforming according to $\mathcal{G}$

- Yet: if for a particular matrix Hamiltonian $\mathcal{H}(\mathcal{K})$ with basis functions $\{\psi_\nu\}$ transforming according to Γ_ψ an IR Γ_I does not appear in $\Gamma^*_\psi \times \Gamma_\psi$, then the tensor operators $\mathcal{K}^I$ may not appear in $\mathcal{H}(\mathcal{K})$.

Basis Matrices

- In general, the basis functions $\{\psi_\nu(\mathbf{r}) : \nu = 1, \ldots, n\}$ include several irreducible representations Γ_J



  $\Rightarrow$ Decompose $\mathcal{H}(\boldsymbol{\mathcal{K}})$ into $n_J \times n_{J'}$ blocks $\mathcal{H}_{JJ'}(\boldsymbol{\mathcal{K}})$, such that
  - rows transform according to IR Γ_J^* (dimension n_J)
  - columns transform according to IR $\Gamma_{J'}$ (dimension $n_{J'}$)

$$\mathcal{H}(\boldsymbol{\mathcal{K}}) = \begin{pmatrix} \mathcal{H}_{cc} & \mathcal{H}_{cv} & \mathcal{H}_{cv'} \\ \mathcal{H}_{cv}^\dagger & \mathcal{H}_{vv} & \mathcal{H}_{vv'} \\ \mathcal{H}_{cv'}^\dagger & \mathcal{H}_{vv'}^\dagger & \mathcal{H}_{v'v'} \end{pmatrix}$$

- Choose basis matrices $X_\nu^{I^*}$ transforming according to the IRs Γ_I^* in $\Gamma_J^* \times \Gamma_{J'}$

$$X_\nu^{I^*} \;\to\; \mathcal{D}_J(g_i^{-1})\, X_\nu^{I^*}\, \mathcal{D}_{J'}(g_i) = \sum_\mu \mathcal{D}_I^*(g_i)_{\mu\nu}\, X_\mu^{I^*}$$

- More explicitly: $\quad (X_\nu^{I^*})_{\lambda\mu} = \left(\begin{matrix} I & J' \\ \nu & \mu \end{matrix}\middle|\begin{matrix} J\,\ell \\ \lambda \end{matrix}\right)^*$

  which reflects the transformation rules for matrix elements $\langle J\lambda|\mathcal{K}_\nu^I|J'\mu\rangle$

$\Rightarrow$ For each block we get $\quad \mathcal{H}_{JJ'}(\boldsymbol{\mathcal{K}}) = \sum_I a_I \sum_\nu X_\nu^{I^*} \mathcal{K}_\nu^I$

Time Reversal

- time reversal $\hat{\theta}$ connects expansion point $\mathbf{k}_0$ and $-\mathbf{k}_0$
- often: $\hat{\theta}\,\psi_{\mathbf{k}_0\lambda}(\mathbf{r})$ and $\psi_{-\mathbf{k}_0\lambda}(\mathbf{r})$ linearly dependent

$$\hat{\theta}\,\psi_{\mathbf{k}_0\lambda}(\mathbf{r}) = \sum_{\lambda'} \mathcal{T}_{\lambda\lambda'}\,\psi_{-\mathbf{k}_0\lambda'}(\mathbf{r})$$

- thus additional condition

$$\mathcal{T}^{-1}\,\mathcal{H}(\zeta\boldsymbol{\mathcal{K}})\,\mathcal{T} = \mathcal{H}^*(\boldsymbol{\mathcal{K}}) = \mathcal{H}^t(\boldsymbol{\mathcal{K}})$$

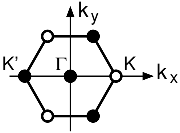
applicable in particular for $\mathbf{k}_0 = -\mathbf{k}_0 = 0$

$\zeta = +1$: $\boldsymbol{\mathcal{K}}$ even under θ
$\zeta = -1$: $\boldsymbol{\mathcal{K}}$ even under θ

- $\mathbf{k}_0 \neq -\mathbf{k}_0$: often $\mathbf{k}_0$ and $-\mathbf{k}_0$ also connected by spatial symmetries R

$$\mathcal{H}_{-\mathbf{k}_0}(\boldsymbol{\mathcal{K}}) = \mathcal{D}(R)\,\mathcal{H}_{\mathbf{k}_0}(R^{-1}\boldsymbol{\mathcal{K}})\,\mathcal{D}^{-1}(R).$$

$$\Rightarrow \quad \mathcal{T}^{-1}\mathcal{H}_{\mathbf{k}_0}(R^{-1}\boldsymbol{\mathcal{K}})\mathcal{T} = \mathcal{H}^*_{\mathbf{k}_0}(\zeta\boldsymbol{\mathcal{K}}) = \mathcal{H}^t_{\mathbf{k}_0}(\zeta\boldsymbol{\mathcal{K}})$$



graphene: $\mathbf{k}_0 = \mathbf{K}$

Example: Graphene

- Electron states at K point: point group C_{3v}

  strictly speaking $D_{3h} = C_{3v}$ + inversion

- "Dirac cone": IR Γ_3 of C_{3v}

  It must be Γ_3 because this is the only 2D IR of C_{3v}

- We have $\Gamma_3^* \times \Gamma_3 = \Gamma_1 + \Gamma_2 + \Gamma_3$ (with $\Gamma_3^* = \Gamma_3$)

  $\Rightarrow$ basis matrices $X_1^1 = \mathbb{1}$; $X_1^2 = \sigma_y$; $X_1^3 = \sigma_z,\ X_2^3 = -\sigma_x$

- Irreducible tensor operators $\mathcal{K}$ up to second order in k:

  $\Gamma_1 : k_x^2 + k_y^2$ $\Gamma_3 : k_x, k_y;\ k_y^2 - k_x^2, 2k_x k_y$ Γ_2: $[k_x, k_y] \propto B_z$

- Hamiltonian here: basis functions $|x\rangle$ and $|y\rangle$

$$\mathcal{H}(\mathcal{K}) = a_{31}(k_x\sigma_z - k_y\sigma_x) + a_{11}(k_x^2 + k_y^2)\mathbb{1} + a_{32}[(k_y^2 - k_x^2)\sigma_z - 2k_x k_y \sigma_x]$$

- More common: basis functions $|x - iy\rangle$ and $|x + iy\rangle$

  $\Rightarrow$ basis matrices $X_1^1 = \mathbb{1}$; $X_1^2 = \sigma_z$; $X_1^3 = \sigma_x,\ X_2^3 = \sigma_y$

$$\mathcal{H}(\mathcal{K}) = a_{31}(k_x\sigma_x + k_y\sigma_y) + a_{11}(k_x^2 + k_y^2)\mathbb{1} + a_{32}[(k_y^2 - k_x^2)\sigma_x + 2k_x k_y \sigma_y]$$

- additional constraints for $\mathcal{H}(\mathcal{K})$ from time reversal symmetry

Graphene: Basis Matrices (D_{3h})

Symmetrized matrices for the invariant expansion of the blocks $\mathcal{H}_{\alpha\beta}$ for the point group D_{3h}.

Block	Representations	Symmetrized matrices	
$\mathcal{H}_{55}$	$\Gamma_5^* \times \Gamma_5$	$\Gamma_1 : \; \mathbb{1}$	no spin
	$= \Gamma_1 + \Gamma_2 + \Gamma_6$	$\Gamma_2 : \; \sigma_z$	
		$\Gamma_6 : \; \sigma_x, \sigma_y$	
$\mathcal{H}_{77}$	$\Gamma_7^* \times \Gamma_7$	$\Gamma_1 : \; \mathbb{1}$	with spin
	$= \Gamma_1 + \Gamma_2 + \Gamma_5$	$\Gamma_2 : \; \sigma_z$	
		$\Gamma_5 : \; \sigma_x, -\sigma_y$	
$\mathcal{H}_{99}$	$\Gamma_9^* \times \Gamma_9$	$\Gamma_1 : \; \mathbb{1}$	
	$= \Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$	$\Gamma_2 : \; \sigma_z$	
		$\Gamma_3 : \; \sigma_x$	
		$\Gamma_4 : \; \sigma_y$	
$\mathcal{H}_{79}$	$\Gamma_7^* \times \Gamma_9$	$\Gamma_5 : \; \mathbb{1}, -i\sigma_z$	
	$= \Gamma_5 + \Gamma_6$	$\Gamma_6 : \; \sigma_x, \sigma_y$	

Graphene: Irreducible Tensor Operators (D_{3h})

Terms printed in bold give rise to invariants in $\mathcal{H}^{\mathbf{K}}_{55}(\mathcal{K})$ allowed by time-reversal invariance. Notation: $\{A, B\} \equiv \frac{1}{2}(AB + BA)$.

Γ_1	$\mathbf{1}$; $\mathbf{k_x^2 + k_y^2}$; $\mathbf{\{k_x, 3k_y^2 - k_x^2\}}$; $k_x\mathcal{E}_x + k_y\mathcal{E}_y$; $\boldsymbol{\epsilon_{xx} + \epsilon_{yy}}$; $\boldsymbol{(\epsilon_{yy} - \epsilon_{xx})k_x + 2\epsilon_{xy}k_y}$; $(\epsilon_{yy} - \epsilon_{xx})\mathcal{E}_x + 2\epsilon_{xy}\mathcal{E}_y$; $\mathbf{s_xB_x + s_yB_y}$; $\mathbf{s_zB_z}$; $\mathbf{(s_xk_y - s_yk_x)\boldsymbol{\mathcal{E}}_z}$; $\mathbf{s_z(k_x\boldsymbol{\mathcal{E}}_y - k_y\boldsymbol{\mathcal{E}}_x)}$;
Γ_2	$\{k_y, 3k_x^2 - k_y^2\}$; $\mathbf{B_z}$; $\mathbf{k_x\boldsymbol{\mathcal{E}}_y - k_y\boldsymbol{\mathcal{E}}_x}$; $(\epsilon_{xx} - \epsilon_{yy})k_y + 2\epsilon_{xy}k_y$; $\boldsymbol{(\epsilon_{xx} + \epsilon_{yy})B_z}$; $\boldsymbol{(\epsilon_{xx} - \epsilon_{yy})\mathcal{E}_y + 2\epsilon_{xy}\mathcal{E}_x}$; $\mathbf{s_z}$; $s_xB_y - s_yB_x$; $(s_xk_x + s_yk_y)\mathcal{E}_z$; $\boldsymbol{s_z(\epsilon_{xx} + \epsilon_{yy})}$;
Γ_3	$B_xk_x + B_yk_y$; $\mathcal{E}_xB_x + \mathcal{E}_yB_y$; $\mathcal{E}_zB_z$; $(\epsilon_{yy} - \epsilon_{xx})B_x + 2\epsilon_{xy}B_y$; $s_xk_x + s_yk_y$; $s_x\mathcal{E}_x + s_y\mathcal{E}_y$; $s_z\mathcal{E}_z$; $s_x(\epsilon_{yy} - \epsilon_{xx}) + 2s_y\epsilon_{xy}$
Γ_4	$B_xk_y - B_yk_x$; $\mathcal{E}_z$; $\mathcal{E}_xB_y - \mathcal{E}_yB_x$; $(\epsilon_{xx} - \epsilon_{yy})B_y + 2\epsilon_{xy}B_x$; $(\epsilon_{xx} + \epsilon_{yy})\mathcal{E}_z$; $s_xk_y - s_yk_x$; $s_x\mathcal{E}_y - s_y\mathcal{E}_x$; $s_y(\epsilon_{xx} - \epsilon_{yy}) + 2s_x\epsilon_{xy}$
Γ_5	B_x, B_y; $B_yk_y - B_xk_x, B_xk_y + B_yk_x$; $k_y\mathcal{E}_z, -k_x\mathcal{E}_z$; $\mathcal{E}_yB_y - \mathcal{E}_xB_x, \mathcal{E}_yB_x + \mathcal{E}_xB_y$; $(\epsilon_{xx} + \epsilon_{yy})(B_x, B_y)$; $(\epsilon_{xx} - \epsilon_{yy})B_x + 2\epsilon_{xy}B_y, (\epsilon_{yy} - \epsilon_{xx})B_y + 2\epsilon_{xy}B_x$; $2\epsilon_{xy}\mathcal{E}_z, (\epsilon_{xx} - \epsilon_{yy})\mathcal{E}_z$; s_x, s_y; $s_yk_y - s_xk_x, s_xk_y + s_yk_x$; $s_yB_z, -s_xB_z$; $s_zB_y, -s_zB_x$; $s_y\mathcal{E}_y - s_x\mathcal{E}_x, s_x\mathcal{E}_y + s_y\mathcal{E}_x$; $(s_x, s_y)(\epsilon_{xx} + \epsilon_{yy})$; $s_x(\epsilon_{xx} - \epsilon_{yy}) - 2s_y\epsilon_{xy}, s_y(\epsilon_{yy} - \epsilon_{xx}) - 2s_x\epsilon_{xy}$

Graphene: Irreducible Tensor Operators (cont'd)

Γ_6	$\mathbf{k_x, k_y}$; $\{\mathbf{k_y + k_x, k_y - k_x}\}, 2\{\mathbf{k_x, k_y}\}$;
	$\{\mathbf{k_x, k_x^2 + k_y^2}\}, \{\mathbf{k_y, k_x^2 + k_y^2}\}$; $B_z k_y, -B_z k_x$;
	$\mathcal{E}_x, \mathcal{E}_y$; $k_y \mathcal{E}_y - k_x \mathcal{E}_x, k_x \mathcal{E}_y + k_y \mathcal{E}_x$;
	$\boldsymbol{\mathcal{E}_y B_z, -\mathcal{E}_x B_z}$; $\boldsymbol{\mathcal{E}_z B_y, -\mathcal{E}_z B_x}$;
	$\boldsymbol{\epsilon_{yy} - \epsilon_{xx}, 2\epsilon_{xy}}$; $\boldsymbol{(\epsilon_{xx} + \epsilon_{yy})(k_x, k_y)}$;
	$\boldsymbol{(\epsilon_{xx} - \epsilon_{yy}) k_x + 2\epsilon_{xy} k_y, (\epsilon_{yy} - \epsilon_{xx}) k_y + 2\epsilon_{xy} k_x}$;
	$2\epsilon_{xy} B_z, (\epsilon_{xx} - \epsilon_{yy}) B_z$;
	$(\epsilon_{xx} - \epsilon_{yy}) \mathcal{E}_x + \epsilon_{xy} \mathcal{E}_y, (\epsilon_{yy} - \epsilon_{xx}) \mathcal{E}_y + \epsilon_{xy} \mathcal{E}_x$;
	$(\epsilon_{xx} + \epsilon_{yy})(\mathcal{E}_x, \mathcal{E}_y)$; $s_z k_y, -s_z k_x$;
	$\boldsymbol{s_y B_y - s_x B_x, s_x B_y + s_y B_x}$; $\boldsymbol{s_z \mathcal{E}_y, -s_z \mathcal{E}_x}$;
	$\boldsymbol{s_y \mathcal{E}_z, -s_x \mathcal{E}_z}$; $\boldsymbol{s_z (k_x \mathcal{E}_y + k_y \mathcal{E}_x), s_z (k_x \mathcal{E}_x - k_y \mathcal{E}_y)}$;
	$\boldsymbol{(s_x k_y + s_y k_x) \mathcal{E}_z, (s_x k_x - s_y k_y) \mathcal{E}_z}$;
	$2 s_z \epsilon_{xy}, s_z (\epsilon_{xx} - \epsilon_{yy})$;

Graphene: Full Hamiltonian

Winkler and Zülicke, PRB **82**, 245313

$\mathcal{H}(\mathcal{K}) = a_{61}(k_x\sigma_x + k_y\sigma_y)$	"Dirac term"
$+ a_{12}(k_x^2 + k_y^2)\mathbb{1} + a_{62}[(k_y^2 - k_x^2)\sigma_x + 2k_xk_y\sigma_y]$	nonlinear + anisotropic corrections
$+ a_{22}(k_x\mathcal{E}_y - k_y\mathcal{E}_x)\sigma_z$	orbital Rashba term
$+a_{21}B_z\sigma_z$	orbital Zeeman term
$+ a_{14}(\epsilon_{xx} + \epsilon_{yy})\mathbb{1} + a_{66}[(\epsilon_{yy} - \epsilon_{xx})\sigma_x + 2\epsilon_{xy}\sigma_y]$	strain-induced terms
$+a_{15}[(\epsilon_{yy} - \epsilon_{xx})k_x + 2\epsilon_{xy}k_y]\mathbb{1}$	
$+a_{67}(\epsilon_{xx} + \epsilon_{yy})(k_x\sigma_x + k_y\sigma_y)$	isotropic velocity renormalization
$a_{68}\{[(\epsilon_{xx} - \epsilon_{yy})k_x + 2\epsilon_{xy}k_y]\sigma_x$ $+[(\epsilon_{yy} - \epsilon_{xx})k_y + 2\epsilon_{xy}k_x]\sigma_y\}$	anisotropic velocity renormalization
$+a_{23}(\epsilon_{xx} + \epsilon_{yy})B_z\sigma_z$	strain - orbital Zeeman
$+a_{24}[(\epsilon_{xx} - \epsilon_{yy})\mathcal{E}_y + 2\epsilon_{xy}\mathcal{E}_x]\sigma_z$	strain - orbital Rashba
$+ a_{21}\, s_z\sigma_z$	intrinsic SO coupling
$+ a_{61}\, s_z(\mathcal{E}_y\sigma_x - \mathcal{E}_x\sigma_y) + a_{62}\,\mathcal{E}_z(s_y\sigma_x - s_x\sigma_y)$	Rashba SO coupling
$+a_{63}\, s_z[(k_x\mathcal{E}_y + k_y\mathcal{E}_x)\sigma_x + (k_x\mathcal{E}_x - k_y\mathcal{E}_y)\sigma_y]$	
$+a_{64}\,\mathcal{E}_z[(s_xk_y + s_yk_x)\sigma_x + (s_xk_x - s_yk_y)\sigma_y]$	
$+a_{11}\,(s_xk_y - s_yk_x)\mathcal{E}_z + a_{12}\, s_z(k_x\mathcal{E}_y - k_y\mathcal{E}_x)$	
$+ a_{26}(\epsilon_{xx} + \epsilon_{yy})s_z\sigma_z$	strain-mediated SO coupling

Symbols

$\mathcal{G}$	group
$\mathcal{U}$	subgroup
$a, b, c, \ldots$	group elements
$i, j, k, \ldots$	indeces labeling group elements
e	unit element (= identity element) of a group
h	order of a group (= number of group elements)
$\mathcal{C}_k$	classes of a group
h_k	number of group elements in class $\mathcal{C}_k$
$\tilde{N}$	number of classes
$\mathcal{D}(g_i)$	matrix representation for group element g_i
$\Gamma = \{\mathcal{D}(g_i)\}$	(irreducible) representation
$I, J, K, \ldots$	indeces labeling irreducible representations
N	number of irreducible representations
$\mu, \nu, \lambda, \ldots$	indeces labeling the elements of representation matrices $\mathcal{D}(g_i)$
n_I	dimensionality of irreducible representation Γ_I
$\chi_I(g_i)$	character of representation matrix for group element g_i
a_K^{IJ}	multiplicity with which Γ_K is contained in $\Gamma_I \times \Gamma_J$
$\mathcal{H}$	Hilbert space, multiband Hamiltonian
$\mathcal{S}_I$	invariant subspace (IR Γ_I)
α, β	we may have multiple irreducible invariant subspaces $\mathcal{S}_I^\alpha$ for one IR Γ_I
$\hat{P}(g_i)$	unitary operator that realizes the symmetry element g_i in the Hilbert space

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IR	irreducible representation