Advanced Quantum Mechanics

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Lecture #2

Symmetries and Quantum Mechanics

Ref : J. P. Elliot and P. G. Dawber, Symmetry in Physics
Sakurai, Modern Quantum Mechanics
Landau and Lifshitz, Quantum Mechanics
Michael Artin, Algebra
Serge Lang, Algebra

Recap of Last Class

- Symmetries as guiding principle
- Shapes and Symmetries: Definition of Symmetry
- Groups: defn. , examples of groups, examples of sets which are NOT groups
- Set of all symmetry transformations have properties of a group
- Group Tables: Combination Rules, Homomorphism and Isomorphism

Conjugacy Classes

Consider a group element G_a. Now consider the set of Group elements $G_b G_a G_b^{-1}$, where G_b runs over all group elements. This set defines a conjugacy class.

- An element of a group belongs to one and only one class
- Identity element is in a class by itself
- Each member of an Abelian group forms a class by themselves

Example:

Group : {1,-1}

Classes: {1},{-1}

	1	-1
1	1	-1
-1	-1	1

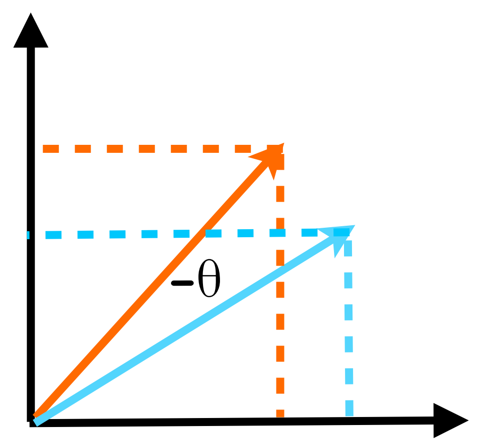
Basics of Group Theory

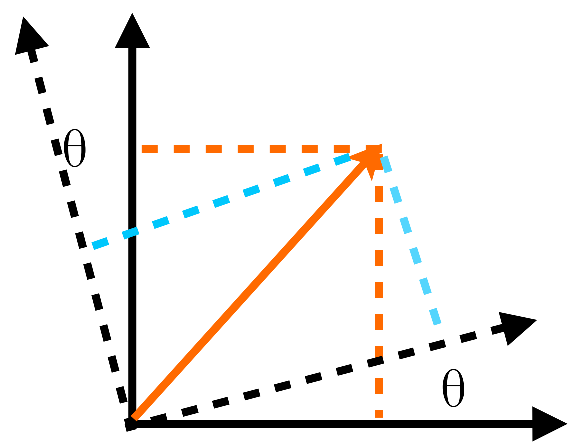
Conjugacy Classes

Consider a group element G_a. Now consider the set of Group elements $G_b G_a G_b^{-1}$, where G_b runs over all group elements. This set defines a conjugacy class.

Example: Rotation Group

Each rotation is characterized by an unit vector for the axis and an angle of rotation $R(\hat{n}, \theta)$





$R^{-1}(\hat{n}, \theta)$ is a rotation of the co-ordinate system about the axis $\hat{n}$ by angle θ

$$R(\hat{k}, \phi) R(\hat{n}, \theta) R^{-1}(\hat{k}, \phi)$$

Rotate co-ord. about k by φ
In rotated basis rotate vectors about n by θ
Rotate co-ord back to original

Overall, we have rotated about some axis (not n in original co-ord system) by θ

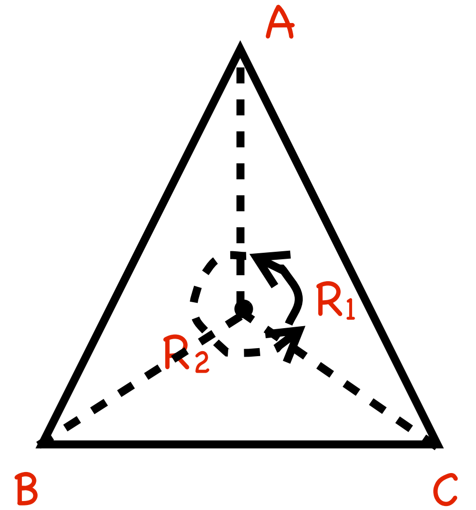
So rotations by the same angle about different axes form a conjugacy class.

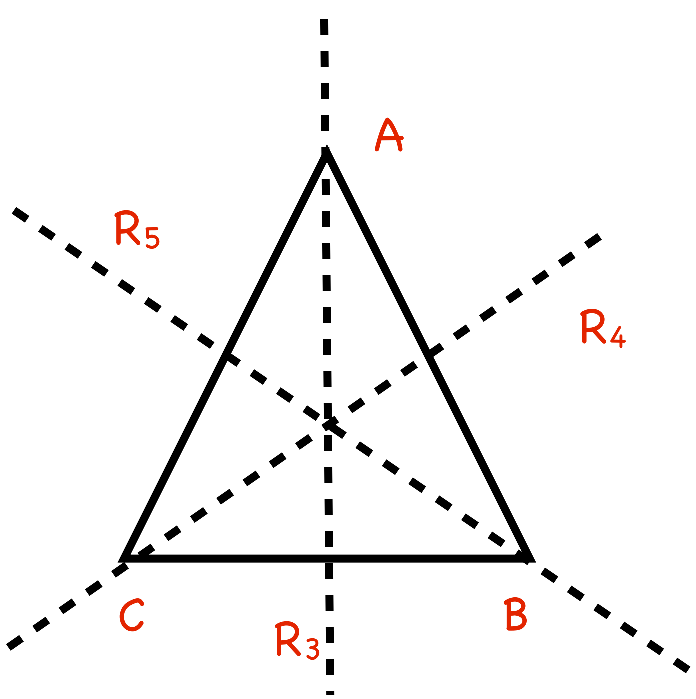
Basics of Group Theory

Conjugacy Classes

Consider a group element G_a. Now consider the set of Group elements $G_b G_a G_b^{-1}$, where G_b runs over all group elements. This set defines a conjugacy class.

Example: **Group D_3**: Symmetries of Equilateral Triangle





	E	R_1	R_2	R_3	R_4	R_5
E	E	R_1	R_2	R_3	R_4	R_5
R_1	R_1	R_2	E	R_4	R_5	R_3
R_2	R_2	E	R_1	R_5	R_3	R_4
R_3	R_3	R_5	R_4	E	R_2	R_1
R_4	R_4	R_3	R_5	R_1	E	R_2
R_5	R_5	R_4	R_3	R_2	R_1	E

Conjugacy Classes: $\{E\}$, $\{R_1,R_2\}$, $\{R_3,R_4,R_5\}$

Note that E is rotation by 0, $\{R_1,R_2\}$ is rotation by $2\pi/3$, and $\{R_3,R_4,R_5\}$ are rotations by π

Representation of Groups

Formal Definition: A mapping from group elements G_a to a set of linear operators on a vector space (matrices !!) T_a is called a Representation of the group if the mapping preserves group multiplication relations.

$G_a \rightarrow T(G_a)$ $G_b \rightarrow T(G_b)$ If $G_a G_b = G_c$, then $T(G_a)\,T(G_b) = T(G_c) = T(G_a G_b)$

Examples:

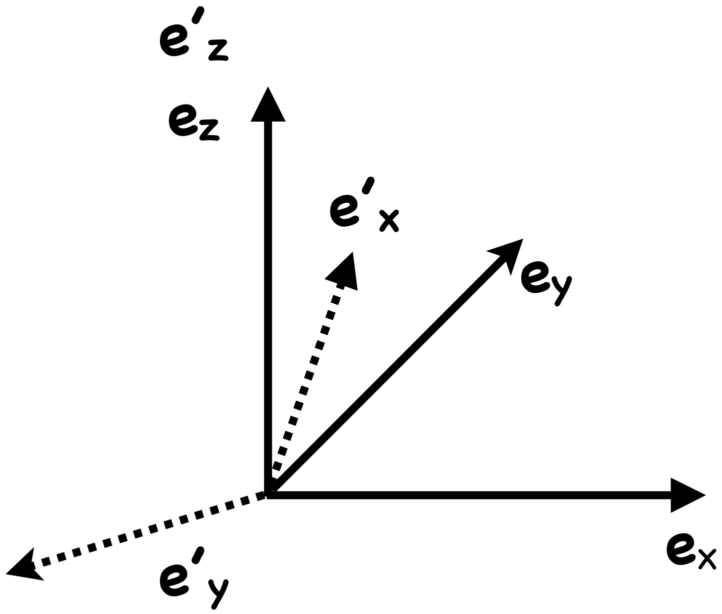
Identity Representation: All group elements map onto 1 (or identity matrix)

Set of Rotations in 2D: $R(\theta) \rightarrow \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$ $R(\theta) \rightarrow \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Each symmetry transformation (which was an abstract concept) corresponds to a linear operator in the Hilbert space and we would like to study the properties of these operators.

Constructing Representation of Groups

Example: Representation of D_3 :



- Take a basis in 3D real vector space, $\mathbf{e}_x$, $\mathbf{e}_y$ and $\mathbf{e}_z$.
- Apply the elements of D_3 to $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ and generate new basis vectors $\mathbf{e'}_x$, $\mathbf{e'}_y$, $\mathbf{e'}_z$.
- The matrix $T_{ij}(G_a) = \langle e_i | e'_j \rangle = \langle e_i | T(G_a) | e_j \rangle$.
- These matrices (one for each transform) form a representation of D_3

$$T_E \to \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad T_{R_1} = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} & 0 \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad T_{R_2} = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} & 0 \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$T_{R_3} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad T_{R_4} = \begin{pmatrix} \frac{1}{2} & -\sqrt{\frac{3}{4}} & 0 \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad T_{R_5} = \begin{pmatrix} \frac{1}{2} & \sqrt{\frac{3}{4}} & 0 \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Check using these matrices and the group multiplication tables, that this is a representation of D_3

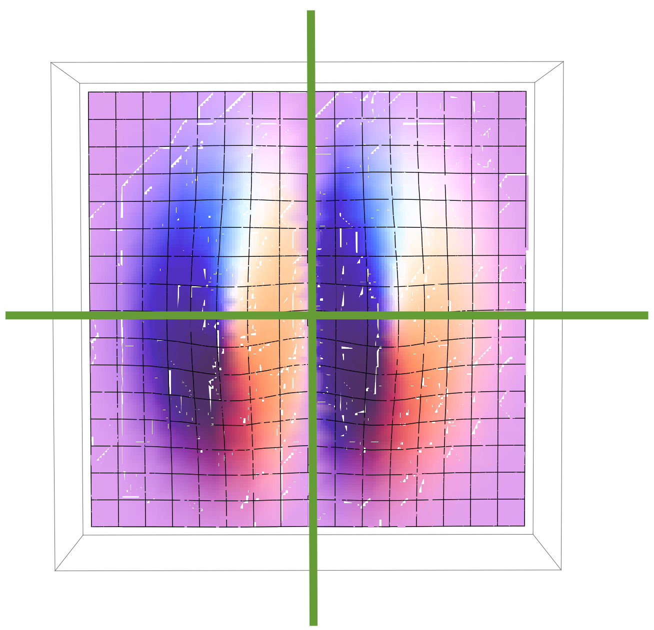
Representations are however, not unique. To see this, let us construct another representation of D_3

Function Spaces and Transformation of wfn.s

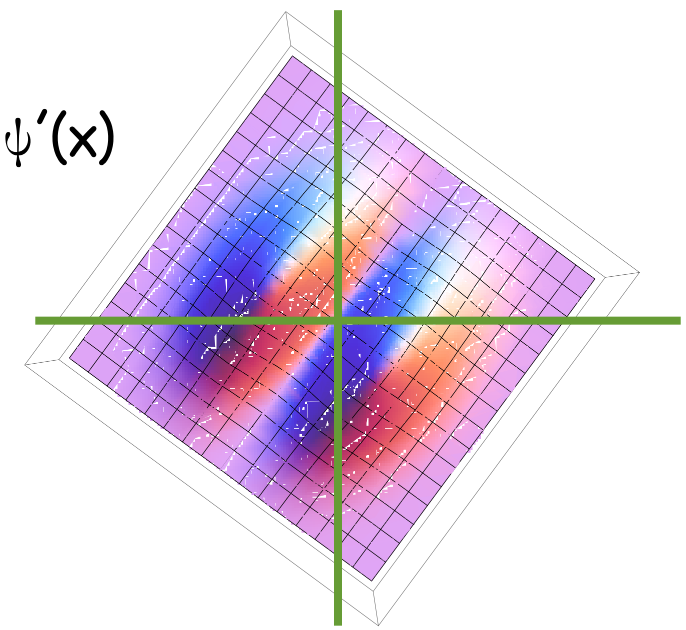
Consider a spatial symmetry (say rotation) which transforms the co-ordinates. How does a function of the co-ordinates (a wavefunction or a field as the case may be) change under this transform?

Rotation of the system followed by the same rotation of co-ordinate axes leads to the same functional form of the wavefunction.

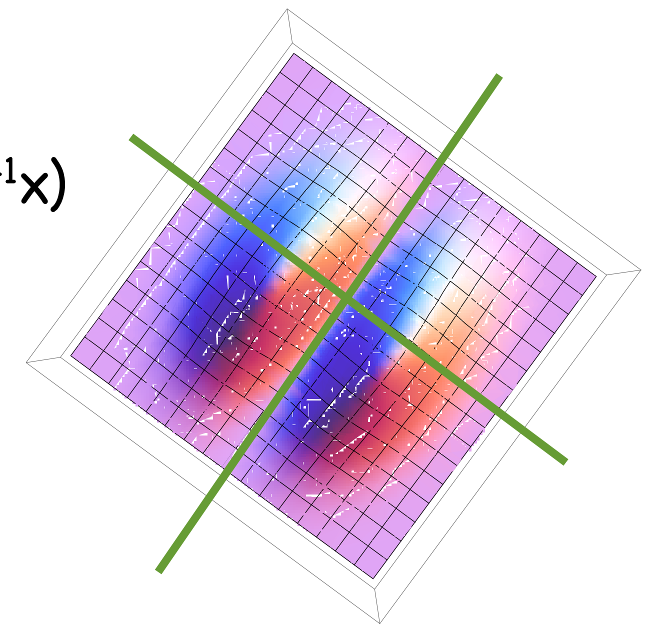
$\psi(x)$



$\psi'(x)$



$\psi(x') = \psi(R^{-1}x)$



So $\psi^{'}(\vec{x}) = \psi(R^{-1}\vec{x})$

More generally: $\psi^{'}(\vec{r}) = \psi(G_b^{-1}\vec{r})$

$$T(G_a)\psi(\vec{r}) = \psi(G_a^{-1}\vec{r})$$

$$T(G_a)T(G_b)\psi(\vec{r}) = T(G_a)\psi(G_b^{-1}\vec{r}) = T(G_a)\psi^{'}(\vec{r})$$

$$= \psi^{'}(G_a^{-1}\vec{r}) = \psi(G_b^{-1}G_a^{-1}\vec{r}) = T(G_aG_b)\psi(\vec{r})$$

preserves Group Multiplication
and provides a representation of G

Constructing Representation of Groups

Example: Another Representation of D_3 :

Consider the space of all quadratic functions of (x,y,z),

$$f(x,y,z)= c_1x^2+c_2y^2+c_3z^2+c_4xy+c_5yz+c_6xz$$

. Then $\{x^2,y^2,z^2,xy,yz,xz\}$ can act as a basis set in this vector space.

$$|\psi\rangle = (c_1, c_2, c_3, c_4, c_5, c_6)^T \rightarrow c_1x^2 + c_2y^2 + c_3z^2 + c_4xy + c_5yz + c_6xz$$

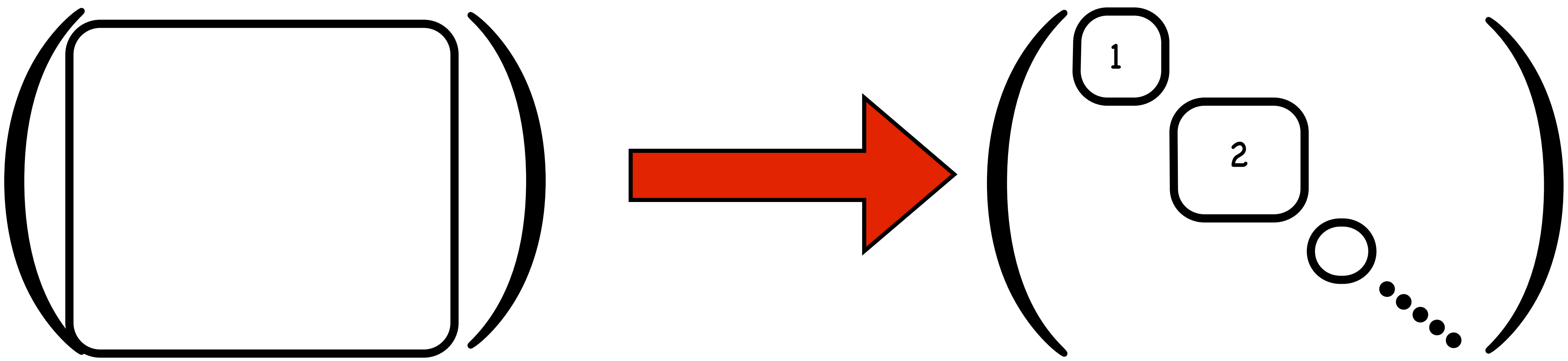
Apply the symmetry transformations of D_3 to x^2,y^2,z^2, xy, yz, xz and generate the new basis set. The dot product of the new and old basis defines the matrix T, one for each transformation.

- We have constructed 2 representations (of 3 and 6 dim) of the same group.
- It is clear that we can look at cubic fn.s and generate a 10 dim. representation of D_3

Is there a more systematic way of studying the properties of representations?

Irreducible Representations

If one writes down a representation of a group, one can change basis and try to reduce the matrices (with same basis trans. for all the matrices) to a block diagonal form. The representation for which this cannot be done is called an irreducible representation. Otherwise it is said to be reducible.



Example: D_3

$$T_E \rightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T_{R_1} = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} & 0 \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T_{R_2} = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} & 0 \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$T_{R_3} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad T_{R_4} = \begin{pmatrix} \frac{1}{2} & -\sqrt{\frac{3}{4}} & 0 \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad T_{R_5} = \begin{pmatrix} \frac{1}{2} & \sqrt{\frac{3}{4}} & 0 \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Irreducible Representations

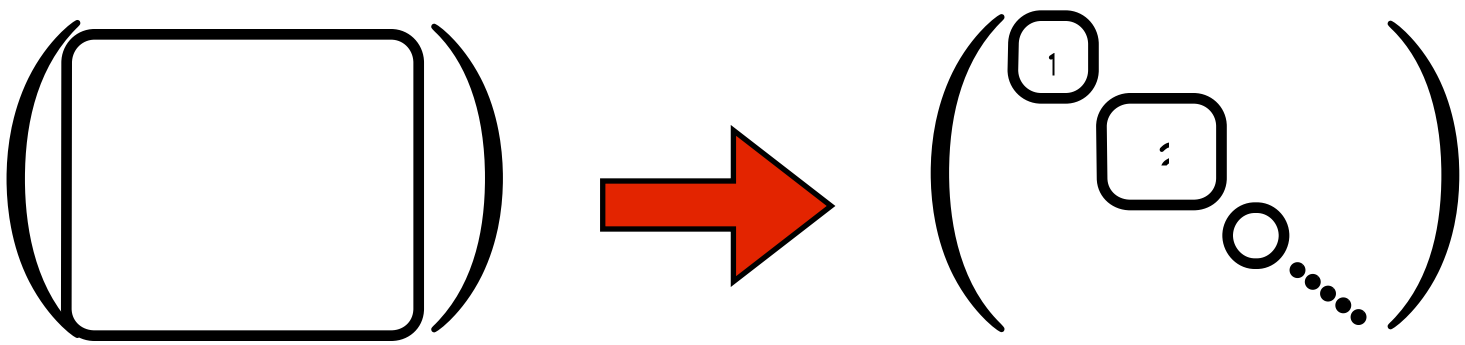
We will study the properties of irreps of a group, rather than all possible representations.

We will show how to reduce a representation into its irreps.

Given a group, how does one find the irreps?

Will not answer this ... assume irreps of groups are known ... true for most groups you would meet in physics .... we will look up tables people have catalogued.

How can we decompose (reduce) arbitrary representations into irreps?



How do we do this?

$$T = T^{(1)} \oplus T^{(2)} \oplus \ldots$$

For finite groups all representations can be built up in this way

How do we translate from groups and representations to info about the quantum system?

Orthogonality Property of Irreps.

Assume that we know the irreps (the sets of irreducible matrices, one for each group element).

We will also assume that these matrices are unitary (for finite groups you can always find unitary irreps). These matrices then satisfy

$$\sum_{a=1}^{g} T_{ip}^{(\alpha)}(G_a) T_{jq}^{(\beta)}(G_a)^* = \delta_{\alpha\beta}\delta_{ij}\delta_{pq}\frac{g}{s_\alpha}$$

Sum over Group Elements (Group Avg.)

order of group

dim. of irrep

Note: Group avg. replaced by appropriate integrals for cont. groups (at least for compact group)

See Elliott and Dawber or std. books on group theory for proof

No restriction on i,p,j,q
Huge number of constraints

The large no. of constraints are at the heart of the ability to predict that certain matrix elements of quantum operators should be zero.

We will use the orthogonality properties to reduce a representation into irreps.

Characters and Orthogonality

Character: The character of a group representation is the set of traces of the representation matrices.

$$\chi_a = \sum_i T_{ii}^{(\alpha)}(G_a)$$ (one for each group element)

$$T(G_b)T(G_a)T(G_b^{-1}) = T(G_b)T(G_a)T^{-1}(G_b)$$ is a similarity transformation under which trace is invariant

So, the elements of a given conjugacy class have the same character

Orthogonality of characters:

$$\sum_{a=1}^{g} T_{ip}^{(\alpha)}(G_a)T_{jq}^{(\beta)}(G_a)^* = \delta_{\alpha\beta}\delta_{ij}\delta_{pq}\frac{g}{s_\alpha}$$

Put p=i, q=j and sum over i,j

$$\sum_{a=1}^{g}\sum_i T_{ii}^{(\alpha)}(G_a)\sum_j T_{jj}^{(\beta)}(G_a)^* = g\delta_{\alpha\beta}$$

$$\sum_{a=1}^{g}\chi^{(\alpha)}(G_a)\chi^{(\beta)}(G_a)^* = g\delta_{\alpha\beta} \qquad \sum_{p=1}^{n} c_p\chi_p^{(\alpha)}\chi_p^{(\beta)*} = g\delta_{\alpha\beta}$$

c_p is the number of elements in the p^{th} conjugacy class

$$\sum_{p=1}^{n} c_p|\chi_p^{(\alpha)}|^2 = g$$

How to reduce Representations

Given a representation (g Matrices) of a group, and irreps of the group, how do we reduce the representation into irreps?

If $T = \oplus_\alpha m^{(\alpha)} T^{(\alpha)}$ (An irrep can occur more than once in a reduction)

Taking Trace $\chi_p = \sum_\alpha m^{(\alpha)} \chi_p^{(\alpha)}$

Using Orthogonality of characters

$$\frac{1}{g}\sum_p c_p \chi_p^{(\beta)*} \chi_p = \frac{1}{g}\sum_p c_p \chi_p^{(\beta)*} \sum_\alpha m^{(\alpha)} \chi_p^{(\alpha)} = \frac{1}{g}\sum_\alpha m^{(\alpha)} \sum_p c_p \chi_p^{(\beta)*} \chi_p^{(\alpha)} = m^{(\beta)}$$

We need to know the characters of all the conjugacy classes for all the irreps of the group. These are tabulated in the character table for the group.

Example: D_3

For finite groups, no. of irreps = no. of conjugacy classes

Columns are conjugacy classes

Rows are irreps

	{E}	{R_1,R_2}	{R_3,R_4,R_5}
$T^{(1)}$	1	1	1
$T^{(2)}$	1	1	-1
$T^{(3)}$	2	-1	0

Identity Class, irrep. matrices are identity matrices, characters give dimension of irrep

Group Representations and QM

In the QM Hilbert space, symmetry transformations correspond to linear operators which form a representation of the group.

Transformation of a quantum state under symmetry operations:

$$|\psi^{'}\rangle = T(G_a)|\psi\rangle$$

How do operators change under a symmetry transform?

$$\hat{A}^{'} = T(G_a)\hat{A}T^{-1}(G_a) = T(G_a)\hat{A}T(G_a^{-1})$$

Defn. of Symmetry in QM:

If $T(G_a)\hat{H}T^{-1}(G_a) = \hat{H}$, then the Hamiltonian has the corresponding symmetries.

Note that symmetry is about invariance of H, not of eigenstates

Group Representations and QM

Defn. of Symmetry in QM:

Note that symmetry is about invariance of H, not of eigenstates

If $T(G_a)\hat{H}T^{-1}(G_a) = \hat{H}$, then the Hamiltonian has the corresponding symmetries.

$$T(G_a)\hat{H}T^{-1}(G_a) = \hat{H} \Rightarrow [T(G_a), \hat{H}] = 0 \quad \Rightarrow \frac{d}{dt}T(G_a) = 0$$

- $T(G_a)$ and H can be diagonalized simultaneously.... classification of energy eigenstates.
  (For a non-Abelian group, $T(G_a)$ and $T(G_b)$ does not commute. We would need to make a choice of eigenbasis.)
- $T(G_a)$ is conserved, but does it represent an observable? ... not necessarily!!
- How many independent conserved quantities would we have?

Note that the symmetry operators themselves transform as $T^{'}(G_b) = T(G_a)T(G_b)T(G_a^{-1})$

Thus, representation operators of elements in a conjugacy class transform amongst themselves.

Invariant Subspaces

Consider now the set of g states, $\{|\psi_a\rangle\}$ where $|\psi_a\rangle = T(G_a)|\psi\rangle$ (one for each group element G_a)

These vectors span a subspace which is invariant under the symmetry operations, i.e. vectors in this (sub)space transform to other vectors in this (sub)space.

Invariant Subspaces and degeneracies:

Consider now an invariant subspace generated from an eigenstate of the Hamiltonian $\hat{H}|\psi\rangle = E|\psi\rangle$

$$\hat{H}|\psi_a\rangle = \hat{H}T(G_a)|\psi\rangle = T(G_a)\hat{H}|\psi\rangle = ET(G_a)|\psi\rangle = E|\psi_a\rangle$$

So these vectors (and their linear combinations) have degenerate eigenvalues. If these vectors are linearly independent, one can make an orthonormal basis set out of their linear combinations (Gram-Schmidt procedure) and get a g dim. representation of the group

In general these vectors are NOT linearly independent, but one can usually find a subset of s < g vectors which are linearly independent. These can then form the basis vectors for a s dim. representation of the group and correspondingly there will be s-fold degenerate states.

This s dimensional invariant subspace corresponds to a s-dim irrep of the symmetry group.

Irreps Eigenstates and Degeneracies

- The eigenstates of a Hamiltonian can be labeled by the irrep.s of its symmetry group.
- If an irrep is s-dimensional, then eigenstates corresponding to that irrep is s-fold degenerate

Applications: Inversion Symmetry

All irreps of Abelian groups are 1-D

- There are 2 irreps given by +1 and -1. (Irreps are 1D matrices or simply numbers)
- Eigenstates are either even (corresponding to +1) or odd (corresponding to -1) under inversion.
- No degeneracy (all irrep.s are 1D)

Examples

1-D SHO:

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega_0^2 \hat{x}^2$$

1D SHO + delta fn.:

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega_0^2 \hat{x}^2 + \lambda\delta(\hat{x})$$

Eigenstates are either even or odd in x

2D Potential :

$$V(x, y) = \lambda xy$$

$$\psi_e(r, \theta) = \sum_{l=even} f_l(r) e^{il\theta}$$

Even eigenstates

$$\psi_o(r, \theta) = \sum_{l=odd} f_l(r) e^{il\theta}$$

Odd eigenstates