An Algebraic Approach to Quantum Systems Using Finite Group Representation

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Good. Let's get started.

Abstract

Undergraduate physics emphasises the Schrödinger's analytic approach in solving and understanding quantum systems. Although briefly mentioned, group-theoretic approach is not emphasised, at least in terms of mathematical rigour. I attempt to kill the two rabbits - rigour and application. Part I develops the necessary formal theory of representation of finite group. In part II: Application, I primarily focus on the behaviour of an electron in various potentials where the spherical symmetry of an atom is broken into finite symmetry where I can readily apply the machinaries that I have developed in part I. Basic notions of group theory, linear algebra and quantum mechanics are assumed.

I.0. Prologue: Group Action on a Vector Space

Definition A *group* G is a set with an associative group operation $f : G \bigotimes G \to G$ that contains an identity element, and an inverse element for each group element $g \in G$.

Remark. The identity element is unique and so is the inverse g^{-1} of $g \in G$. For future reference, we denote $1 \in \mathbb{N}$ as an ordinary number or as the group identity. We denote $\mathbb{1}$ as the identity operator of a linear map.

Definition $\pi : G \to Perm(X)$ is called *group action* if π is a group homomorphism such that $\pi_1 x = x$, $\forall x \in X$.

Consider the cyclic group $G = C_n = (\rho)(\cong \mathbb{Z}/n\mathbb{Z})$ where G is generated by ρ. Let G act on a 2-dimensional Euclidean space, or more formally, define $\pi : G \to Perm(\mathbb{R}^2)$ such that

$$\pi_\rho \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos(\frac{2\pi}{n})x - \sin(\frac{2\pi}{n})y \\ \sin(\frac{2\pi}{n})x + \cos(\frac{2\pi}{n})y \end{pmatrix} \in \mathbb{R}^2.$$

This suggests the following:

$$\pi_\rho = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}, \text{ where } \phi = \frac{2\pi}{n},$$

an *active* transformation on $\mathbb{R}^2$ as opposed to *passive* transformation.

Remark. Strictly speaking, G consists of abstract group elements. The π_ρ *represents* the elements (and hence G) by matrices. Note that this G-representation by π_ρ depends on the basis of $\mathbb{R}^2$. I.e., had we used a different basis, we would have obtained a different *representation* of G.

This combines group action and matrices, or in general, group theory and linear algebra. In terms of application, representation theory enriches the algebraic language of group theory with computational power. Let us recall the following theorem from linear algebra that plays a fundamental role in representation theory throughout.

Theorem *$Hom(V, W)$ and $M_{mn}(\mathbb{C})$ form a vector space over $\mathbb{C}$, and are isomorphic. Similarly, $GL(V) \cong GL_n(\mathbb{C})$, where $dim_{\mathbb{C}} V = n$.*

We will generally assume that a vector space is of finite dimension over $\mathbb{C}$, and similarly a group of finite order, unless otherwise stated. Now we introduce the coordinate-free definition of representation.

I.1. Group and Representation

Definition A *representation* of G is a group homomorphism $\gamma : G \to GL(V)$ for some vector space V.

e.g.) Let $G = C_n$, $V_0 = \mathbb{C}$. $\gamma_g = 1$, $\forall g \in G$ defines a *trivial representation*. Notice that $dim(V) = 1$ yields an ordinary function, because $GL(V) \cong C^*$. In fact, let us say that a representation is of *degree* n if $dim(V) = n$.

e.g.) With the same G, $V_1 = \mathbb{C}^2$. $\gamma_\rho = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}$ where $\phi = \dfrac{2\pi}{n}$ defines a representation of G. Hence, the example given at the prologue is a group representation.

e.g.) With the same G, let $V_2 = \mathbb{C}$. Since $o(\rho) = n$, $o(\gamma_\rho) = n$ (o is the order notation in group theory). In other words $\gamma_\rho^n = 1$. This limits the values of γ_ρ to be the roots of unity. In fact, $\gamma_\rho = \xi_n^k$, $\xi_n = e^{\frac{2\pi ki}{n}}$ for $k = 0, 1, ...n-1$ defines n *inequivalent, irreducible* represenations.

The examples illustrate the two following points: 1° The choice of V is not unique. 2° For a fixed group, there exist many representations.

On the other hand, in analogy with the Unique Factorisation Theorem of $\mathbb{N}$, we want to classify a given representation by primes, or irreducible representations, or simply *irreps* as a shorthand. In fact, this decomposition of a complicated object into *prime elements* is ubiquitous and fundamental in mathematics. Before presenting formal definitions, let the following example on the symmetry group of H_2 molecule motivate further discussions.

e.g.) Although the *full symmetry group* of H_2 involves the identity, 180° rotation and infinitely many rotations through the H_2, let us ignore the infinite rotations. I.e., the symmetry group is C_2, not $D_{\infty h}$, the usual crystallographic notation. Let $C_2 = \{1, \tau\}$, where τ transposes the two H-atoms. Consider the following:

1. *1-D representation*: $\gamma_\tau = -1$ (What is γ_1?)
2. *2-D representation*: $\mathbb{D}_\tau = \begin{pmatrix} -5 & 2 \\ -12 & 5 \end{pmatrix} \in GL_2(\mathbb{C})$ (What is $\mathbb{D}_1$?)

It should be *intuitive* that a 1-D representation is irreducible (even without knowing its definition), and that reducing a representation, roughly speaking, corresponds to reducing its degree. Hence, the given 1-D representation is in a satisfactory form since we wish to classify all irreps of C_2. What about the represenation by $\mathbb{D}$?

Consider the following: $\sigma : G \to GL_2(\mathbb{C})$ where $\sigma_g = P\gamma_g P^{-1}$ where P is a similarity transformation by $\begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix}$. Then, clearly $\sigma_1 = \mathbb{1}$. What about σ_τ?

$$\begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} -5 & 2 \\ -12 & 5 \end{pmatrix} \begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \text{ a block matrix!}$$

Evidently, σ is another 2-D representation. Furthermore, since a similarity transformation corresponds to coordinate transformation, $\mathbb{D}$ and σ *encode* two sets of similar matrices of the *same* linear transformation in two *different* basis vectors. Question: Are $\mathbb{D}$ and σ *genuinely* different?

Definition Two representations $\gamma : G \to GL_n(\mathbb{C})$ and $\mathbb{D} : G \to GL_m(\mathbb{C})$ are *equivalent* if $\exists$ a similarity transformation $P \in M_{mn}(\mathbb{C})$ such that $P\gamma_g P^{-1} = \mathbb{D}_g \ \forall g$.

Remark 0. In 1-dimension, the number of coordinate transformations is limited; a similarity transformation is an identity operator. I.e., in 1-dimension, $\gamma \sim \mathbb{D} \iff \gamma = \mathbb{D}$.

Remark 1. Use the notation $\gamma \sim \mathbb{D}$ to denote equivalence (and surely, this defines an equivalence relation). Note that from this definition, a coordinate-free definition of equivalence follows naturally. (What is it?)

Remark 2. Recall that a block matrix (necessarily a square matrix) diagonalises a given vector space; there are no *cross terms*. For example,

$$\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} ax \\ by \end{pmatrix}$$

Hence, a matrix action (block matrix) on a vector space corresponds to a matrix acting on each *orthogonal* subspaces separately and then bringing them altogether by *direct sum*. This concept leads to a useful definition:

Definition Given a representation $\gamma : G \to GL(V)$ and $W \leq V$, a subspace of V, W is *G-invariant* if $\gamma_g w \in W \ \forall g \in G, \forall w \in W$. We also say γ fixes W.

To finish the discussion, notice that $\mathbb{D} \sim \sigma \sim \gamma^0 \bigoplus \gamma$ where γ^0 is the trivial representation where the *direct sum* of two representations is to be understood as forming $n+m$ by $n+m$ block matrices, given n-dimensional and m-dimensional representations. By the previous discussion, $\gamma^0 \bigoplus \gamma$ fixes $W_i = \mathbb{C}, i = 1, 2$ where $W_1 \bigoplus W_2 = \mathbb{C}^2$. Hence $\mathbb{D}$ encodes a set of matrices that acts on two orthogonal subspaces of V independently by allowing no cross-terms. In fact, $\mathbb{D}$ is reducible by two irreps, γ^0 and γ, as the notation of direct sum suggests.

Definition $\gamma : G \to GL(V)$ is *reducible* by $\gamma^1 : G \to GL(V_1)$ and $\gamma^2 : G \to GL(V_2)$ if γ fixes $V_i \leq V$ for $i = 1, 2$, $V_1 \bigoplus V_2 = V$ and $\gamma|_{V_i} = \gamma^i$ for $i = 1, 2$. Write $\gamma \sim \gamma^1 \bigoplus \gamma^2$.

Definition $\gamma : G \to GL(V)$ is *irreducible* if γ fixes no proper subspace of V. (Hence, by definition, a 1-D representation is irreducible.)

Remark. Why can't we define *irreducible* as *not reducible*? A careful examination of the two definitions shows that they are not related by negation.

e.g.) Let $G = (\mathbb{Z}, +)$ (an infinite group!), $V = \mathbb{C}^2$. *Claim:* $\gamma : n \mapsto \begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix}$ is neither irreducible nor reducible.

$$\begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ 0 \end{pmatrix} = \begin{pmatrix} x \\ 0 \end{pmatrix} \ \forall x \in \mathbb{C}$$

γ fixes $\mathbb{C} \leq \mathbb{C}^2$, where the subspace is to be understood as an isomorphism by embedding. $\therefore \gamma$ is not irreducible.

Suppose γ is reducible. By some similarity transformation, $\begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix} \sim \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$ for some $a, b \in \mathbb{C}$ where the constants depend on $n \in \mathbb{Z}$. I.e., each γ_n is diagonalisable. Let us apply the following lemma from linear algebra:

Lemma $A \in M_n(\mathbb{C})$ is diagonalisable $\iff$ $m_A(t)$, the minimal polynomial of A, has no repeated roots.

Characteristic polynomial: $p_A(t) = det(A - tI) = t^2 - 2t + 1 = (t-1)^2$

Since $m_A(t) | p_A(t)$, $m_A(t) = (t-1)^2$ or $m_A(t) = t - 1$.

Clearly, $\begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix} - 1 = \begin{pmatrix} 0 & n \\ 0 & 0 \end{pmatrix} \neq 0$.

$\therefore m_A(t) = (t-1)^2$ and $\begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix}$ is not diagonalisable. $\Rightarrow\Leftarrow$

This example goes against our common sense, but if we assume G finite, our intuition stands correct. To investigate further, we need the following definition.

Definition Given an inner product space V, $\gamma : G \to GL(V)$ is *unitary* if

$$\left\langle w \,\middle|\, \gamma_g^\dagger \gamma_g \,\middle|\, v \right\rangle = \langle w \,|\, v \rangle \;\forall v, w \in V, \forall g \in G.$$

Remark 0. We employ Dirac's braket notation for inner product. This comes in handy when we later apply these concepts to quantum mechanics.

1. $v \in V$ is associated with $|v\rangle \in V$. The dual vector of $|v\rangle$ is $\langle v| \in V^*$. The dual vector of $\gamma_g |v\rangle$ is $\langle v| \gamma_g^\dagger$ where $\gamma_g^\dagger$ is the *Hermitian conjugate* of γ_g. In this essay, we freely exploit this one-to-one correspondence between V and V^*, justified by the *Riesz Representation Theorem* applied to Hilbert space. More will follow regarding Hilbert space when we apply group representation to quantum systems.

Remark 1. Unitary operations preserve norm and angle, as symmetry operations usually do. In particular, all *proper rotations*, rotations whose determinant is 1, are unitary operations. Hence, unitary representation of a symmetry group plays a fundamental role in applications that contain symmetries as we will see.

Remark 2. By definition, a linear map $A : V \to V$ is unitary if $A^\dagger A = \mathbb{1}$.

e.g.) Consider a time-independent hamiltonian H. The Schrödinger Equation $H|\psi(t)\rangle = i\hbar \dfrac{\partial |\psi(t)\rangle}{\partial t}$ yields a time-evolution operator $U(t) = e^{-i\frac{H}{\hbar}t}$, by directly solving the first-order differential equation.

$$U^\dagger U = e^{i\frac{H}{\hbar}t} e^{-i\frac{H}{\hbar}t} = \mathbb{1}.$$

$\therefore$ The time-evolution operator is unitary.

Theorem

1. *A representation of finite group is unitary up to a re-definition of a given inner product.*
2. *A unitary representation is either irreducible or reducible.*

proof 1. Given $\gamma : G \to GL(V)$, assume V is an inner product space. Define $(w|v) = \left\langle w \,\middle|\, \gamma_\alpha^\dagger \gamma_\alpha \,\middle|\, v \right\rangle$ where we adopt the summation convention with the index α; greek letters are adopted to denote summation. The sum is well-defined since G is finite.

$$(w|\gamma_g^\dagger \gamma_g|v) = \left\langle w \,\middle|\, \gamma_g^\dagger \gamma_\alpha^\dagger \gamma_\alpha \gamma_g \,\middle|\, v \right\rangle = \left\langle w\gamma_{\alpha g}^\dagger \gamma_{\alpha g} v \right\rangle = \left\langle w \,\middle|\, \gamma_\beta^\dagger \gamma_\beta \,\middle|\, v \right\rangle = (w|v)$$

proof 2. Given $\gamma : G \to GL(V)$, a unitary representation of finite G, assume γ is not irreducible. Then, there exists $W \leq V$ such that $\gamma_g w \in W, \forall g \in G, \forall w \in W$. Note $V = W \bigoplus W^\perp$, an internal direct sum. We want to show that γ fixes $W^\perp$. Let $w \in W$ and $u \in W^\perp$. Then,

$$\langle \gamma_g u \,|\, w \rangle = \left\langle u \,\middle|\, \gamma_{g^{-1}} w \right\rangle = 0 \implies \gamma_g u \in W^\perp,$$

since γ is unitary and $\gamma_{g^{-1}} w \in W$. $\therefore \gamma$ fixes $W^\perp$ and γ is reducible.

QED

Now we have all ingredients to answer the following question: is a representation of G completely reducible into irreps?

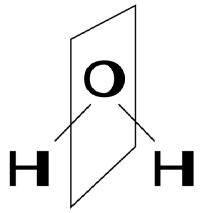
Theorem: Unique Factorisation *Let $\gamma : G \to GL(V)$ be a representation of a finite group. Then $\gamma \sim \bigoplus_{i=1}^s \gamma^{(i)}$ where $\gamma^{(i)} : G \to GL(V_i)$ is irreducible $\forall i$ and $V = \bigoplus_1^s V_i$. Such decomposition into irreducibles is unique.*

proof Induct on $n = deg(\gamma)$. Given a representation of degree n+1, assume that γ is not irreducible. Then, γ is reducible, since γ is unitary WLOG. The decomposition yields a representation of degree $\leq$ n, to which we apply the induction hypothesis. Then follows the result promptly. We come back to uniqueness later.

QED

With the machinery discussed so far, let us ask the following question: when identifying the full symmetry group of a molecule, how do we know that two group elements are genuinely identical (or different)?

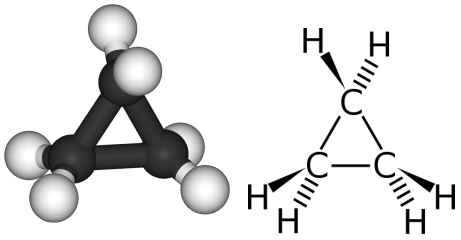
Consider a water molecule. Its symmetry group is $C_{2v}(\cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}) = \left\{1, C_2, \sigma_v, \sigma_v^{'}\right\}$ (v for vertical with respect to the *principal axis*). C_2 is evidently the 180° rotation about the principal axis, the axis of highest order of rotation, through the oxygen O molecule. σ_v is the following reflection:



With this picture in mind, one can guess what $\sigma_v^{'}$ is: a reflection across a plane containing all entire H_2O molecule.

However, the action of 1 and $\sigma_v^{'}$ on the molecule looks identical. After all, no atoms move. Are they truly identical?

Consider the following cyclopropane molecule: C_3H_6.



The principal axis is a 3-fold rotation through the plane containing all three carbon atoms. In fact, it is customary to define $\sigma_v^{'}$ as the reflection across that plane (the symbol σ_h is used as well for horizontal). Here, the identity and $\sigma_v^{'}$ are not the same. The confusion vanishes if we consider the group elements to act on the *entire* $\mathbb{R}^3$ space, not just on given molecules, and indeed that is exactly what we mean by $GL_3(\mathbb{R})$. Hence, to show the equality of two group elements, we need to consider infinitely many model molecules, or perhaps exploit representation.

Suppose σ_h acts on the xy-plane in $\mathbb{R}^3$. Then,

$$\sigma_h = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \mathbb{1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\therefore \sigma_h \neq \mathbb{1}$$

Now, let us investigate group representations of a cyclic group $C_n \cong \mathbb{Z}/n\mathbb{Z}$. By the previous example, $\gamma_\rho = \xi_n^k$, $\xi_n = e^{\frac{2\pi k i}{n}}$ for $k = 0, 1, ...n-1$ defines n inequivalent irreps. Let us accept the fact that an irrep of an abelian group is of dimension one (We will prove it). Then, since the image of the generator satisfies $z^n = 1$, these are the only irreps. Let us consider the following *character table* with $n = 3$.

	1	C	C^2
χ_0	1	1	1
χ_1	1	ξ_3	ξ_3^2
χ_2	1	ξ_3^2	ξ_3

Note that we have χ, not γ in the columns.

I.2. Character, Schur's Lemma, Orthogonality Relation Theorem

Definition Given $\gamma : G \to GL(V)$, define $\chi_\gamma : G \to \mathbb{C}$ such that $\chi_\gamma(g) = Tr(\gamma_g)$. χ_γ is called the *character* of γ. Use the shorthand $\chi_{\gamma i} = \chi_i$ where the i's label the irreps of G.

Lemma

1. $\chi_\gamma(gxg^{-1}) = \chi_\gamma(x)\ \forall x, g \in G$
2. $\gamma \sim \mathbb{D} \Rightarrow \chi_\gamma = \chi_\mathbb{D}$
3. $\chi_\gamma(1) = deg(\gamma)$

Remark In fact, a character function fits into a bigger class of functions called *class function*. Say $f : G \to \mathbb{C}$ is a class function if $f(gxg^{-1}) = f(x)\ \forall x, g \in G$. Let Z(G) denote the collection of class functions, to which we come back later.

e.g.) Let us compute the character of $R : G \to GL(\mathbb{C}G)$, the regular representation where $\mathbb{C}G$ denotes *group algebra* over the complex field. (Recall that R_g acts on $\mathbb{C}G$ by left action.) Fix $h \in G \backslash \{ 1 \}$. To calculate the trace, find the matrix elements.

$$(R_h)_{ij} = \langle i \,|\, R_h \,|\, j \rangle \text{ where } |i\rangle = g_i, \text{ a basis element of } \mathbb{C}G$$

In particular, we are interested in j=i.

$$R_h g_i = h g_i = c_\alpha g_\alpha, c_\alpha \in \mathbb{C}$$

$$\text{Since } h \neq 1,\ c_i = 0\ \forall i$$
$$\Rightarrow \chi_R(h) = \langle \alpha \,|\, R_h \,|\, \alpha \rangle = 0.$$
$$\therefore \text{ In general, } \chi_R(g) = |G|\delta_{1g}, \text{ the Kronecker delta.}$$

Character tables in applied fields such as chemistry carry one extra columns with spatial functions called *basis functions*. For example, with $G = C_3$,

	1	C	C^2	
χ_0	1	1	1	z
χ_1	1	ξ_3	ξ_3^2	$x + iy$
χ_2	1	ξ_3^2	ξ_3	$x - iy$

Under a transformation by group action, these basis functions *transform* as one of the irreps. To clarify, consider a 3-fold rotation by C_3 about the z-axis. Under group actions by all group elements, it is intuitive that the function z is invariant.

$$1z = \mathbf{1}z,\ Cz = \mathbf{1}z,\ C^2 z = \mathbf{1}z,$$

We say that z transforms as γ^0. Note the character of (1,1,1). Using a similar argument, we show the following:

1. $x + iy$ transforms as γ^1.
2. $x - iy$ transforms as γ^2.

proof We use the following trick. Given f(x), where $x \in \mathbb{R}^3$, suppose we perform a coordinate transformation by A: $x' = Ax$. Let us describe a new scalar field under a new coordinate x'.

$$g(x') = f(x) \Rightarrow g(x') = f(A^{-1}x') \Rightarrow g(x) = f(A^{-1}x)$$

The spatial variable x now denotes the former x'. Let $f(x, y, z) = x + iy$ and let us perform a *passive* transformation where the coordinate axes move.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$
$$\Rightarrow A = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\Rightarrow A^{-1} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\Rightarrow A^{-1}x = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x\cos\phi - y\sin\phi \\ x\sin\phi + y\cos\phi \\ z \end{pmatrix}$$

$$\Rightarrow g(x,y,z) = f(x\cos\phi - y\sin\phi, x\sin\phi + y\cos\phi, z) \quad (1)$$
$$= x\cos\phi - y\sin\phi + i(x\sin\phi + y\cos\phi) \quad (2)$$
$$= e^{i\phi}(x+iy) \quad (3)$$

In particular, $\phi = \frac{2\pi}{3} \Rightarrow e^{i\phi} = \xi_3$.
$1(x+iy) = 1(x+iy)$, $C(x+iy) = \xi_3(x+iy)$, $C^2(x+iy) = \xi_3^2(x+iy)$
$\therefore f(x,y,z) = x+iy$ transforms as γ^1, according to the character table.

QED

Up to equation(1), the proof goes through with a general function f and an angle ϕ about the z-axis. Hence the second claim can be proved trivially by substituting $f(x,y,z) = x - iy$ at equation(1).

Let $a_1 = x+iy, a_2 = x-iy, a_3 = z$. Then, a general function $F(a_1,a_2,a_3) = f(x,y,z)$ under a ϕ rotation transforms as follows:

$$f(x,y,z) = F(a_1,a_2,a_3) \xrightarrow{\phi}$$
$$\text{f(xcos}\phi - y\sin\phi, x\sin\phi + y\cos\phi, z) = F(e^{i\phi}a_1, e^{-i\phi}a_2, a_3)$$

Furthermore, it is trivial to check that x,y,z can be described as a linear combination of a_1, a_2, a_3. This tells us that had we defined a function using the basis functions as our independent variables, then the function would transform nicely under the group action.

As an example, consider the wavefunction of a hydrogen atom $\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$. In particular, consider the angular function, or the spherical harmonics: $Y_l^m(\theta,\phi)$ where the quantum numbers l (orbital angular momentum) and m (magnetic quantum number) have been added after applying the boundary conditions of H-atom (the nature of BC is not important for our discussion). One can look up the spherical harmonics table online and notice that they are written in terms of basis functions for rotations: $x+iy, x-iy, z$. To be more exact, they are written in terms of $\cos\theta, \sin\theta, e^{i\phi}$.

$$(\frac{a_1}{a_2})^{\frac{1}{2}} = (\frac{x+iy}{x-iy})^{\frac{1}{2}} = (\frac{(r\sin\theta\cos\phi) + i(r\sin\theta\sin\phi)}{(r\sin\theta\cos\phi) - i(r\sin\theta\sin\phi)})^{\frac{1}{2}} = (\frac{r\sin\theta e^{i\phi}}{r\sin\theta e^{-i\phi}})^{\frac{1}{2}} = e^{i\phi}$$
$$(\frac{a_1a_2}{r^2})^{\frac{1}{2}} = (\frac{r^2\sin^2\theta}{r^2})^{\frac{1}{2}} = \sin\theta$$
$$\frac{a_3}{r} = \cos\theta$$
where r is a constant on the sphere of radius r.

One might be curious why we only consider a z-axis rotation. After all, $SO(3)$ is an infinite group of rotations in infinitely many axes. In dimension 3, a rotation of ϕ about a plane spanned by $\{e_1, e_2\}$, two linearly independent unit vectors, and another plane spanned by $\{f_1, f_2\}$ are related by a similarity transformation.

Since characters are invariant under conjugacy classes, we can WLOG consider a rotation by ϕ about the xy-plane (z-axis).

Let us investigate the orthogonality relation amongst rows and columns. It is puzzling that the dot products are zero. Pure mathematics texts fully delve into the proof whilst texts on application tend to gloss over this material. To gain a sufficient insight, we shall aim for the Aristotelian mean. Our guiding questions are as follows: what is the most natural algebraic structure on which orthogonality is defined?

$\gamma_g \in U_n(\mathbb{C})$ from a given representation, WLOG unitary, $\gamma : G \to U_n(\mathbb{C})$ yields $\{\gamma_{ij}(g)\}_{1\leq i,j\leq n}$, i.e., $n \times n$ complex numbers. Equivalently, we have $\{\gamma_{ij}\}_{1\leq i,j\leq n}$ where each element is an ordinary function $\gamma_{ij} : G \to \mathbb{C}$. This collection of functions that take a group element into $\mathbb{C}$ forms an algebraic structure where we can add, scale and perform dot product: inner product space.

Lemma

1. Let $\mathbb{C}^G \equiv \{f : G \to \mathbb{C}\}$. Then, $\mathbb{C}^G$ is a vector space (how do we define addition and scaling?). Moreover, $Z(G) \leq \mathbb{C}^G$.
2. $\langle \psi \,|\, \varphi \rangle \equiv \dfrac{\psi(\alpha)^* \varphi(\alpha)}{|G|}$ defines an inner product where $|\varphi\rangle, |\psi\rangle \in \mathbb{C}^G$ and the index α denotes summation.
3. $Span\,\{\delta_g\}_{g\in G} \equiv \mathbb{C}\,\{\delta_g\}_{g\in G} = \mathbb{C}^G$ where $\delta_g : G \to \mathbb{C}$ such that $\delta_g(x) = \delta_{xg}$, the kronecker delta. $\therefore$ $dim_{\mathbb{C}}(\mathbb{C}^G) = |G|$. Similarly, $\dim(Z(G)) = |Cl(G)|$, where Cl(G) denotes the collection of conjugacy classes of G.

Going back to the character table of C_3, we note that $\chi_i \in \mathbb{C}^G$. It is easily verified that $\langle \chi_j \,|\, \chi_i \rangle = \delta_{ij}$, the kronecker delta.

In fact, it is not coincidental that $\{\chi_i\}$ forms an *orthonormal* set. Orthonormality is a quintessential concept in quantum mechanics, to which we come back later. For now, we delve into more theories.

Consider two quantum states $|\Psi\rangle$, $|\psi\rangle$. The two states are fundamentally distinguishable if $\langle \psi \,|\, \Psi \rangle = 0$, i.e., if the inner product is zero. On the other hand, $\langle \Psi \,|\, \Psi \rangle = 1$ (normalisation is always assumed).

Since every representation of a finite group is completely reducible, consider two inequivalent, irreps $\gamma : G \to U_n(\mathbb{C})$, $\mathbb{D} : G \to U_m(\mathbb{C})$, from which we have $\{\gamma_{ij}\}_{1\leq i,j\leq n}$, $\{\mathbb{D}_{kl}\}_{1\leq k,l\leq m} \subseteq \mathbb{C}^G$. Then, take the braket $\langle \mathbb{D}_{kl} \,|\, \gamma_{ij} \rangle$. Given that γ_{ij} and $\mathbb{D}_{kl}$ are induced by genuinely different representations, what would $\langle \mathbb{D}_{kl} \,|\, \gamma_{ij} \rangle$ be?

Theorem: Orthogonality Relation *Given γ and $\mathbb{D}$ as above,*

1. $\langle \mathbb{D}_{kl} \,|\, \gamma_{ij} \rangle \equiv 0$
2. $\langle \gamma_{kl} \,|\, \gamma_{ij} \rangle = \dfrac{\delta_{ki}\delta_{lj}}{n}$, *where n is the degree of γ.*

The proof of this theorem follows from *Schur's Lemma*, on which several remarks are presented. First, we can only have a finite number of $i = 1, 2, ..., s$ where $\gamma^{(i)} : G \to GL(V_i)$, inequivalent irreps, because each $\gamma^{(i)}$ contributes d_i^2 elements of $\mathbb{C}^G$, d_i = degree of $\gamma^{(i)}$. Hence, $\sum_{i=1}^{s} d_i^2 \leq dim_{\mathbb{C}}(\mathbb{C}^G) = |G|$. We need the following definition to fully understand Schur's lemma.

Definition Given two representations $\gamma : G \to GL(V)$, $\mathbb{D} : G \to GL(W)$, $L \in Hom(V, W)$ intertwines γ and $\mathbb{D}$ as follows: $L\gamma_g = \mathbb{D}_g L \;\forall g \in G$. L is called an *intertwining operator*.

Remark. Of course, $\gamma = \mathbb{D} \Rightarrow$ L commutes with the representation γ. In fact, the collection of intertwining operators form a subspace of Hom(V,W). For future discussions, denote this subspace as A_I.

Theorem: Schur's Lemma *Let $\gamma : G \to GL(V)$ and $\mathbb{D} : G \to GL(W)$ be unitary irreps. Then,*

1. $\gamma \nsim \mathbb{D} \Rightarrow L = 0$
2. $\gamma \sim \mathbb{D} \Rightarrow dim_{\mathbb{C}} A_I = 1$
3. $\gamma = \mathbb{D} \Rightarrow L = \mathbb{1}$ up to a constant in the complex field.

proof cf. Steinberg for 1,3. The proof of 2° requires a slick trick, not mentioned in the main text. Let $L \in A$. Definition of intertwining operator $\Rightarrow L\gamma_g = \mathbb{D}_g L$; $\gamma \sim \mathbb{D} \Rightarrow \exists$ T, a vector isomorphism, such that $\gamma_g = T^{-1}\mathbb{D}_g T \ \forall g \in G$. Consider $T^{-1}L \in$ End(V). If $T^{-1}L \in A$ (which it is, and kindly left as an exercise), then $T^{-1}L = \alpha\mathbb{1}$ for some $\alpha \in \mathbb{C}$ by claim 3. $\therefore$ L is spanned by T. The rest of the proof is trivial.

QED

e.g.) Time to keep my promise that an irrep of an abelian group is of dimension one. Since $[\gamma_g, \gamma_h] = \gamma_g\gamma_h - \gamma_h\gamma_g = \gamma_{gh} - \gamma_{hg} = \gamma_{gh} - \gamma_{gh} = 0$, apply the third statement of Schur's Lemma. The irreducibility condition forces the conclusion.

QED

Equipped with Schur's Lemma, we can prove the orthogonality theorem. Due to the lengthy computation involved, we omit the proof, but I give one last remark. The main question is as follows: whilst Schur's Lemma concerns commutation, the orthogonality theorem concerns inner product of functions derived from representations. How do we connect the two seemingly different concepts *intuitively*?

Consider $x, y \in \mathbb{C}^n$ and a diagonal matrix, for simplicity say $\mathbb{1} \in GL_n(\mathbb{C})$. Notice $y^\dagger \mathbb{1} x = \sum_1^n y_i^* x_i = \langle y \,|\, x \rangle$, where the braket is the usual L_2 norm on the Euclidean space. This illustrates that a quadratic form by a diagonal matrix yields a result that has the form of an inner product.

Now consider $\mathbb{D}_\alpha L \gamma_{\alpha^{-1}} \in Hom(V, W)$ where L $\in$ Hom(V,W), $\gamma, \mathbb{D}$ defined as usual and the summation convention. Considering that we take unitary representations WLOG, this is in the desired quadratic form, provided that L is diagonal, or of the form that yields inner product as before. In fact, we take $L = E_{ki} \in M_{mn}(\mathbb{C})$, a matrix whose ki-element is 1 and the rest zero. Then, by straightforward computation, we can find the lj-element as follows:

$$[\mathbb{D}_\alpha E_{ki} \gamma_{\alpha^{-1}}]_{lj} = |G| \, \langle \mathbb{D}_{kl} \,|\, \gamma_{ij} \rangle, \text{ an inner product of } \gamma_{ij} \text{ and } \mathbb{D}_{kl}!$$

Now Schur's Lemma kicks in since $\mathbb{D}_\alpha E_{ki} \gamma_{\alpha^{-1}}$ genuinely *intertwines* γ and $\mathbb{D}$ (an easy exercise). Then, follows the theorem promptly. Let us apply this concept to the character table.

Theorem $\langle \chi_j \,|\, \chi_i \rangle = \delta_{ij}$ *where we assume the usual notation.*

proof

$$\begin{aligned}
\langle \chi_j \,|\, \chi_i \rangle &= \frac{\chi_j(\alpha)^* \chi_i(\alpha)}{|G|} \\
&= \frac{Tr(\gamma_\alpha^{(j)})^* Tr(\gamma_\alpha^{(i)})}{|G|} \\
&= \frac{\gamma_{\beta\beta}^{(j)}(\alpha)^* \gamma_{\gamma\gamma}^{(i)}(\alpha)}{|G|} \\
&= \left\langle \gamma_{\beta\beta}^{(j)} \,\middle|\, \gamma_{\gamma\gamma}^{(i)} \right\rangle = \delta_{ij}
\end{aligned}$$

In short, the character vectors of irreducible representations are orthonormal.

QED

Corollary *Unique Factorisation Theorem for a representation of a finite group*

proof We reduce a given representation completely as follows:

$$\gamma \sim \bigoplus_{i=1}^{s} m_i \gamma^{(i)},$$
where we consider multiplicities.

Taking the character of the equivalence relation, $\chi_\gamma = m_\alpha \chi_\alpha$. It follows promptly that $m_i = \langle \chi_i \,|\, \chi_\gamma \rangle$. Hence, the multiplicity coefficients are uniquely defined.

QED

Now we finish the theory of character and $\mathbb{C}^G$ by completely classifying the basis of $\mathbb{C}^G$ and $Z(G)$.

Consider the regular representation $R : G \to GL(\mathbb{C}G)$ (To apply the orthogonality theorem or Schur's lemma, R needs to be unitary, which is an easy exercise). By our previous calculation, $\chi_R(g) = |G|\delta_{1g}$.

$$\text{By UFT, } R \sim \bigoplus_{i=1}^{s} m_i \gamma^{(i)} \text{ where } \left\{ \gamma^{(\alpha)} \right\}_\alpha \text{: the irreps of G.}$$

$$m_i = \langle \chi_i \,|\, \chi_R \rangle = \frac{\chi_i(\alpha)^* \chi_R(\alpha)}{|G|} = d_i$$

$$\Rightarrow \therefore R \sim \bigoplus_{i=1}^{s} d_i \gamma^{(i)}$$

$$\chi_R = \sum_{i=1}^{s} d_i \chi_i$$

$$\chi_R(1) = \sum_{i=1}^{s} d_i \chi_i(1)$$

$$|G| = \sum_{i=1}^{s} d_i^2$$

Previously, we have established that $\left\{ \gamma_{ij}^{(k)} \right\}_{1 \le i,j \le d_k}^{1 \le k \le s}$ forms an orthonormal set (up to normalisation) of size $\sum_1^s d_i^2$. Hence, we have proved the following:

Theorem $\left\{ \gamma_{ij}^{(k)} \right\}_{1 \le i,j \le d_k}^{1 \le k \le s}$ *is an orthogonal basis for* $\mathbb{C}^G$ (Normalise!). Hence, $\sum_1^s d_i^2 = |G|$

Corollary $\{ \chi_i \}_{1 \le i \le s}$ is an orthonormal basis for Z(G).

proof Follows from the previous theorem; the orthonormality has been shown previously.

Remark. In practice, to completely classify all inequivalent irreps of a finite G, we always begin with the following equalities, aided by the orthogonality theorem:

$$\sum_1^s d_i^2 = |G|,\ s = |Cl(G)|.$$

As an example, let us completely classify $G = S_3$, the symmetry group on $\{1, 2, 3\}$. Two irreps are readily apparent: 1° Trivial representation. 2° Even-odd permutation, i.e., $\gamma_\sigma = \pm 1$, where $+1$ corresponds to even permutation, and -1 odd. Hence the following:

	1	σ	σ^2	τ_{12}	τ_{23}	τ_{13}
χ_1	1	1	1	1	1	1
$\chi_\pm$	1	1	1	-1	-1	-1
χ_2	a	b	b	c	c	c

Note that σ denotes (123), a 3-cycle. Note the multitude of b's and c's since a character is a class function. Since S_n has $p(n)$ conjugacy classes, where $p(n)$ denotes partition function for integers, we have a total of 3 irreps. Since the sum of $(degrees)^2$ add up to the order of G, we have the following: $1^2+1^2+a^2 = 6 \Rightarrow a = 2$, i.e., χ_2 corresponds to a 2-dimensional irrep. Moreover, by orthogonality of characters, we have the following:

$$\begin{gathered}\langle \chi_1 \,|\, \chi_2 \rangle = 0,\ \langle \chi_\pm \,|\, \chi_2 \rangle = 0 \\ \Rightarrow 2 + 2b + 3c = 0,\ 2 + 2b - 3c = 0 \\ \Rightarrow b = -1, c = 0 \\ \therefore\end{gathered}$$

	1	2σ	3τ
χ_1	1	1	1
$\chi_\pm$	1	1	-1
χ_2	2	-1	0

The updated table has 3 numerical columns rather than 6. Using the fact that a character is a class function, we suppress the table by grouping into conjugacy classes.

Often times, we represent S_n by n-dimensional representation given by permutation matrices. For example, when $n = 3$, the following defines a representation:

$$\sigma \mapsto \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},\ \tau_{12} \mapsto \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

We decompose this γ into irreps as follows: $\gamma \sim A\gamma^1 \bigoplus B\gamma^\pm \bigoplus C\gamma^2$

$$\begin{aligned}\Rightarrow A = \langle \chi_1 \,|\, \chi_\gamma \rangle &= \frac{1}{6}(3 + 0 + 0 + 1 + 1 + 1) = 1 \\ B = \langle \chi_\pm \,|\, \chi_\gamma \rangle &= \frac{1}{6}(3 + 0 + 0 - 1 - 1 - 1) = 0 \\ C = \langle \chi_2 \,|\, \chi_\gamma \rangle &= \frac{1}{6}(6 + 0 + 0 + 0 + 0 + 0) = 1\end{aligned}$$

$$\Rightarrow \therefore \gamma \sim \gamma^1 \bigoplus \gamma^2$$

This example motivates the following useful corollary:

Corollary *Given $\gamma : G \to U_n(\mathbb{C})$, γ is an irrep $\Leftrightarrow \langle \chi_\gamma \,|\, \chi_\gamma \rangle = 1$.*

proof γ is an irrep. $\Leftrightarrow \gamma \sim \gamma^i$ for some irrep of G $\Leftrightarrow 1 = \langle \chi_i \,|\, \chi_\gamma \rangle = \langle \chi_\gamma \,|\, \chi_\gamma \rangle$

QED

Remark 0. For the γ above, $\langle \chi_\gamma \,|\, \chi_\gamma \rangle = \frac{1}{6}(9 + 0 + 0 + 1 + 1 + 1) = 2 \neq 1$, which implies that γ is reducible.

Remark 1. How did I know that there exist two 1-dimensional representation other than six of them? Note $|Cl(S_3)| = 3$, the total number of inequivalent irreps. A more general procedure for identifying all 1-dimensional representation will be studied later.

II.0. The Necessary Minimal Background for Quantum Mechanics

Before we delve into quantum phenomena, let us digress from the rigorous study of group representation to the basic notions of non-relativistic quantum mechanics. Some of the most important ideas that we shall use are the following:

1. **Identification of System** We associate a *Hilbert space* $\mathcal{H}$ to a given physical system, from which a complete understanding of the system is obtained, at least in principle. To a complicated composition of many systems, we associate the tensor product of Hilbert spaces $\bigotimes_{i=1}^{n} \mathcal{H}_i$ of each respective system.

2. **Eigen-Problem** We associate a *Hermitian operator* to an *observable*, or the experimental values that we can obtain in labs, where the observables are simply the spectrum of the Hermitian operator. In particular, a Hamiltonian operator is Hermitian.

3. **Probability** Wavefunctions are defined as follows: $\Psi(x) \equiv \langle x \,|\, \Psi \rangle$. $|\Psi(x)|^2$ yields probability density, given Ψ is normalised.

4. **Uncertainty** Hermitian operators commute $\iff$ They are simultaneously diagonalisable. Physically, this means we can observe two quantites A and B simultaneously if the corresponding Hermitian operators commute.

Remark 0. $\mathcal{H}$ is a Banach space (complete normed vector space) with an inner product such that the norm is defined by the inner product as follows: $\|\Psi\| = \langle \Psi \,|\, \Psi \rangle^{1/2}$. Hence, $\mathcal{H}$ is by definition Banach, but the converse may not hold. A more exact definition/description of Banach/Hilbert space can be found in Folland as listed in the reference.

Remark 1. Given a linear operator $T \in GL(\mathcal{H})$, the $T^\dagger$ is called *Hermitian conjugate operator* if $\langle \psi \,|\, T \,|\, \varphi \rangle = \left\langle \varphi \,\middle|\, T^\dagger \,\middle|\, \psi \right\rangle^*$ where the $*$ denotes a complex conjugate. T is a Hermitian if $T^\dagger = T$.

Remark 2. Wavefunctions are basis-dependent. The most typical bases are position and momentum.

In this essay, we study both infinite and finite-dimensional $\mathcal{H}$. If $\mathcal{H}$ is finite-dimensional, its linear maps are automatically continuous. We take Hilbert's approach by assuming that all linear maps are continuous, i.e., consider bounded operators. We also assume that $\mathcal{H}$ has a countable dense subset, i.e., *separable*.

e.g.) The simplest form of infinite-dimensional $\mathcal{H}$ is a set of measurable wavefunctions $\{\psi(x)\}$ defined on the Lebesgue measure space $(\mathbb{R}, \mathcal{L}, m)$ such that $\int |\psi|^2 < \infty$.

With the following lemma, we finish laying out the general framework of quantum mechanics.

Lemma

1. A Hermitian operator H diagonalises a given Hilbert space $\mathcal{H}$ into *orthogonal* subspaces. Each eigenspace corresponds to a *real* eigenvalue.

2. $\mathcal{H}$ contains an orthonormal basis.

3. $\mathcal{H}$ is separable $\iff$ $\mathcal{H}$ contains a *countable* orthonormal basis. This justifies our previous assumption on the separability of $\mathcal{H}$.

4. $\forall\, |\Psi\rangle \in \mathcal{H}, |\Psi\rangle = \langle \psi_\alpha \,|\, \Psi \rangle \, |\psi_\alpha\rangle$ where the summation is over any orthonormal basis; $\mathcal{H}$ is complete.

II.1. Hamiltonian Group and its Application

Definition Let $H \in GL(\mathcal{H})$ denote Hamiltonian. Then a set of $R \in GL(\mathcal{H})$ such that $[R, H] = 0$ is called the *Hamiltonian group*.

Remark. Commuting with the Hamiltonian is a big deal. They describe the full symmetry of the given system.

Lemma G_H, a Hamiltonian group, is indeed a group.

proof Assume $R_1, R_2 \in G_H$. Then, $[R_1 R_2, H] = [R_1, H] R_2 + R_1 [R_2, H] = 0 + 0 = 0 \in GL(\mathcal{H})$. The verification of other axioms is omitted.

Given a system, suppose we have identified $\mathcal{H}$ by solving $H|\psi\rangle = E|\psi\rangle$. I.e., we have $\{|\psi_n\rangle\}_{n\geq 0}$, a countable orthonormal energy basis, and the corresponding $\{E_n\}_{n\geq 0}$. Choose an arbitrary energy E_n with degeneracy d_n, or the dimension of E_n-eigenspace; for simplicity, let us drop the $_n$ notation. Notice the following:

$$\begin{aligned} &HR\left|\psi^{(i)}\right\rangle = RH\left|\psi^{(i)}\right\rangle = RE\left|\psi^{(i)}\right\rangle = ER\left|\psi^{(i)}\right\rangle \\ \implies\ &R\left|\psi^{(i)}\right\rangle \in V_E, \text{ the E-eigenspace, } \forall R \in G_H \text{ and } 1 \leq i \leq d. \end{aligned}$$

This proves that V_E is a G_H-invariant subspace $\forall E$. This is nice, because we managed to reduce the domain of our interest to a finite-dimensional V_E for a fixed E from, possibly, an infinite-dimensional $\mathcal{H}$. For most cases, there are no further invariant subspaces proper to this V_E, a phenomenon which we call *normal degeneracy*; the representation, say γ, induced by V_E is irreducible. However, if such induced representation is reducible, i.e., if V_E splits into the direct sum of subspaces on which γ is irreducible, we call that *accidental degeneracy*. As an example, the Hamiltonian with the Coulomb potential, in particular a H-atom without perturbation, carries such accidental degeneracy. This indicates that G_H that has been identified is not the full symmetry group for a particular system. For our applications, we assume that G_H is the full symmetry group, i.e., that there is no *hidden* symmetry. Even if there exists such hidden symmetry, we can consider the symmetry group H that we found as a subgroup of the full G_H. Now comes group representation.

Theorem *Define γ_{ij}^k as follows: $R_k|\psi_j\rangle = \gamma_{\alpha j}^k|\psi_\alpha\rangle$ where the sum is over all degeneracy within the given energy eigenspace of degeneracy d. This defines a unitary irrep $\gamma : G_H \to U_d(\mathbb{C})$*

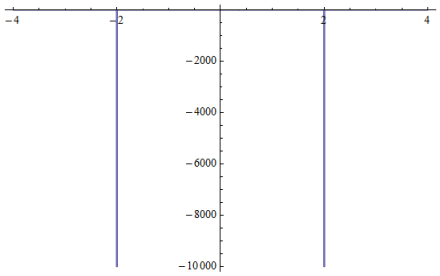
The proof is a straightforward computation showing unitarity and group homomorphism. If γ were reducible, then we can find a vector with the same energy outside of the given energy eigenspace, an accidental degeneracy. However, since we assume normal degeneracy, γ is an irrep.

Notice that the level of degeneracy equals the degree of irrep. Given a quantum system, we will associate each energy eigenspace with an irrep of G_H. Without knowing the specific nature of such eigenspace, its dimension equals the degree of its associated irrep by the previous remark.

Algebraic Approach to the Double Delta Potential

A single electron bounded under Coulomb potential, for example a H-atom, experiences a spherical symmetry, but what happens once that symmetry is lost?

Suppose we have two identical stationary atoms with net positive charges sitting in a one-dimensional line, i.e., a double delta-function potential (A single delta potential is done beautifully in Griffith). We denote the left atom as 1 and the right atom as 2.



For this problem, we can obtain an analytic solution by solving the SE with $V(x) = -\alpha(\delta(x+a)+\delta(x-a))$, where $\alpha > 0$ denotes the strength of delta-potential, in three different regions with a special handling of boundary conditions at $x = \pm a$ where the derivative of $\psi(x)$ is discontinuous; this is mouthful and overly computational which we are not going to do! We will use the analytic solution for a single delta potential

and group representation to approximate the solution for a bounded state as opposed to a scattered state. The solution for a bounded state of a single delta potential at the origin is given as follows:

$$\boxed{\psi(x) = \frac{(m\alpha)^{1/2}}{\hbar} e^{-m\alpha|x|/\hbar^2}, E = -\frac{m\alpha^2}{2\hbar^2}}$$

We approximate by employing a technique widely used in physical chemistry called LCAO, *linear combination of atomic orbital*. Let $|1\rangle$ be the pure state in the absence of atom 2, and $|2\rangle$ defined similarly. We make the assumption that the effect of two potentials on an electron is related to the linear combination of each potential, i.e., $|\psi\rangle = A|1\rangle + B|2\rangle \in \mathcal{H}$ for some $A, B \in \mathbb{C}$ where $|\psi\rangle$ is an eigenstate for some energy E. Of course, normalisation implies $|A|^2 + |B|^2 = 1$. This is clearly an approximation that treats the effect of delta potential on the particle separately; in reality, this is not true since both delta potentials affect the particle altogether.

Since the problem is given in the position basis, we look for a transformation on x such that the Hamiltonian is invariant under such transformation. Note that the potential is an even function. It turns out that $G_H = S_2 = \{1, \tau\}$ where $x \xrightarrow{1} x$ and $x \xrightarrow{\tau} -x$.

The character table for G_H is trivial:

	1	τ
χ_1	1	1
χ_{-1}	1	-1

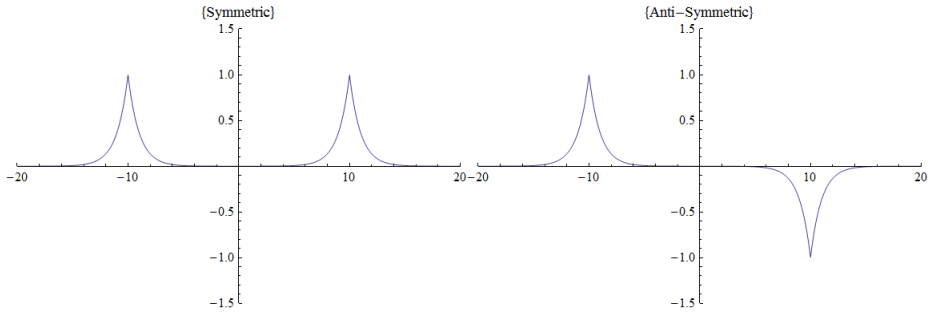
The character tells us that there are two different modes of vibrations, all of which are non-degenerate where we take for granted that solutions of 1-dimensional Schrödinger equation are non-degenerate. We also take for granted that the ground state almost always contains the full symmetry of G_H. Hence, χ_1 mode corresponds to the ground state, and χ_{-1} to the excited state. Since all irreps are of degree 1, it yields the following equations that look like eigenvalue problem:

$$\begin{aligned}
\chi_1 : \tau[A|1\rangle + B|2\rangle] &= A|2\rangle + B|1\rangle = A|1\rangle + B|2\rangle \\
\chi_{-1} : \tau[A|1\rangle + B|2\rangle] &= A|2\rangle + B|1\rangle = -A|1\rangle - B|2\rangle \\
\implies A[|1\rangle - |2\rangle] &= B[|1\rangle - |2\rangle] \\
A[|1\rangle + |2\rangle] &= -B[|1\rangle + |2\rangle] \\
\implies A &= B \\
A &= -B \\
\implies \chi_1 : (A, B) &= (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}) \\
\chi_{-1} : (A, B) &= (\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}) \\
\therefore |\psi_1\rangle &= \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle \\
|\psi_{-1}\rangle &= \frac{1}{\sqrt{2}}|1\rangle - \frac{1}{\sqrt{2}}|2\rangle
\end{aligned}$$

If pure states are all we want, we are done. To obtain, say, the probability that a particle lies on some interval, then we need a wavefunction. Since we already know the solution for a single potential, the transition from abstract vectors to wavefunctions is easy. We also note that $x = x_1 - a$ and $x = x_2 + a$.

$$\begin{aligned}
\psi_1(x) = \langle x | \psi_1 \rangle &= \tfrac{1}{\sqrt{2}}\psi_1(x_1) + \tfrac{1}{\sqrt{2}}\psi_2(x_2) = \tfrac{1}{\sqrt{2}}\psi_1(x+a) + \tfrac{1}{\sqrt{2}}\psi_2(x-a) \\
&= \frac{(m\alpha)^{1/2}}{\sqrt{2}\hbar}\left[e^{-m\alpha|x+a|/\hbar^2} + e^{-m\alpha|x-a|/\hbar^2}\right]
\end{aligned}$$

$$\psi_{-1}(x) = \langle x \,|\, \psi_{-1} \rangle = \tfrac{1}{\sqrt{2}}\psi_1(x_1) - \tfrac{1}{\sqrt{2}}\psi_2(x_2) = \tfrac{1}{\sqrt{2}}\psi_1(x+a) - \tfrac{1}{\sqrt{2}}\psi_2(x-a)$$
$$= \frac{(m\alpha)^{1/2}}{\sqrt{2}\hbar}\left[e^{-m\alpha|x+a|/\hbar^2} - e^{-m\alpha|x-a|/\hbar^2}\right]$$

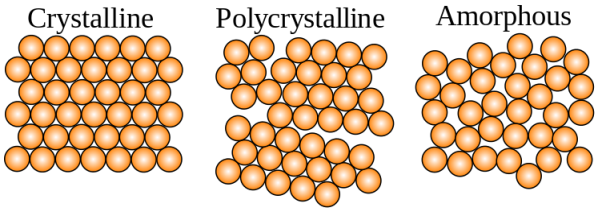


Figures, not scaled. Left: ψ_1; Right:ψ_{-1}

Pros and cons of LCAO are evident for this particular problem. *Pros*: Computation involves no complicated integrals, but merely a simple algebra. Group theoretic approach gives us a clear qualitative picture of the system. *Cons*: The solution is numerically off. Based on the analytic solution, there must be two bound states, and yet this approach gives us an energy of zero for the asymmetric state (Linearity of the Hamiltonian operator implies that energy is additive).

Symmetry within a Crystal and Bloch's Theorem

The previous example dealt with the behaviour of an electron under 2 periodic potentials. Now we study N periodic potentials where N is big; typically, it is to an order of Avogadro's number: 6.02×10^{23} atoms/mol. The periodicity of potential is naturally plausible when we study crystals, or solids with a regular structure with lattices. For example, diamond and NaCl are crystals. A glass is not; it is an amorphous solid. We begin our analysis with dimension 1; a generalisation to dimension 3 will be apparent.



Wikipedia: Crystal

Assume N stationary atoms are equally spaced by some number $a \in \mathbb{R}$ on the real line at $0, a, 2a, ...(N-1)a$ and call this interval Ω. The Hamiltonian is as follows: $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$. We set the boundary condition as follows: $\psi(x+Na) = \psi(x)$, a cyclic BC. Some authors describe this as *making a ring* by connecting the beginning and an end. It is more natural to think that we are *sampling* a portion of crystal from a given extended solid structure. Hence the following:

$$\boxed{H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x); \psi(x+Na) = \psi(x); V(x+a) = V(x)}$$

Claim: Define $R \in GL(\mathcal{H})$ such that $R\psi(x) = \psi(x+a)$. Then, $[R, H] = 0$.
proof

$$RH(x)\psi(x) - H(x)R\psi(x) = ER\psi(x) - H(x)\psi(x+a)$$
$$= \mathrm{E}\psi(x+a) - H(x+a)\psi(x+a)$$
$$= \mathrm{E}\psi(x+a) - E\psi(x+a) = 0$$

We used an eigenfunction, instead of a general square-integrable function, in the proof above. This is justified, because $\mathcal{H}$ is complete.

Since $[R, H] = 0$, $[R^n, H] = 0$ for $n \in \mathbb{N}$, but noting that $R^N = \mathbb{1}$, $G_H = \left\{\mathbb{1}, R, R^2, ..., R^{N-1}\right\} \cong \mathbb{Z}/N\mathbb{Z}$, an abelian group! In fact, $\gamma^{(n)}(R) = e^{\frac{2\pi ni}{N}}$, $0 \leq n \leq N-1$ defines N irrep. Due to the one-to-one correspondence between an irrep and an eigenfunction of the Hamiltonian, we can completely classify all eigenfunctions as follows: $\psi_n(x)$.

$$R\psi_n(x) = \psi_n(x+a) = e^{\frac{2\pi ni}{N}}\psi_n(x) = e^{iK_n a}\psi_n(x)$$
$$\boxed{\therefore \psi_n(x+a) = e^{iK_n a}\psi_n(x);\ K_n = \tfrac{2\pi n}{Na}, x \in \Omega, 0 \leq n \leq N-1}$$

This is a 1-dimensional manifestation of **Bloch's Theorem**. An identification of $\psi(x)$ on $[0, a]$ extends completely to Ω, and this approximation is rather good as along as N is big and we are not too close toward the end. Now let us generalise!

Let $\overrightarrow{a_1}, \overrightarrow{a_2}, \overrightarrow{a_3}$ denote three position vectors in $\mathbb{R}^3$ that denote lattices of the given crystal's unit cell. Since crstals have a periodic structure, these vectors completely determine the geometry. Assume for simplicity that we again have N stationary atoms at each sites. Then, the periodicity of potential and the cylic BC are as follows:

$$\boxed{V(\overrightarrow{r} + \overrightarrow{a}) = V(\overrightarrow{r}); \psi(\overrightarrow{r} + N\overrightarrow{a}) = \psi(\overrightarrow{r})} \text{ where } \overrightarrow{a} = \overrightarrow{a_1} + \overrightarrow{a_2} + \overrightarrow{a_3}$$

We can re-do the problem by noting that G_H is the direct product of three $\mathbb{Z}/N\mathbb{Z}$, for each spatial coordinate, and then taking the *direct product representation* of $(\mathbb{Z}/N\mathbb{Z})^3$. We will instead read off the answer from the 1-dimensional solution.

$$\begin{aligned}\psi_{n_1,n_2,n_3}(\overrightarrow{r} + \overrightarrow{a}) &= e^{\frac{2\pi n_1 i}{N}} e^{\frac{2\pi n_2 i}{N}} e^{\frac{2\pi n_3 i}{N}} \psi_{n_1,n_2,n_3}(\overrightarrow{r}) \\ &= e^{i\frac{2\pi n_1}{Na_1}a_1} e^{i\frac{2\pi n_2}{Na_2}a_2} e^{i\frac{2\pi n_3}{Na_3}a_3} \psi_{n_1,n_2,n_3}(\overrightarrow{r}) \\ &= \mathrm{e}^{i(K_{n_1}a_1 + K_{n_2}a_2 + K_{n_3}a_3)} \psi_{n_1,n_2,n_3}(\overrightarrow{r}) \\ = e^{i\overrightarrow{K}_{n_1,n_2,n_3}\cdot\overrightarrow{a}} \psi_{n_1,n_2,n_3}(\overrightarrow{r}) &\text{ where K is defined as before.}\end{aligned}$$

Grouping the indices together as a single index n, the **Bloch's Theorem** reads as follows:

$$\boxed{\psi_n(\overrightarrow{r} + \overrightarrow{a}) = e^{i\overrightarrow{K}_n\cdot\overrightarrow{a}}\psi_n(\overrightarrow{r})}$$

Remark 0. The theorem is a manifestation of symmetry induced by the periodicity of crystals.

Remark 1. Group representation classifies eigenstates into similar categories by labelling them with *quantum numbers*.

Perturbation, Selection Rule, Energy-Splitting

Other than Coulomb potential, the quantum harmonic oscillator is another essential potential that is spherically symmetric, i.e., $G_H = SO(3)$. Let us work in dimension 3 where $V(x, y, z) = \frac{m}{2}w^2(x^2 + y^2 + z^2)$. Suppose we have drilled down the Schrödinger equation and have obtained the complete solution, the Hermite polynomials. The energy of an electron in an energy eigenstate will not change unless we *perturb* the system. Under a small perturbation by an external electric field, we can test in a lab that only certain transitions in eigenstates occur by observing the spectral lines whose frequency is given by $hf = |E_f - E_i|$. This phenomenon must be related to the harmonic potential; clearly, a zero potential, i.e., a free particle, would yield a different result. How does group representation explain this phenomenon?

Let us write the perturbation by an external field E_{ext} as H'. Let $\hat{p}$, $\hat{E}$ denote the electric dipole operator and the external field operator, respectively. Then, H' is as follows:

$$H' = -\hat{p}\cdot\hat{E} \equiv -p_xE_x \bigotimes p_yE_y \bigotimes p_zE_z = -e\left[xE_x \bigotimes yE_y \bigotimes zE_z\right]$$
$$= \text{-e } [E_x x \bigotimes E_y y \bigotimes E_z z] \in GL(\mathcal{H}_x \bigotimes \mathcal{H}_y \bigotimes \mathcal{H}_z)$$
where we can commute E_{ext} and position since E is external, and $e = 1.6 \times 10^{-19}C$.

Let $|n_xn_yn_z\rangle \equiv |n_x\rangle \bigotimes |n_y\rangle \bigotimes |n_z\rangle \in \mathcal{H}_x \bigotimes \mathcal{H}_y \bigotimes \mathcal{H}_z$ denote an eigenstate where $n_i \geq 0$ for $i = 1, 2, 3$. Then,

$$|n_xn_yn_z\rangle \xrightarrow{\text{Perturbation}} \left|n'_xn'_yn'_z\right\rangle = H' \left|n_xn_yn_z\right\rangle$$

As discussed before, two states are *genuinely* different if $\left\langle n_xn_yn_z \,\middle|\, n'_xn'_yn'_z\right\rangle = 0$. Now that H' *intertwines* the eigenstates, instead of leaving them invariant as the original H, we need to compute $\left\langle n_xn_yn_z \,\middle|\, H' \,\middle|\, n'_xn'_yn'_z\right\rangle$ to determine the *overlap* of the two states. Hence, such inner product determines whether or not a transition between eigenstates is possible or forbidden.

Given $|\psi\rangle$ and $|\varphi\rangle \in \mathcal{H}$, $\langle\psi \,|\, \varphi\rangle = 0$ if $|\psi\rangle$ and $|\varphi\rangle$ transform as different irrep of G_H, i.e., if $\gamma^{|\psi\rangle} \neq \gamma^{|\varphi\rangle}$. Let $\gamma^{H'}$ denote the irrep by which the perturbation transforms; H' is simply an operator that transforms in a certain way under the group action by G_H, in contrast to the unperturbed H^0 that is invariant under the group action by G_H, that is, H^0 transforms as the trivial representation. Based on this discussion, $\left\langle n_xn_yn_z \,\middle|\, H' \,\middle|\, n'_xn'_yn'_z\right\rangle = 0$ if the decomposition of $\gamma^{H'} \bigotimes \gamma'$ into the irreps of G_H does not contain γ.

Now, the problem. Note that the product states split into three Cartesian coordinates.

$$\left\langle n_xn_yn_z \,\middle|\, H' \,\middle|\, n'_xn'_yn'_z\right\rangle = A\,\langle n_x \,|\, x \,|\, n'_x\rangle \left\langle n_y \,\middle|\, y \,\middle|\, n'_y\right\rangle \langle n_z \,|\, z \,|\, n'_z\rangle \text{ for some A} \in \mathbb{R}$$

On each 1-dimensional space, the Hamiltonian group is the good old $S_2 \cong \mathbb{Z}/2\mathbb{Z}$ since the potential $\frac{m}{2}w^2x^2$ is even. Admittedly, S_2 is a subgroup of the full symmetry group. One might prove by contradiction or construction that S_2 is indeed the full G_H on a 1-dimensional space. For this application, I am not interested in a highly general transformation. Rather, I am interested in solving the problem, that is, how group representation explains a spectroscopic phenomenon, and the subgroup S_2 is sufficient for our purpose.

χ_1 denotes the symmetric irrep, and χ_{-1} the anti-symmetric irrep. We want $\left\langle n_xn_yn_z \,\middle|\, H' \,\middle|\, n'_xn'_yn'_z\right\rangle = 0$. This occurs when WLOG $\langle n_x \,|\, x \,|\, n'_x\rangle = 0$. Under spatial *inversion*, $x \to -x \implies$ x transforms as χ_{-1}. Suppose n'_x transforms as χ_{-1}. Then $\gamma^{H'} \bigotimes \gamma'$transforms as χ_1; after all, the direct product of two anti-symmetric irreps must be symmetric. Then, $\langle n_x \,|\, x \,|\, n'_x\rangle = 0$ if $|n_x\rangle$ transforms anti-symmetrically. To generalise, $\langle n_x \,|\, x \,|\, n'_x\rangle = 0$ if $|n_x\rangle$ and $|n'_x\rangle$ transform either as χ_1 or χ_{-1} *together*. In the function space, $|n_x\rangle$'s are given by the Hermite polynomials, which are even when n is even, and odd when n odd. Hence, $\langle n_x \,|\, x \,|\, n'_x\rangle = 0$ if n_x, n'_x are both even or both odd.

Is the transition from $n_1 = 0$ to $n_2 = 3$ possible? For this, we need an extra help from the Hermite polynomials. Hermite polynomials form a complete orthogonal basis on $L^2(\mathbb{R})$ with respect to the weight function $w(x) = e^{-x^2}$.

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)w(x)dx = \sqrt{\pi}2^n n!\delta_{nm}$$

On the function space, $|n'_x\rangle$ corresponds to a degree n_1 Hermite polynomial, and $|n_x\rangle$, a degree n_2 Hermite polynomial for some $n_1, n_2 \geq 0$. WLOG let $n_2 \geq n_1$. Then x $|n'_x\rangle$ corresponds to a degree $n_1 + 1$ polynomial that can be written as follows:

$$xH_{n_1}(x) = \textstyle\sum_{k=0}^{n_1+1} c_kH_k(x), \text{ for some } c_k \in \mathbb{R}$$
$$\implies \langle n_x \,|\, x \,|\, n'_x\rangle = \textstyle\int_{-\infty}^{\infty} H^*_{n_2}(x)xH_{n_1}(x)dx = \sum_{k=0}^{n_1+1}\left[c_k \int_{-\infty}^{\infty} H^*_{n_2}(x)H_{n_1}(x)dx\right]$$

Hence, if $\langle n_x \,|\, x \,|\, n'_x\rangle \neq 0$, i.e., the transition is possible, then $n_2 = n_1$ or $n_2 = n_1 + 1$. Generally, if we set no inequality between n_1 and n_2, we have $|n_1 - n_2| \leq 1$. However, the difference cannot be zero based on the previous discussion. Hence, the selection rule:

$$\boxed{\Delta n = 1}$$

Under an external electric field perturbation, transition occurs only if the above relation holds.

Now let us revert back to the Couloumb potential. Consider a H-atom placed in a quasi−2−dimensional crystal whose unit cell is a square. The spherical invariance of H^0 is now broken into $G_H = D_4$ after we perturbed the system by trapping it in a cell. Admittedly, this is an assumption on the new G_H; the point group can be an octahedral group, cubic group or etc; it need not be D_4. However, due to the geometry of quasi−2−dimensional square cell, $G_H = D_4$. Hence,

$$H^0 \xrightarrow{\text{Perturbation}} H = H^0 + H'$$

Usually H' splits the degeneracies of energy levels. To analytically compute by how much they split, we need more machinaries, but symmetry is enough to give us a qualitative understanding of the perturbed system.

For our next discussion, we note that the Coulomb potential yields a quantum number l whose eigenstates form a $2l+1$-dimensional energy eigenspace. Using these states as the basis, $SO(3)$ yields an irreducible spin representation for each spin l. What is its irreducible character? Are the irreducible characters orthonormal, albeit the group being infinite? Without getting into the study of Lie group and Haar measure, we use the following results without proof:

$$\chi^{(l)}(\phi) = \frac{\sin\left[(l+\frac{1}{2})\phi\right]}{\sin(\phi/2)} \tag{4}$$

$$\left\langle \chi^{(l_1)} \,\middle|\, \chi^{(l_2)} \right\rangle \equiv \frac{1}{2\pi}\int_0^{2\pi} (1-\cos\phi)\chi^{(l_1)*}\chi^{(l_2)}d\phi = \delta_{l_1 l_2} \tag{5}$$

Suppose we are interested in how the three degeneracies in a $j = l = 1$ split. The $l = 1$ angular momentum representation will generally not be an irrep once H' is introduced. We decompose the $l = 1$-irrep into the irreps of D_4. First, we need the character table of D_4:

	1	$2C_4$	C_4^2	$2C_2^{d_1}$	$2C_2^{d_2}$
χ_1	1	1	1	1	1
χ_2					
χ_3					
χ_4					
χ_5					

The C_4 denotes $\pi/2$ anti-clockwise rotation whereas $C_2^{d_1}$ and $C_2^{d_2}$ denote the reflections, diagonal and non-diagonal. For our purposes, the exact nature of each group element is not important and the table construction is an easy, yet laborious, exercise using the orthogonality relations. Here we present a technique for identifying all 1-dimensional representations.

Let $\gamma : G \to G_1$ be a group homomorphism. Let N be a normal subgroup of G such that N is contained in K, the kernel of γ, i.e., $\mathrm{N} \subseteq K \triangleleft \mathrm{G}$. Consider $gN \in G/N$. Noting that $\mathrm{gN} \subseteq \mathrm{gK}$ and $\bar{\gamma} : G/K \to G_1$, define $\tilde{\gamma} : G/N \to G_1$ such that $\tilde{\gamma}(gN) = \bar{\gamma}(gK) = \gamma(g)$. This defines a homomorphism on G/N where $N \subseteq K$.

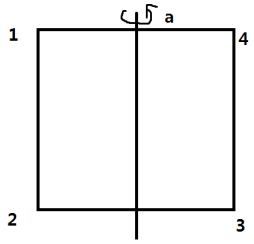
Conversely, suppose $\gamma : G/N \to G_1$, a homomorphism on G/N, is given. Let $\pi : G \to G/N$ be the canonical homomorphism. Then, define $\tilde{\gamma} = \gamma \circ \pi : G \to G_1$. This defines a homomorphism on G. Hence, assuming $N \subseteq K$, there exists a bijection between $\gamma : G \to G_1$ and $\gamma : G/N \to G_1$.

Now we focus on 1-d representation by $G_1 = C^*$. Note $\gamma|_{[G,G]} = 1$, i.e., $[G,G] \subseteq K$, where $[G,G]$ is the normal subgroup generated by commutators. Hence, we can identify all 1-d irreps of G with the irreps of $G/[G,G]$. Let us invoke the following lemma: G/N is abelian $\iff$ N contains $[G,G]$. Hence, $G/[G,G]$ is abelian and therefore there are $|G/[G,G]|$ 1-d irreps of G.

Before completing the D_4 table, let us answer the following question posed before: why are there two 1-d irreps for S_3?

By the even/odd permutation homomorphism, $S_n/A_n \cong \mathbb{Z}/2\mathbb{Z}$, an abelian group. $\therefore [S_n, S_n] \subseteq A_n$, where A_n is the kernel of such homomorphism. Conversely, consider $(ij)(kl) \in A_n$ where each element denotes transposition. Let $u = (li), v = (lj), w = (kj), t = (kl)$. Then, $(ij)(kl) = [u, v][w, t] \in [S_n, S_n]$. Using this argument, it is trivial to show $A_n \subseteq [S_n, S_n]$. $\therefore A_n = [S_n, S_n]$. Hence, there are $|S_n/[S_n, S_n]| = |S_n/A_n| = 2$ one-dimensional irrep of $S_n \forall n \geq 2$. These irreps are the trivial representation and the even/odd permutation representation.

Now we complete the D_4 table. Let ρ be the $\frac{\pi}{4}$ anti-clockwise rotation and a the following operation:



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Then, one can show that $[a, \rho] = \rho^2$ by a simple computation. It is also true that $(\rho) \triangleleft D_4$ since $\dfrac{|D_4|}{|(\rho)|} = 2$, where (ρ) is a subgroup generated by ρ. Consider $D_4/(\rho) \cong \mathbb{Z}/2\mathbb{Z}$, an abelian group $\implies [D_4, D_4] \subseteq (\rho)$ since (ρ) must contain the commutator subgroup. Since $[a, \rho] = \rho^2 \in [D_4, D_4]$, this implies $[D_4, D_4]$ is a subgroup of order 2 or 4. Suppose the latter. Then, since $[D_4, D_4]$ is a subgroup of (ρ), $[D_4, D_4] = (\rho)$. There are $|D_4/(\rho)| = \frac{8}{4} = 2$ one-dimensional irrep. Since we have 5 conjugacy classes,

$$1^2 + 1^2 + x^2 + y^2 + z^2 = |D_4| = 8 \implies x^2 + y^2 + z^2 = 6,$$

where x,y,z ≥ 2 are degrees of irreps. However,

$$x^2 + y^2 + z^2 \geq 2^2 + 2^2 + 2^2 = 12 \implies 6 \geq 12$$
$$\therefore [D_4, D_4] \cong \mathbb{Z}/2\mathbb{Z} \text{ and we have } \tfrac{8}{2} = 4 \text{ one-dimensional irreps.}$$

Since $C_2^{d_1}, C_2^{d_2} \in D_4$ are transpositions,

$$\chi(\tau^2) = \chi(\tau)\chi(\tau) = \chi(1) = 1 \implies \chi(\tau) = \pm 1$$

Since each transposition can take two values independently and we have 4 inequivalent 1-d irreps, the following must be true:

	1	$2C_4$	C_4^2	$2C_2^{d_1}$	$2C_2^{d_2}$
χ_1	1	1	1	1	1
χ_2	1			-1	-1
χ_3	1			1	-1
χ_4	1			-1	1
χ_5					

Let $a = C_2^{d_1}, b = C_2^{d_2}$. Then, since $ab = \rho$,

$$\chi(\rho) = \chi(ab) = \chi(a)\chi(b) = \pm 1$$
$$\chi(\rho^2) = \chi(\rho)\chi(\rho) = 1$$

	1	$2C_4$	C_4^2	$2C_2^{d_1}$	$2C_2^{d_2}$
χ_1	1	1	1	1	1
χ_2	1	1	1	-1	-1
χ_3	1	-1	1	1	-1
χ_4	1	-1	1	-1	1
χ_5	a	b	c	d	e

The rest is an application of orthogonality.

$$1^2 + 1^2 + 1^2 + 1^2 + a^2 = 8 \implies \boxed{a = 2}$$

$$\begin{aligned} 2 + b + c + d + e &= 0 \\ 2 + b + c - d - e &= 0 \\ 2 - b + c + d - e &= 0 \\ 2 - b + c - d + e &= 0 \end{aligned}$$

$$\implies \boxed{\{b, c, d, e\} = \{0, -2, 0, 0\}}$$

	1	$2C_4$	$\vdots$ C_4^2	$2C_2^{d_1}$	$2C_2^{d_2}$
χ_1	1	1	1	1	1
χ_2	1	1	1	-1	-1
χ_3	1	-1	1	1	-1
χ_4	1	-1	1	-1	1
χ_5	2	0	-2	0	0

Using the previous result on the irrep of angular momentum,

$$\chi^{(l=1)}(\phi) = \frac{\sin\left[(3/2)\phi\right]}{\sin(\phi/2)}$$

In the order of the character table, we have $\phi = \left\{0, \frac{\pi}{2}, \pi, \pi, \pi\right\}$
to which $\chi^{(l=1)} = \{3, 1, -1, -1, -1\}$.

The angles correspond to the group elements of D_4, namely $1, C_4, C_4^2, C_2^{d_1}, C_2^{d_2}$. One can show $\chi^{(l=1)} = \chi_2 + \chi_5$. Hence,

$$\gamma^{(l=1)} \sim \gamma^{(2)} \bigoplus \gamma^{(5)}$$

Note that χ_2 and χ_5 correspond to the irreps of degree 1 and 2, respectively. Hence, the degeneracy of 3 states splits into 2 distinct energy eigenspaces where one eigenspace maintains a degeneracy of 2 states and another eigenspace is non-degenerate. Again, group representation is insufficient to tell us of the relative energy ordering of the split states.

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