# Chapter 2

## Representations

In the last chapter we learned something about the structure of the groups themselves, but we are really interested in how the symmetry groups act on the eigenstates of a physical Hamiltonian. The set of states corresponding to a given eigenvalue of degeneracy  $\ell$  forms a vector space of dimension  $\ell$ . The result of applying the symmetry operation to any of these states gives a state with the same energy eigenvalue, and thus a state in the same  $\ell$ -dimensional vector space. The symmetry acts linearly on the states,

$$S(\alpha |\psi_1\rangle + \beta |\psi_2\rangle) = \alpha S(|\psi_1\rangle) + \beta S(|\psi_2\rangle),$$

so the operators are linear operators on a vector space, and may be considered  $\ell \times \ell$  matrices acting on this eigenspace.

Let  $\{e_i, i=1,...,\ell\}$  be an orthonormal basis of the vector space. If  $A \in G$  is one of the symmetry operators, it will act on  $e_i$  to give a linear combination of the basis vectors,

$$Ae_i = \sum_j e_j T_{ji}(A).$$

Notice the order of the indices on T. If  $\psi = \sum \psi_i e_i$  is an arbitrary vector in the eigenspace, and if  $\psi' = \sum \psi'_i e_i = A\psi$ , then

$$\psi' = \sum \psi_i' e_i = A \sum \psi_i e_i = \sum \psi_i A e_i = \sum_{ij} \psi_i T_{ji}(A) e_j,$$

or

$$\psi_j' = \sum_k T_{jk}(A)\psi_k,$$

by the linear independence of the  $e_j$ 's. Note the order of the indices now.  $T_{ij}$  can be considered the matrix element  $T_{ij}(A) = \langle e_i | A | e_j \rangle$ .

We can find the composition law for these matrices by noting that

$$ABe_{i} = \sum_{k} e_{k} T_{ki}(AB) = A(Be_{i}) = A\left(\sum_{j} e_{j} T_{ji}(B)\right) = \sum_{j} T_{ji}(B) Ae_{j}$$

$$= \sum_{j} T_{ji}(B) \sum_{k} T_{kj}(A) e_{k},$$
so
$$T_{ki}(AB) = \sum_{j} T_{kj}(A) T_{ji}(B),$$
or
$$T(AB) = T(A)T(B),$$

where the multiplication is just ordinary matrix multiplication. Thus we have a homomorphism from the group G onto a group of  $\ell \times \ell$  nonsingular matrices. This is called an  $\ell$ -dimensional representation of the group G.

If no two elements of G are mapped into the same matrix, then the homomorphism  $G \to T = \{T(A) | A \in G\}$  is an isomorphism,  $G \cong T$ , and we call the representation **faithful**. An example of an unfaithful representation for any group is the homomorphism  $g \in G \mapsto \mathbb{I}$ , in which every element is mapped into the identity matrix. This trivial representation is called the **identity representation** of the group.

Note that for any representation

$$T(1)T(A) = T(1A) = T(A)$$
, so  $T(1) = 1_{\ell \times \ell}$ ,

as T(A) is nonsingular. Also

$$T(A^{-1})T(A) = T(A^{-1}A) = T(\mathbb{1}) = \mathbb{1}$$
, so  $T(A^{-1}) = [T(A)]^{-1}$ .

If R is an  $\ell$ -dimensional representation of G, and if S is a fixed nonsingular  $\ell \times \ell$  matrix, then

$$T(A) := S^{-1}R(A)S$$
 for all  $A \in G$ ,

is also clearly an  $\ell$ -dimensional representations of G. Two representations related by such a fixed similarity transformation are **equivalent representations**.

Consider an *n*-dimensional representation T of G on a vector space  $L_n$ . Suppose we take a particular vector v and act on it with all the elements T(A) and then consider the vector space  $L_m$  spanned by these vectors, *i.e.* the space of all linear combinations of  $\{T(A)v|A\in G\}$ . Surely  $L_m$  is contained in  $L_n$ , but it might be the whole of  $L_n$  or it might be a proper subspace<sup>1</sup>, of dimension m < n. Clearly  $L_m$  is closed under the action of the group, as for any  $A \in G$ , the action of A on an arbitrary vector  $\sum a_B T(B)v$  in  $L_n$  is  $A: \sum a_B T(B)v \mapsto \sum a_B T(A)T(B)v = \sum a_B T(AB)v$ , which is included in the definition of  $L_m$ . If we choose a new basis for  $L_n$  such that the first m basis vectors span the subspace  $L_m$ , we see that

$$T(A)e_i = \sum_{j=1}^{m} e_j T_{ji}(A)$$
 for  $i \le m$ 

or  $T_{ii}(A) = 0$  for all  $i \leq m, j > m, A \in G$ . So T has the form

$$T(A) = \begin{pmatrix} D^{(1)}(A) & X(A) \\ 0 & D^{(2)}(A) \end{pmatrix}$$
 (2.1)

with  $D^{(1)}$  an  $m \times m$  matrix,  $D^{(2)}$  an  $(n-m) \times (n-m)$  matrix, and X an  $m \times (n-m)$  matrix.

If we check how two such matrices multiply we can easily show that  $D^{(1)}(AB) = D^{(1)}(A)D^{(1)}(B)$  and  $D^{(2)}(AB) = D^{(2)}(A)D^{(2)}(B)$ , so  $D^{(1)}$  and  $D^{(2)}$  are m and n-m dimensional representations respectively, and our original representation T is said to be a **reducible representation**. The subspace  $L_m$  is called an **invariant subspace**. If there is no proper subspace of  $L_n$  which is closed under action by the group, we say that T is an **irreducible representation**.

We expect symmetry transformations on our hilbert space to be unitary transformations, preserving the norm of the states. Then because we asked that  $e_i$  be an orthonormal basis, the matrices T(A) will be unitary matrices, and the representation is called a **unitary representation**. We will now prove that any finite dimensional representation of a finite group is equivalent to a unitary representation. This will also be true for infinite groups if we can define finite invariant integration measures, but this we will consider later.

Consider a representation T of a finite group G. Define the matrix

$$H = \sum_{A \in G} T(A)T^{\dagger}(A).$$

<sup>&</sup>lt;sup>1</sup>A subspace of a vector space is a subset closed under addition and scalar multiplication. A **proper subspace** is a subspace which is not the whole space and not just the point {0}.

H is clearly hermitian so it can be diagonalized by a unitary U,  $H_d = U^{-1}HU$ ,  $(H_d)_{ij} = d_i\delta_{ij}$ . So

$$d_{i} = (H_{d})_{ii} = \sum_{A} \sum_{k} (U^{-1}T(A))_{ik} (T^{\dagger}(A)U)_{ki}$$
$$= \sum_{A} \sum_{k} |(T^{\dagger}(A)U)_{ki}|^{2} > 0,$$

as  $U^{-1}=U^{\dagger}$  because U is unitary, and both T and U are nonsingular. Thus we can define  $\left(H_d^{1/2}\right)_{ij}=d_i^{1/2}\delta_{ij}$  and  $V=UH_d^{1/2}$  will provide the similarity transformation from T to an equivalent unitary representation  $\Gamma$ . Let

$$\Gamma(A) = V^{-1}T(A)V = H_d^{-1/2}U^{-1}T(A)UH_d^{1/2}.$$

Then

$$\begin{split} \Gamma(A)\Gamma^{\dagger}(A) &= H_d^{-1/2}U^{-1}T(A)\underbrace{UH_d^{1/2}H_d^{1/2}U^{-1}}_{H=\sum_B T(B)T^{\dagger}(B)}T^{\dagger}(A)UH_d^{-1/2} \\ &= H_d^{-1/2}U^{-1}\underbrace{\sum_B T(A)T(B)T^{\dagger}(B)}_{H}T^{\dagger}(A)UH_d^{-1/2} \\ &= H_d^{-1/2}H_dH_d^{-1/2} = \mathbb{I}, \end{split}$$

where in the first line we used that  $H_d$  is hermitean and U is unitary, and in the second that the underbraced sum is  $\sum_B T(AB)T^{\dagger}(AB) = \sum_B T(B)T^{\dagger}(B) = H$ , where the first equality is due to the left invariance of sums over all the elements in the group.

This is the first example we have seen, but far from the last, of the usefulness of summing over all the elements of a group with equal weight. For a Lie group, one with elements indexed by a continuous parameter, we will need carefully to give meaning to a sum with equal weights over all elements. We will need to define an invariant integration measure. We will then find that for compact Lie groups, for which the total group volume in finite, we can again find a similarity transformation, so that we will have proven:

**Theorem:** Any finite dimensional representation of a finite group or of a compact Lie group is equivalent to a unitary representation.

If T was reducible, so is  $\Gamma$ , as there is still an invariant proper subspace. The necessary change of basis to get  $\Gamma$  into the form of eq. 2.1 can be chosen unitary, so the new form is also unitary. But then

$$\Gamma(A) = (\Gamma(A^{-1}))^{\dagger} = \begin{pmatrix} D^{(1)\dagger}(A^{-1}) & 0 \\ X^{\dagger}(A^{-1}) & D^{(2)\dagger}(A^{-1}) \end{pmatrix}.$$

But we know that the lower left block of  $\Gamma$  is zero, so X=0, and the representation is block diagonal,

$$\Gamma(A) = \begin{pmatrix} D^{(1)} & 0\\ 0 & D^{(2)} \end{pmatrix}.$$

A representation which can be successively reduced in this manner to a block diagonal form of two or more irreducible representations is said to by **fully reducible**. We say that  $\Gamma$  is the **direct sum** of the irreducible representations.

We will find physics examples after we prove

#### 2.1 Schur's First Lemma

Any matrix which commutes with all the matrices of an irreducible representation of a finite or compact Lie group must be a multiple of the identity.

We can assume we have made the similarity transformation so that our representives  $\Gamma(A)$  are unitary. Whether or not the commuting M is a multiple of the identity will not be affected by this similarity transformation. Then if  $[M, \Gamma(A)] = 0$  for all  $A \in G$ ,

$$\Gamma(A)M = M\Gamma(A), \quad \text{and also } M^\dagger\Gamma^\dagger(A) = \Gamma^\dagger(A)M^\dagger.$$

We multiply the last equation by  $\Gamma(A)$  on the left and on the right, using the fact that  $\Gamma(A)$  is unitary, we get

$$\Gamma(A)M^{\dagger} = M^{\dagger}\Gamma(A),$$

so  $M^{\dagger}$  also commutes with all  $\Gamma(A)$ , and so do the hermitean matrices  $H_{+} = M + M^{\dagger}$  and  $H_{-} = i(M^{\dagger} - M)$ . Now either of these hermitean matrices can be diagonalized by a unitary matrix  $U, H = UDU^{-1}$ , where  $D_{ij} = d_{i}\delta_{ij}$ . But

we can also transform our representation  $\Gamma$  by U, defining a new representation  $\Gamma'(A) = U^{-1}\Gamma(A)U$ , which is still irreducible and unitary, and  $[\Gamma'(A), D] = U^{-1}[\Gamma(A), H]U = 0$ . Thus

$$(\Gamma'(A)D)_{ij} = \Gamma'(A)_{ij}d_j = (D\Gamma'(A))_{ij} = \Gamma'(A)_{ij}d_i \Rightarrow \Gamma'(A)_{ij}(d_j - d_i) = 0.$$

Now either all the  $d_i$  are equal, in which case D is a multiple of the identity, or  $\Gamma'(A)_{ij} = 0$  for all A, except for i and j in the same block, that is for i and j having the same d. But that would mean  $\Gamma'(A)$  is reducible, and so is  $\Gamma(A)$ , which contradicts the hypothesis. This argument works for both  $H_+$  and  $H_-$ , and tells us that both must be multiples of the identity, as must be  $M = H_+ + iH_-$ .

This lemma has a useful contrapositive: if a matrix M which is not a multiple of the identity matrix commutes with all the representatives of elements in the group, the representation must be reducible.

As an example of reducibility and the use of Schur's Lemma, consider the three dimensional rotation group. This is a continuous (infinite) group. The elements may be parameterized by a 3-vector  $\vec{\omega}$ , and the group elements written as

$$g(\vec{\omega}) = e^{i\vec{\omega}\cdot\vec{L}},$$

where  $L_j$  are the angular momentum operators<sup>2</sup>. [As we shall define later, these are generators of a Lie algebra, not generators of the group in the sense we have used so far, e.g. in  $D_4 = \langle C, m_x \rangle$ .] As we know from quantum mechanics, the  $L_j$  do not commute with each other, but  $L^2 = \sum_j L_j^2$  does commute with all the  $L_j$ , and therefore with all the group elements  $g \in SO(3)$ .

Thus  $L^2$  acts as a constant value on any irreducible representation of the rotation group. That is, all the states in an irreducible representation are eigenstates of  $L^2$  with eigenvalue<sup>3</sup>  $\ell(\ell+1)$ ,  $\ell=0,1,2,...$ 

Now consider a 3-D isotropic harmonic oscillator with  $H = \vec{p}^2/2m + \frac{1}{2}k\vec{r}^2$ . The motion in the three cartesian coordinates decouple, so the state of the

<sup>&</sup>lt;sup>2</sup>We are taking  $\hbar=1$  here if we wish to associate  $L_j$  with the quantum mechanical operator  $-i\hbar \sum_{kq} \epsilon_{jkq} r_k \partial_q$ .

<sup>&</sup>lt;sup>3</sup>Systems with fermions can lie in ray representation rather than a true representation of SO(3). Then the value of  $\ell$  can be half an odd integer. This possibility arises because the phase of the wavefunction is unphysical, and it is not required that every rotation which leaves space unchanged, such as rotation by  $2\pi$ , leave the wavefunction unchanged, but only that it leaves  $|\psi^2|$  unchaged. This will be discussed later, when we discuss the simple-connectedness of Lie groups.

system can be described by the product of states of one dimensional harmonic oscillators, specified by the excitation levels  $n_j, j = 1, 2, 3$ . Thus the energy is given by  $E = \hbar \omega (\sum_j n_j + 3/2)$ . The ground state (0,0,0) is nondegenerate, while the first excited state is triply degenerate, with occupation numbers (1,0,0), (0,1,0), and (0,0,1). These form an  $\ell = 1$  irreducible representation of the rotation group. The third level has six states  $|(2,0,0)\rangle, |(0,2,0)\rangle, |(0,0,2)\rangle, |(1,1,0)\rangle, |(1,0,1)\rangle$  and  $|(0,1,1)\rangle$ . This cannot be an irreducible representation. In terms of the raising and lowering operators  $a_j^{\dagger}$  and  $a_j$  for each direction, the number operator  $N = n_x + n_y + n_z = \sum_j a_j^{\dagger} a_j$  and the angular momentum generators are  $L_i = -i \sum_{jk} \epsilon_{ijk} a_j^{\dagger} a_k$ , so

$$L^{2} = -\sum_{i} \sum_{jk} \epsilon_{ijk} a_{j}^{\dagger} a_{k} \sum_{\ell m} \epsilon_{i\ell m} a_{\ell}^{\dagger} a_{m} = -\sum_{jk} a_{j}^{\dagger} a_{k} a_{j}^{\dagger} a_{k} + \sum_{jk} a_{j}^{\dagger} a_{k} a_{k}^{\dagger} a_{j}$$

$$= \sum_{jk} \left( -a_{j}^{\dagger} (a_{j}^{\dagger} a_{k} + \delta_{jk}) a_{k} + a_{j}^{\dagger} (a_{k}^{\dagger} a_{k} + 1) a_{j} \right)$$

$$= -\left( \sum_{j} a_{j}^{\dagger^{2}} \right) \left( \sum_{k} a_{k}^{2} \right) - N + \sum_{j} a_{j}^{\dagger} (N + 3) a_{j}$$

$$= -\left( \sum_{j} a_{j}^{\dagger^{2}} \right) \left( \sum_{k} a_{k}^{2} \right) + 2N + \sum_{j} a_{j}^{\dagger} \underbrace{N a_{j}}_{a_{j}(N-1)}$$

$$= -\left( \sum_{j} a_{j}^{\dagger^{2}} \right) \left( \sum_{k} a_{k}^{2} \right) + N^{2} + N.$$

Now  $N=n_x+n_y+n_z$  is 2 on all the six states under discussion. In the last expression, the first term vanishes on the  $|(1,1,0)\rangle$  state and its cousins, and gives  $-2(|(2,0,0)\rangle + |(0,2,0)\rangle + |(0,0,2)\rangle$ ) when acting on any of the states  $|(2,0,0)\rangle$ ,  $|(0,2,0)\rangle$ , or  $|(0,0,2)\rangle$ . Thus on the state proportional to  $(|(2,0,0)\rangle + |(0,2,0)\rangle + |(0,0,2)\rangle)$  it acts as -6, cancelling the  $N^2 + N$  contribution, while on the two states orthogonal to this it gives zero. So we see that  $L^2$  is not a constant on the space of twice-excited states, but divides it into two subspaces, a singlet with  $L^2=0$  and a five dimensional space with  $L^2=6$ . That is, the second excited state of the isotropic oscillator is decomposed into an  $\ell=0$  irreducible representation and an  $\ell=2$  irreducible representation of the rotation group.

It is also a very interesting idea to apply this kind of consideration to the energy eigenstates of the nonrelativistic hydrogen atom.

## 2.2 Schur's Second Lemma

If  $\Gamma^i$  and  $\Gamma^j$  are irreducible unitary representations of G, of dimensions  $\ell_i$  and  $\ell_j$  respectively, and if

$$\Gamma^i(A)M = M\Gamma^j(A)$$
 for all  $A \in G$ ,

then either M=0 or  $\Gamma^i\cong\Gamma^j$  and M is nonsingular.

Proof: Take hermitian conjugate:

$$M^{\dagger}\Gamma^{i\dagger}(A) = \Gamma^{j\dagger}(A)M^{\dagger}. \quad \text{right multiply by } M, \text{use } \Gamma^{j\dagger}(A) = \Gamma^{j}(A^{-1})$$

$$M^{\dagger}\underbrace{\Gamma^{i}(A^{-1})M}_{M\Gamma^{j}(A^{-1})} = \Gamma^{j}(A^{-1})M^{\dagger}M \quad \text{for all} \quad A^{-1} \in G, \text{ so}$$

$$M^{\dagger}M = \lambda \mathbb{I}$$

by Schur's first lemma, and the fact that  $\Gamma^j$  is irreducible. If  $\lambda=0$ ,  $\operatorname{Tr} M^\dagger M=0=\sum_{ij}(M^\dagger)_{ij}M_{ji}=\sum_{ij}|M_{ji}|^2$ , so M=0. If  $\ell_i=\ell_j$  and  $\lambda\neq 0$ , M is nonsingular, and provides the similarity transformation that proves  $\Gamma^i\cong\Gamma^j$ . If  $\ell_i\neq\ell_j$  and  $\lambda\neq 0$ , then  $\ell_i>\ell_j$ , because  $M^\dagger$  cannot be an onto map from a smaller space to a larger one. But we could have done our argument slightly differently, premultiplying by M instead of postmultiplying

$$MM^\dagger\Gamma^i(A^{-1})=M\Gamma^j(A^{-1})M^\dagger=\Gamma^i(A^{-1})MM^\dagger$$

for all  $A^{-1} \in G$ , so we also have  $MM^{\dagger} = \lambda' \mathbb{I}$ . Then either  $\lambda' = 0$  (and as  $MM^{\dagger}M = M\lambda = \lambda' M$ , so is  $\lambda$ ), or  $MM^{\dagger}$  has an image which is all of the *i*-dimensional space, which implies the *j*-dimensional space on which M acts is at least of dimension i, in contradiction with what we showed first.

## 2.3 The Great Orthogonality Theorem

Let  $\Gamma^i$  and  $\Gamma^j$  be irreducible unitary representations of a group G, of finite dimensions  $\ell_i$  and  $\ell_j$  respectively. Let X be a fixed  $\ell_i \times \ell_j$  matrix, and

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

[If G is a continuous group with an invariant measure,  $\int d\mu f(BA) = \int d\mu f(A)$  for any B and f, replace the  $\sum_{A \in G}$  by  $\int d\mu$  and the rest of this argument will go through OK.]

Then for any B,

$$\Gamma^{i}(B)M = \sum_{A} \Gamma^{i}(B)\Gamma^{i}(A)X\Gamma^{j}(A^{-1})\Gamma^{j}(B^{-1})\Gamma^{j}(B)$$

$$= \sum_{A} \Gamma^{i}(BA)X\Gamma^{j}((BA)^{-1})\Gamma^{j}(B)$$

$$= M\Gamma^{j}(B).$$

Thus by Schur's second lemma, if  $\Gamma^i$  is not equivalent to  $\Gamma^j$ , M=0 for any X. In particular, take any  $b \leq \ell_i$  and  $d \leq \ell_j$ , and let  $X_{ef} := \delta_{eb}\delta_{fd}$ . Then

$$M_{ac} = \sum_{A \in G} \Gamma_{ab}^{i}(A) \Gamma_{dc}^{j}(A^{-1}) \quad \text{must vanish}$$
so  $0 = \sum_{A \in G} \Gamma_{ab}^{i}(A) \Gamma_{cd}^{j*}(A) \quad \text{(for } \Gamma^{i} \ncong \Gamma^{j}),$  (2.2)

as  $\Gamma^j$  is a unitary representation.

On the other hand, if  $\Gamma^i$  and  $\Gamma^j$  are the same representation, then Schur's first lemma tells us  $M_{ac}=c\delta_{ac}$ . Tracing,

$$c \ell_i = \sum_{A \in G} \sum_a \Gamma_{ab}^i(A) \Gamma_{da}^i(A^{-1}) = \sum_{A \in G} \Gamma_{db}^i(\mathbb{I}) = g \delta_{bd},$$

where g is the order of G, so  $c = g\delta_{bd}/\ell_i$ , and

$$\sum_{A \in G} \Gamma_{ab}^{i}(A) \Gamma_{cd}^{i*}(A) = \frac{g}{\ell_i} \delta_{ac} \delta_{bd}. \tag{2.3}$$

If we understand the index i to run over all **inequivalent** irreducible representations, we can write both results (2.2) and (2.3) as

$$\sum_{A \in G} \Gamma_{ab}^{i}(A) \Gamma_{cd}^{j*}(A) = \frac{g}{\ell_{i}} \delta_{ij} \delta_{ac} \delta_{bd}. \tag{2.4}$$

This is known as the **great orthogonality theorem**. [Note: for the continuum version, if  $\int d\mu 1 = V$ ,

$$\int d\mu \Gamma_{ab}^{i}(A) \Gamma_{cd}^{j*}(A) = \frac{V}{\ell_{i}} \delta_{ij} \delta_{ac} \delta_{bd}.$$

In what sense is this orthogonality? Think of the space of all complexvalued functions of the group elements. Define a norm on this space of functions by  $(f,h) = \sum_{A \in G} f^*(A) h(A)$ , or for a compact Lie group,  $(f,h) = \int d\mu f^*(A(\mu)) h(A(\mu))$ . Then the great orthogonality theorem tells us that

$$\sqrt{\frac{\ell_i}{g}}\Gamma^i_{ab}(A)$$

form an orthonormal set of vectors in the vector space of all functions on the group.

If the group  $G = \{A_1, ... A_g\}$  has a finite number of elements, one orthonormal basis for functions on G is the set  $e_{\alpha}$  of functions  $e_{\alpha}(A_{\beta}) = \delta_{\alpha\beta}$ , for  $\alpha$  and  $\beta = 1, ..., g$ . This set clearly spans the space of all functions, as for any  $\psi$ ,

$$\psi = \sum_{\alpha} \psi(A_{\alpha})e_{\alpha}$$
, that is  $\psi(B) = \sum_{\alpha} \psi(A_{\alpha})e_{\alpha}(B)$ 

and is linearly independent. Thus the space of functions  $L_G$  on G is g-dimensional. The orthonormal set we got from the great orthogonality theorem has dimension  $\sum_i \ell_i^2$ , so it must be true that  $\sum_i \ell_i^2 \leq g$ . We will soon show it is an equality.

In general, if we have a set of functions  $\psi_j(A)$  on the group, we can define the operation of the group on these functions by

$$(B\psi_j)(A) := \psi_j(AB).$$

The order is important, in order to preserve the group multiplication law,  $(CB)\psi = C(B\psi)$ . To show this let both functions act on A.

$$((CB)\psi)(A) = \psi(ACB), \quad (C(B\psi))(A) = (B\psi)(AC) = \psi(ACB) \quad \text{good!}.$$

If you had tried to define  $(B\psi)(A) := \psi(BA)$ , (wrong!), you would not find  $(CB)\psi = C(B\psi)$ .

Now the function  $B\psi$  is a function of the group elements. Although it is not the function  $\psi$ , it is certainly in the space of all functions on the group. Thus the space  $L_G$  of all functions on the group provides a representation of the group, g dimensional. Let us use the basis  $e_{\alpha}$ . Then the function  $Be_{\alpha}$  can be expanded with coefficients we call  $\Gamma_{\beta\alpha}^{\text{reg}}(B)$  of the basis vectors  $e_{\beta}$ ,  $Be_{\alpha} = \sum_{\beta} \Gamma_{\beta\alpha}^{\text{reg}}(B)e_{\beta}$ . Acting on  $A_{\gamma}$ , we have

$$Be_{\alpha}(A_{\gamma}) = \sum_{\beta} \Gamma_{\beta\alpha}^{\text{reg}}(B) \underbrace{e_{\beta}(A_{\gamma})}_{\delta_{\beta\gamma}} = e_{\alpha}(A_{\gamma}B) = \delta_{A_{\gamma}B, A_{\alpha}}.$$

So we see

$$\Gamma_{\gamma\alpha}^{\rm reg}(B) = \delta_{A_{\gamma}B, A_{\alpha}}$$
.

This representation is called the **regular representation** of the group. Included in this space of all functions on G is a set of functions

$$\psi_b(A) = \Gamma^i_{ab}(A),$$

where i is any of the irreducible representations of G and a is a fixed index  $a \in [1, \ell_i]$ . This set of  $\ell_i$  functions transform by

$$(B\psi_b)(A) = \psi_b(AB) = \Gamma^i_{ab}(AB) = \sum_c \Gamma^i_{ac}(A)\Gamma^i_{cb}(B) = \sum_c \psi_c(A)\Gamma^i_{cb}(B),$$

so  $B\psi_b = \sum_c \psi_c \Gamma^i_{cb}(B)$ , and this set transforms like the  $i^{\text{th}}$  irreducible representation.

Actually we see that we have  $\ell_i$  such sets of functions, one set for each a, and they are guaranteed linearly independent by the Great Orthogonality Theorem. Thus we see that each irreducible representation  $\Gamma^i$  appears at least  $\ell_i$  times in the reduction of the regular representation. This again tells us that  $\sum_i \ell_i^2 \leq g$ . Very soon, we shall see that it appears  $exactly \ \ell_i$  times and  $\sum_i \ell_i^2 = g$ .

Any function on the group is a linear combination of the  $e_{\alpha}$  which provide the basis of the regular representation. In particular, the function  $f_B: G \to \mathbb{C}$  given by  $f_B(A) = \delta_{A,B}$  is just the  $(\mathbb{I},B)$  element in the regular representation  $\Gamma^{\text{reg}}$  as we have defined it. But the regular representation is reducible, so it is equivalent to a direct sum of irreducible representations:  $\Gamma^{\text{reg}} = S^{-1}\left(\bigoplus_{i,n_i}\Gamma^i\right)S$ , where  $\left(\bigoplus_{i,n_i}\Gamma^i\right)$  is essentially a block diagonal matrix with  $n_i$  blocks for each irreducible representation  $\Gamma^i$ , each block an  $\ell_i \times \ell_i$  matrix function on the group. This direct sum matrix thus has two compound indices, each one a combination of i giving the irreducible representation,  $n=1,\ldots,n_i$  telling which one of the  $n_i$  copies, and a or b giving which basis vector within that representation. Thus  $S=S_{(i,n,b),\beta}$  and

$$\Gamma_{\alpha\beta}^{\text{reg}} = \sum_{i,n,a,b} \left( S^{-1} \right)_{\alpha,(i,n,a)} \Gamma_{ab}^{i} S_{(i,n,b),\beta},$$

and if we define  $a_{ab}^i(B) = \sum_n (S^{-1})_{\mathbf{1},(i,n,a)} S_{(i,n,b),B}$  we have

$$\sum_{iab} a_{ab}^{(i)}(B) \Gamma_{ab}^{i}(A) = \Gamma_{\mathbf{1},B}^{\text{reg}}(A) = \delta_{A,B}.$$
 (2.5)

Multiply this by  $\Gamma_{cd}^{j*}(A)$  and sum over  $A \in G$ ,

$$\Gamma_{cd}^{j*}(B) = \sum_{iab} a_{ab}^{(i)}(B) \underbrace{\sum_{A} \Gamma_{ab}^{i}(A) \Gamma_{cd}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A) \Gamma_{cd}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A) \Gamma_{cd}^{j*}(A)}}_{\underbrace{f_{ab}^{j*}(A) \Gamma_{cd}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A) \Gamma_{cd}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{ab}^{j*}(A)}_{\underbrace{f_{$$

using the Great Orthogonality Theorem. When we insert this back into (2.5), we have

$$\delta_{AB} = \sum_{iab} \frac{\ell_i}{g} \Gamma^i_{ab}(A) \Gamma^{i*}_{ab}(B), \qquad (2.6)$$

which is sort of orthonormality of the g vectors  $\Gamma(A)$  (A is an index here) in the  $\sum \ell_i^2$  dimensional space indexed by (i,a,b). In particular, g vectors in a  $\sum_i \ell_i^2$  dimensional space can be independent, which they are, only if  $g \leq \sum_i \ell_i^2$ . Perhaps it would be clearer to say this: Using (2.6), any function on G

$$f(A) = \sum_{B} \delta_{AB} f(B) = \sum_{iab} \left( \frac{\ell_i}{g} \Gamma_{ab}^{i*}(B) \Gamma_{ab}^{i}(A) \right) f(B)$$
$$= \sum_{iab} \left( \frac{\ell_i}{g} \Gamma_{ab}^{i*}(B) f(B) \right) \Gamma_{ab}^{i}(A),$$

is a linear combination of the  $\sum \ell_i^2$  functions  $\Gamma_{ab}^i(A)$ , so these are a complete set of functions on G, and that space is g-dimensional. So again  $g \leq \sum_i \ell_i^2$ . But we have already shown  $g \geq \sum_i \ell_i^2$ , so we have an important statement about the full set of irreducible representations and their dimensions:

$$g = \sum_{i} \ell_i^2. \tag{2.7}$$

## 2.4 Characters

We have seen that two representations are considered equivalent if they are related by a similarity transformation  $\Gamma^{(1)}(A) = U\Gamma^{(2)}(A)U^{-1}$  for all  $A \in G$ .

To characterize a representation we are not interested in all the equivalent forms, so we would like something invariant under similarity. This is done by defining the **character** of a representation  $\Gamma$  to be a function  $\chi: G \to \mathbb{C}$  on the group given by

$$\chi(A) = \operatorname{Tr} \Gamma(A).$$

Note  $\chi$  is a complex-valued function on the group, not a matrix-valued function as  $\Gamma$  is. Also note it is obviously unaffected by similarity transformations. But this has an important consequence on the function  $\chi$  — namely, if A and B are conjugate group elements, i.e.  $A = C^{-1}BC$  for some  $C \in G$ , then

$$\chi(A) = \operatorname{Tr} \Gamma(A) = \operatorname{Tr} \Gamma(C^{-1}BC) = \operatorname{Tr} \left(\Gamma^{-1}(C)\Gamma(B)\Gamma(C)\right) = \operatorname{Tr} \Gamma(B)$$
  
=  $\chi(B)$ .

Thus the character is actually only a function on the conjugacy classes of the group.

Now the great orthogonality theorem (2.4)

$$\sum_{A \in G} \Gamma_{ab}^{i}(A) \Gamma_{cd}^{j*}(A) = \frac{g}{\ell_i} \delta_{ij} \delta_{ac} \delta_{bd}$$

can be traced in ab and in cd, to give

$$\sum_{A \in G} \chi^{i}(A) \chi^{j*}(A) = \frac{g}{\ell_{i}} \delta_{ij} \underbrace{\sum_{ac} \delta_{ac} \delta_{ac}}_{\ell_{i}} = g \delta_{ij}.$$

Thus two different representations have different characters—in fact they form a set of linearly independent functions on the conjugacy classes of the group. Thus the number of inequivalent irreducible representations of G must be  $\leq$  the dimension of the space<sup>4</sup> of complex functions on the classes of G, which is just the number of classes of G.

Suppose we have a representation which might be reducible. Then  $\Gamma = \bigoplus_i a_i \Gamma^i$ , which means

$$\underbrace{\Gamma^{i_1} \bigoplus \Gamma^{i_1} \bigoplus \dots \bigoplus \Gamma^{i_1}}_{a_{i_1} \text{ times}} \bigoplus \Gamma^{i_2} \dots$$

<sup>&</sup>lt;sup>4</sup>Over the field of complex numbers

That is, we know in principle that  $\Gamma$  is reducible to a direct sum of irreducible representations, but we haven't done it. Now we will see how to extract the  $a_i$ 's.

The representation  $\Gamma$  has a character  $\chi$ , so for each possible irreducible representation  $\Gamma^j$  which might be included in the direct sum, we can form

$$\sum_{A \in G} \chi^{j*}(A)\chi(A) = \sum_{i} a_i \sum_{A \in G} \chi^{j*}(A)\chi^{i}(A) = \sum_{i} a_i g \delta_{ij} = g a_j, \qquad (2.8)$$

SO

$$a_j = \frac{1}{g} \sum_{A \in G} \chi^{j*}(A) \chi(A). \tag{2.9}$$

If  $\Gamma$  is in fact irreducible, one a will come out one and the others zero. For the one j which gives  $a_j = 1$ ,  $\chi^j = \chi$ , so

$$\sum_{A \in G} \chi^*(A)\chi(A) = g \quad \text{if } \chi \text{ is irreducible.}$$

In fact, this is an "if and only if" statement, for

$$\sum_{A \in G} \chi^*(A) \chi(A) = \sum_{ij} a_i a_j \sum_{A \in G} \chi^{i*}(A) \chi^j(A) = g \sum_{ij} a_i a_j \delta_{ij} = g \sum_{ij} a_i^2.$$

If this is g, exactly one  $a_i$  is one and the others must be zero.

Let us return to the regular representation, which is a  $g \times g$  matrix representation

$$\Gamma_{\alpha\beta}^{\text{reg}}(B) = \delta_{A_{\alpha}B, A_{\beta}}.$$

The diagonal elements are  $\Gamma_{\alpha\alpha}^{\text{reg}}(B) = \delta_{A_{\alpha}B, A_{\alpha}} = \delta_{B,\mathbf{I}}$ , so

$$\chi^{\text{reg}}(\mathbb{I}) = \sum_{\alpha=1}^{g} (\mathbb{I})_{\alpha\alpha} = g, \qquad \chi^{\text{reg}}(B) = 0 \text{ for } B \neq \mathbb{I}.$$

For each irreducible representation  $\Gamma^i$  of G,  $\chi^i(\mathbb{1}) = \ell_i$ , so the number of times that representation occurs in the regular representation is

$$a_i = \frac{1}{g} \sum_{A} \chi^i(A) \chi^{\text{reg}}(A) = \frac{1}{g} \chi^i(\mathbb{I}) \chi^{\text{reg}}(\mathbb{I}) = \ell_i,$$

as we already realized from establishing that our original inequality  $g \ge \sum \ell_i^2$  was in fact saturated,  $g = \sum \ell_i^2$ . This equality now reflects just that the

dimension of the regular representation is the sum of the dimensions of its irreducible components:

$$\dim \Gamma^{\text{reg}} = g = \sum_{i} a_{i} \dim \Gamma^{i} = \sum_{i} \ell_{i}^{2}.$$

The characters also form a basis for functions on the conjugacy classes. Let  $\{C_k\}$  be the conjugacy classes<sup>5</sup> of G, and

$$f: \{\mathcal{C}_k\} \to \mathbb{C}$$

be an arbitrary function on the classes. Then  $\tilde{f}: G \to \mathbb{C}$  defined by  $\tilde{f}(A) = f(\mathcal{C}(A))$ , where  $\mathcal{C}(A)$  is the conjugacy class containing A, is a map from the group into the complex numbers. As any such function is a linear combination of the  $\Gamma^i_{ab}$ 's,  $\tilde{f}(A) = \sum_{iab} c^i_{ba} \Gamma^i_{ab}(A)$  for some set of coefficients  $c^i_{ba}$ . Because  $\tilde{f}(B^{-1}AB) = \tilde{f}(A)$ , we have

$$\sum_{iab} c_{ba}^{i} \Gamma_{ab}^{i}(A) = \sum_{iab} c_{ba}^{i} \Gamma_{ab}^{i}(B^{-1}AB) = \sum_{iabrs} c_{ba}^{i} \Gamma_{ar}^{i}(B^{-1}) \Gamma_{rs}^{i}(A) \Gamma_{sb}^{i}(B).$$

But the  $\Gamma^i_{ab}$  are a set of linearly independent functions, so

$$c_{sr}^{i} = \sum_{ab} c_{ba}^{i} \Gamma_{ar}^{i}(B^{-1}) \Gamma_{sb}^{i}(B),$$

for any B, or in matrix form

$$c^i = \Gamma^i(B)c^i\Gamma^i(B^{-1}), \quad \text{or } c^i\Gamma^i(B) = \Gamma^i(B)c^i.$$

But then Schur's first lemma tells us  $c^i \propto \mathbb{I}$ , or  $c^i_{ba} = k^i \delta_{ab}$ , and

$$\tilde{f}(A) = \sum_{i} k^{i} \sum_{a} \Gamma_{aa}^{i}(A) = \sum_{i} k^{i} \chi^{i}(A),$$

or  $f = \sum_i k^i \chi^i$  is a linear combination of the characters, and consequently the number of irreducible representations is the same as the number of conjugacy classes.

 $<sup>^5</sup>$ Here I am using k as an index that runs over the conjugacy classes, not the representations. We shall show that there are the same number of classes and irreducible representations, but there is no *natural* isomorphism between classes and irreducible representations.

<sup>&</sup>lt;sup>6</sup>By the cyclic invariance of a trace, Tr(MN) = Tr(NM) with N = B and  $M = B^{-1}A$ .

The equation (2.8) can be thought of as an orthogonality statement for the characters. As the character of each element in a conjugacy class is the same, if we define  $\eta_{\mathcal{C}}$  to be the number of elements in the class  $\mathcal{C}$ , we have

$$\sum_{k} \eta_{\mathcal{C}_k} \chi^i(\mathcal{C}_k) \chi^{j*}(\mathcal{C}_k) = g \delta_{ij}.$$

The fact that any function on classes can be expressed as a linear combination of characters enables us to write

$$\delta_{kk'} = \sum_{i} a_i(\mathcal{C}_{k'}) \chi^i(\mathcal{C}_k)$$

Multiply by  $\eta_{\mathcal{C}_k} \chi^{j*}(\mathcal{C}_k)$  and sum over k,

$$\eta_{\mathcal{C}_{k'}}\chi^{j*}(\mathcal{C}_{k'}) = \sum_{i} a_i(\mathcal{C}_{k'}) \sum_{k} \eta_{\mathcal{C}_k}\chi^i(\mathcal{C}_k)\chi^{j*}(\mathcal{C}_k) = ga_j(\mathcal{C}_{k'}),$$

so 
$$a_j(\mathcal{C}_{k'}) = \frac{\eta_{\mathcal{C}_{k'}}}{q} \chi^{j*}(\mathcal{C}_{k'})$$
, and

$$\delta_{kk'} = \sum_{i} \frac{\eta_{\mathcal{C}_{k'}}}{g} \chi^{i*}(\mathcal{C}_{k'}) \chi^{i}(\mathcal{C}_{k}).$$

This tells us

$$\sqrt{\frac{\eta_{\mathcal{C}}}{g}} \; \chi^i(\mathcal{C})$$

is a complete orthonormal basis on the set of conjugacy classes.

#### 2.5 Examples

Now we will use these results to find the irreducible representations, first finding their characters, of the group  $D_4$ .

 $D_4$  has 5 classes and 8 elements. Thus  $\sum_1^5 \ell_i^2 = 8$ , with each  $\ell_i$  a positive integer. Except for ordering, the only solution is  $\ell_1 = \ell_2 = \ell_3 = \ell_4 = 1$ ,  $\ell_5 = 2$ , so there are four one-dimensional representations and one two-dimensional one.

Let us make a table. We take the first representation to be the identity representation,  $A \mapsto 1$  for all A.

- (a) So  $\chi^1(\mathcal{C}) = 1$  for all  $\mathcal{C}$ .
- (b) For all five representations,  $\chi^i(\{\mathbb{1}\}) = \ell_i$ .

$\chi$ Class $\eta_k$	{ <b>1I</b> }	$\{C, C^3\}$	$\{C^2\}$ 1	$\{m_x, m_y\}$	$\begin{cases} \{\sigma_+, \sigma\} \\ 2 \end{cases}$
$\chi_1$	$1_{\rm a}$	$1_{\rm a}$	$1_{\rm a}$	$1_{\rm a}$	$1_{\rm a}$
$\chi_2$	$1_{\rm b}$	$-1_{\rm d}$	$1_{\rm c}$	$-1_{ m d}$	$1_{\rm d}$
$\chi_3$	$1_{\rm b}$	$-1_{\rm d}$	$1_{\rm c}$	$1_{ m d}$	$-1_{\rm d}$
$\chi_4$	$1_{\rm b}$	$1_{\mathrm{d}}$	$1_{\rm c}$	$-1_{\rm d}$	$-1_{\rm d}$
$\chi_5$	$2_{\mathrm{b}}$	0	-2	0	0

(c) The one dimensional representations are the same as their characters, so  $\chi$  is a unitary  $1 \times 1$  matrix  $e^{i\phi}$ . As  $(C^2)^2 = m_x^2 = \sigma_+^2 = 1$ , and  $C^3 = (C)^3$ , we have

$$(\chi_i(\{C^2\}))^2 = (\chi_i(\{m_x, m_y\}))^2 = (\chi_i(\{\sigma_+, \sigma_-\}))^2 = 1$$

$$(\chi_i(\{C\}))^3 = (\chi_i(\{C^3\})) = (\chi_i(\{C\}))$$
 for  $i = 1, ..., 4$ 

so the characters of  $C^2$ ,  $m_x$  and  $\sigma_{\pm}$  are  $\pm 1$  and  $\chi_i(C) = \pm 1$  or 0, with 0 only possible for  $\chi_5$ . But recall  $\sum_k \chi_1(\mathcal{C}_k)\chi_j(\mathcal{C}_k) = 0$  for j = 2, 3, 4, so  $1 + \chi_j(C^2) + 2(\pm 1 \pm 1 \pm 1) = 0$ , which is impossible for  $\chi_i(C^2) = -1$ . So  $\chi_2(C^2) = \chi_3(C^2) = \chi_4(C^2) = 1$ .

(d) Then, again for j = 2, 3, 4, as  $2 + 2 \left[ \chi_j(C) + \chi_j(m_x) + \chi_j(\sigma_{\pm}) \right] = 0$ , we must have two of them -1 and one +1. We need three solutions and there are only three, so except for the order in naming  $\chi_j$ , j = 2, 3, 4, the first four lines are determined.

The last row must be orthogonal, with weights  $\eta_k$ , to each of the rows above, four linear conditions on the four unknowns, and is determined easily. In particular, orthogonality to  $\sum_{1}^{4} \chi_j$  gives  $\chi_5(C^2)$ , and then to  $\chi_1 + \chi_j$  for j = 2, 3, 4 gives the rest.

To find the representations, instead of just the characters, is in this case fairly simple. The one dimensional ones are just the characters.  $\Gamma^{(5)}(C^2)$  is unitary with trace -2, so it can only be  $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$ .  $\Gamma^{(5)}(m_x)$  is traceless, unitary, and has square 1. Any  $2 \times 2$  matrix can be written as  $a + \vec{b} \cdot \vec{\sigma}$  in terms of the Pauli matrices<sup>7</sup>, and tracelessness gives a = 0, that the square = 1 gives  $|\vec{b}| = 1$ . The different directions are all equivalent, all similar to

 $\sigma_z$ , and we are only interested in finding the representation up to similarity, so we take  $\Gamma^{(5)}(m_x) = \sigma_z$ .  $\Gamma^{(5)}(m_y) = \Gamma^{(5)}(m_x)\Gamma^{(5)}(C^2) = -\sigma_z$ . Now  $\Gamma^{(5)}(m_xCm_x) = \Gamma^{(5)}(C^3) = \Gamma^{(5)}(C^2)\Gamma^{(5)}(C) = -\Gamma^{(5)}(C)$ , so  $\Gamma^{(5)}(m_x) = \sigma_z$  anticommutes with  $\Gamma^{(5)}(C)$ . Thus  $\Gamma^{(5)}(C) = a\sigma_x + b\sigma_y$ , with  $a^2 + b^2 = -1$  because  $\Gamma^{(5)}(C^2) = -\mathbb{I}$ , and  $(a^*\sigma_x + b^*\sigma_y)(a\sigma_x + b\sigma_y) = \mathbb{I}$  as it needs to be unitary. This implies  $|a|^2 + |b|^2 = 1$  and  $a^*b$  real. Then we can take  $a = i\cos\theta$ ,  $b = i\sin\theta$ . Using a similarity transformation with  $e^{i\theta\sigma_z}$  permits us to choose  $\theta = -\pi/2$ ,  $\Gamma^{(5)}(C) = -i\sigma_y$ . As  $m_x$  and C generate the group, we need only multiply to find

Note that this forms a group of  $2 \times 2$  matrices, but it is not the group found in the first homework problem of assignment 1, because the  $\sigma_x$  and  $\sigma_z$  terms have real coefficients here.

In general finding the characters and representations may be more involved. The book by Joshi describes a tool based on products of classes, but I will leave that up to you, should you ever need it.

We originally motivated representations by considering spaces of solutions of the Schrödinger equation, and the group  $D_4$  by considering an electron in a periodic square lattice with a single impurity. What have we learned that might help us in solving this problem? Recall that for a one dimensional problem, parity reduced the problem from finding a general function of one variable to finding either a symmetric or an antisymmetric function of one variable. On the other hand, a problem with spherical symmetry has a much greater reduction, from a function of three variables to a function of r only.

For the  $D_4$  symmetry we have only a very finite group, so we can't expect to reduce the space of functions  $\psi(x,y)$  on which we start to ones of a single variable. But the energy eigenstates must transform as a representation of the group, which can be broken into irreducible representations. The wave functions  $\psi(x,y)$  then need to have appropriate behavior under  $x \to -x$   $(m_y)$ , under  $y \to -y$   $(m_x)$ , and under  $x \leftrightarrow y$   $(\sigma_+)$ .

If the symmetry group were only the symmetries of a rectangle,  $\langle m_x, m_y \rangle \cong \mathbb{Z}_2 \times \mathbb{Z}_2$ , we would just learn in each cartesian coordinate what we learned in the one dimensional case with parity:  $\psi$  could be broken into functions

either even or odd in each of the two variables x and y, according to the representations  $\Gamma(m_x)$  and  $\Gamma(m_y)$ . Here we know more, however.

Consider first the identity representation. A wave function in this representation is unchanged under change in sign of x or of y, so it is a function of  $x^2$  and  $y^2$ , but it is also unchanged under interchange of x and y, so it is a *symmetric* function of them,

$$\psi(x,y) = S(x^2,y^2) = S(y^2,x^2)$$
 for the identity representation.

The other one dimensional representations are also easily expressed in terms of an arbitrary such S:

The fifth representation involves *two* functions,  $\psi_1$  and  $\psi_2$ , which transform by

$$\Gamma(m_y) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$
 under  $x \leftrightarrow -x$ , so  $\begin{cases} \psi_1(x,y) = xg(x^2,y) \\ \psi_2(x,y) = h(x^2,y) \end{cases}$ 

$$\Gamma(m_x) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
 under  $y \leftrightarrow -y$ , so  $\begin{cases} \psi_1(x,y) = xg'(x^2,y^2) \\ \psi_2(x,y) = yh'(x^2,y^2) \end{cases}$ 

Finally, we know it transforms as

$$\Gamma(\sigma_+) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
 under  $x \leftrightarrow y$ , so  $g'(x^2, y^2) = h'(y^2, x^2)$ ,

or

$$\psi_1(x,y) = xk(x^2, y^2)$$
  
$$\psi_2(x,y) = yk(y^2, x^2)$$

The group theory is not able to tell us anything about the function  $S(x^2, y^2)$  except that it is symmetric, or anything about k. For more you need to actually consider the Hamiltonian itself.

### 2.6 Point, Space, and Crystallographic Groups

The example we just discussed,  $D_4$ , is an example of a crystallographic point group. There is much interest in condensed matter physics in crystals, which are periodic lattices invariant under translations by

$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \qquad n_j \in \mathbb{Z}.$$

where the  $\vec{a}_j$  are three primitive translation vectors which give the edges of a unit cell, and the crystal is unchanged by translating an integer number of unit cells in any direction. By itself, this symmetry is enough to force the wave functions to be given in terms of Block waves.

But there may also be symmetries which leave one point invariant, consisting of rotations and reflections. The symmetries of this kind which are also compatible with the lattice are called **crystallographic** groups. These are a subset of the **point groups**, groups of rotations and reflections which leave one point invariant.

The combination of a crystallographic group with the translation group is called a **space** group.

In three dimensions there are only 32 possible crystallographic groups. Point groups such as  $C_5$ , rotations though 72° about a given axis, or the symmetries of an icosahedron, are incompatible with extension to an infinite lattice, though the latter might be quite useful in discussing excited states of a buckyball.

I am not going to say more about these groups, but they do have many applications in physics.

The book by Tinkham discusses these in detail.

#### 2.7 Direct Products of Representations

Often a group acts separately on factorizable pieces of the wave function. For example, if we wish to consider the states of two electrons in our lattice, the total wave function  $\psi(x_1, y_1, x_2, y_2)$  could be written as a sum of products  $\sum_i a_i \phi_i(x_1, y_1) \rho_i(x_2, y_2)$ .  $\phi_i$  and  $\rho_i$  can be separately decomposed into irreducible representations of the group, and the group acts on  $\psi$  by the direct product, because it acts together on both  $\vec{r}_1$  and  $\vec{r}_2$ . The vector space

upon which the group is acting here is the tensor product of the space of all functions of  $\vec{r}_1 = (x_1, y_1)$  with the space of all functions of  $\vec{r}_2$ .

Perhaps it would be better to consider first a finite-dimensional example. The electron of a hydrogen atom in an  $\ell=1$  state is in a three-dimensional space with basis vectors  $|m\rangle$ , m=-1,0,1. The rotation group acts on this space in a three-dimensional representation to be further discussed later. At the same time, the electron has a spin degree of freedom in a two-dimensional space with basis  $\{|\uparrow\rangle,|\downarrow\rangle\}$ , or  $|s\rangle$ ,  $s=\pm\frac{1}{2}$ . A full description of the state of the electron lies in a six-dimensional space whose basis is most naturally written as  $\{|m,s\rangle\}$  or

$$|-1,\uparrow\rangle$$
,  $|-1,\downarrow\rangle$ ,  $|0,\uparrow\rangle$ ,  $|0,\downarrow\rangle$ ,  $|1,\uparrow\rangle$ ,  $|1,\downarrow\rangle$ ,

though of course we could still index these basis vectors as  $e_1, ..., e_6$ . Now some operators, such as the orbital angular momentum  $\vec{L}$ , may act only on part of the composite index,  $\langle m', s' | L | m, s \rangle = L_{m'm} \delta_{s's}$ , while others might only act on the spin,  $\langle m', s' | S | m, s \rangle = S_{s's} \delta_{m'm}$ , but in general an operator  $\mathcal{O}$ ,  $e.g. \ \vec{L} \cdot \vec{S}$ , is a  $6 \times 6$  matrix  $\mathcal{O}_{(m's'),(ms)} = \langle m', s' | \mathcal{O} | m, s \rangle$ . The six dimensional space on which it acts is the **tensor product** of the three dimensional space of orbital angular momentum states and the two dimensional space of spin.

Under a rotation<sup>8</sup> A, the state of the electron will be acted on by a six dimensional representation

$$\Gamma_{m's',ms}(A) = \Gamma_{m'm}^{\ell=1}(A)\Gamma_{s's}^{s=\frac{1}{2}}(A),$$

which is the **direct product**,

$$\Gamma(A) = \Gamma^{\ell=1}(A) \bigotimes \Gamma^{s=\frac{1}{2}}(A).$$

More generally we will consider the product of two irreducible representations of any group,

$$\Gamma(A) = \Gamma^{i}(A) \bigotimes \Gamma^{j}(A).$$

This is clearly a representation, because the matrix sum over the tensor product index is just an independent sum over the indices of each subspace.

 $<sup>^8\</sup>mathrm{I}$  am being sloppy here. The fermion wave function is not, strictly speaking, transforming under the rotation group, because under a rotation by  $2\pi$  it is not invariant but changes sign. So what we are really dealing with here are representations of the "covering group" of the rotation group, which is  $\mathrm{SU}(2)$  rather than  $\mathrm{SO}(3)$ . This will be discussed later, page  ${\sim}60$ .

If r, s, t are indices in the  $\ell_i$  dimensional space on which  $\Gamma^i$  acts and a, b, c indices for the  $\ell_i$  dimensional space on which  $\Gamma^j$  acts,

$$\Gamma_{ra,sb}(AB) = \Gamma_{rs}^{i}(AB)\Gamma_{ab}^{j}(AB) = \sum_{t} \Gamma_{rt}^{i}(A)\Gamma_{ts}^{i}(B) \sum_{c} \Gamma_{ac}^{j}(A)\Gamma_{cb}^{j}(B)$$

$$= \sum_{tc} \Gamma_{rt}^{i}(A)\Gamma_{ac}^{j}(A)\Gamma_{ts}^{i}(B)\Gamma_{cb}^{j}(B) = \sum_{tc} \Gamma_{ra,tc}(A)\Gamma_{tc,sb}(B)$$

$$= (\Gamma(A)\Gamma(B))_{ra,sb}.$$

The character of the product representation is simple:

$$\chi(A) = \operatorname{Tr} \Gamma(A) = \sum_{ra} \Gamma(A)_{ra,ra} = \left(\sum_{r} \Gamma_{rr}^{i}(A)\right) \left(\sum_{a} \Gamma_{aa}^{j}(A)\right) = \chi^{i}(A)\chi^{j}(A).$$

Now the product of two irreducible representations need not be irreducible, but it must be equivalent to a direct sum of irreducible representations. For example, for the case of the electron with orbital angular momentum 1 and also spin, the full rotation group has representations labelled by j, and our six dimensional space is a sum of a  $j = \frac{1}{2}$  and a  $j = \frac{3}{2}$  representation,

$$\Gamma^{\ell=1} \bigotimes \Gamma^{s=\frac{1}{2}} \cong \Gamma^{j=\frac{1}{2}} \bigoplus \Gamma^{j=\frac{3}{2}}.$$

More generally,

$$\Gamma^{i}(A) \bigotimes \Gamma^{j}(A) \cong \bigoplus_{k} a_{k}^{ij} \Gamma^{k}(A),$$

where each representation may appear  $a_k^{ij}$  times in this sum, called the Clebsch-Gordon series. The non-negative integers  $a_k^{ij}$  are called Clebsch-Gordon coefficients by mathematicians but not by physicists, who mean something else, which we will discuss later, by that term.

From the formula (2.9) for the number of times a given irreducible representation occurs in an arbitrary one, the coefficients are easily calculated:

$$a_k^{ij} = \frac{1}{g} \sum_{A \in G} \chi^i(A) \chi^j(A) \chi^{k*}(A).$$

We reserve our discussion of the physics of this decomposition until after we have learned to construct irreducible representations of infinite groups.