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Chapter 3

Group Theory and Quantum Mechanics

As a refresher on various True Facts about linear algebra relevant to quantum mechanics, please review the Appendix §3.3.

3.1 Hilbert Space and Group Symmetries

3.1.1 Classification of the basis states

The realization of symmetries in quantum mechanics is expressed through the action of unitary operator representations $\hat{U}(G)$ of some symmetry group G which act on the Hilbert space \mathcal{H} of states. If $[\hat{H}, \hat{U}(g)] = 0$ for all $g \in G$, *i.e.* the Hamiltonian commutes with all symmetry operations from G , its eigenspectrum arranges into multiplets, each of which transforms according to some IRREP Γ of G , with corresponding degeneracy d_Γ . Thus, at the outset, one thing group theory can do for us is to provide us with a useful set of basis states $|\Gamma\mu, l\rangle$ in \mathcal{H} which are identified by three labels (Γ, μ, l) :

- (i) The representation index Γ labels an IRREP of the symmetry group G .
- (ii) The basis index $\mu \in \{1, \dots, d_\Gamma\}$ labels the basis states within the Γ representation.
- (iii) The additional index l labels different invariant subspaces transforming according to the same representation. This allows for other quantum numbers not associated with the group symmetry.

Where do these basis states come from? We can generate them via the projection method, which we will discuss in §3.1.5 below.

Such a basis can greatly simplify the diagonalization of our quantum Hamiltonian \hat{H} , because, as we shall see,

$$\langle \Gamma\mu, l | \hat{H} | \Gamma'\mu', l' \rangle = \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} H_{ll'}^\Gamma \quad . \quad (3.1)$$

However, in general the projection method does not guarantee that the basis states $|\Gamma\mu, l\rangle$ are orthogonal. Rather, we have

$$\langle \Gamma\mu, l | \Gamma'\mu', l' \rangle = \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} O_{ll'}^\Gamma, \quad (3.2)$$

where $O_{ll'}^\Gamma$ is the *overlap matrix*. Group theory tells us that basis states which transform according to different IRREPS are necessarily orthogonal, but it says nothing about the overlap of basis states transforming according to two copies of the same IRREP. Thus, we are left with the task of simultaneously diagonalizing the two Hermitian matrices H^Γ and O^Γ , i.e. solving the linear system $H_{ll'}^\Gamma \phi_{l'}^{\Gamma s} = E_{\Gamma s} O_{ll'}^\Gamma \phi_{l'}^{\Gamma s}$, where s labels the eigenvalue and corresponding eigenfunctions of the s^{th} occurrence of the IRREP Γ . The eigenstates of \hat{H} then satisfy $\hat{H} |\Gamma\mu, s\rangle = E_{\Gamma s} |\Gamma\mu, s\rangle$ with $\langle \Gamma\mu, s | \Gamma'\mu', s' \rangle = \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} \delta_{ss'}$. The index s is necessary because any given IRREP generally occurs several times in the eigenspectrum. This means we can write

$$\hat{H} = \sum_{\Gamma, s} E_{\Gamma, s} \hat{H}^{\Gamma, s}, \quad \hat{H}^{\Gamma, s} \equiv \sum_{\mu} |\Gamma\mu, s\rangle \langle \Gamma\mu, s|, \quad (3.3)$$

where $\hat{H}^{\Gamma, s}$ is the projector onto the s^{th} occurrence of IRREP Γ .

Example: The Hamiltonian $\hat{H} = \frac{p^2}{2m} + V(x)$ commutes with the operators $\{1, P\}$, where $P = P^{-1} = P^\dagger$ is the parity operator, with $P x P = -x$ and $P p P = -p$. Thus, $[\hat{H}, P] = 0$ and we can classify all eigenstates of \hat{H} by representations of \mathbb{Z}_2 , of which there are only two: Γ_1 (trivial) and Γ_2 (sign). Both IRREPS are one-dimensional, so the μ index is unnecessary. Starting with any set $\{\psi_l(x)\}$ of L^2 -integrable functions on \mathbb{R} , we can project onto the trivial (symmetric) and sign (antisymmetric) representations of \mathbb{Z}_2 , forming $\varphi_{l, \pm} \equiv \psi_l(x) \pm \psi_l(-x)$. While the \mathbb{Z}_2 symmetry guarantees that $\langle \varphi_{l, \sigma} | \varphi_{l', \sigma'} \rangle$ vanishes if $\sigma \neq \sigma'$, there is no symmetry consideration guaranteeing that basis states within the same IRREP are orthonormal¹.

Diagonalizing \hat{H} within each of these subspaces yields the *orthonormal* eigenfunctions $\psi_s^{(\Gamma_1)}(x) = \langle x | \Gamma_1 s \rangle$ and $\psi_s^{(\Gamma_2)}(x) = \langle x | \Gamma_2 s \rangle$ may be taken to be the s^{th} lowest energy eigenfunctions in the even and odd parity sectors, respectively. These energy eigenstates interleave, with the n^{th} energy level having $n - 1$ nodes and parity eigenvalue $P = (-1)^{n-1}$.

Example': In later chapters we shall discuss representations of Lie groups, but you already know that for $G = \text{SU}(2)$, the representations are classified by total spin $S \in \frac{1}{2}\mathbb{Z}$, and that the dimension of each spin- S representation is $d_S = 2S + 1$. In a system of N spin- $\frac{1}{2}$ objects, with N even, one can form representations with integer $S \in \{0, 1, \dots, \frac{1}{2}N\}$. The number of spin- S multiplets is given by²

$$M_S = \binom{N}{\frac{1}{2}N + S} - \binom{N}{\frac{1}{2}N + S + 1}. \quad (3.4)$$

Each of these M_S multiplets is $(2S+1)$ -fold degenerate. The Hilbert space basis vectors may be expressed as $|S, m, l\rangle$, where S labels the representation, $m \in \{-S, \dots, +S\}$ is the polarization, and l labels the M_S different spin- S multiplets.

¹For example, we could take $\varphi_{l,+}(x) = A_l x^{2l} e^{-x}$ and $\varphi_{l,-}(x) = B_l x^{2l+1} e^{-x}$.

²This expression counts the difference in the number of states with $S^z = S$ and with $S^z = S + 1$. The difference is the number of multiplets in which $S^z = S$ appears but not $S^z = S + 1$, and is therefore the number of spin- S multiplets.

3.1.2 Accidental degeneracies

In general,

- ◇ For a Hamiltonian \hat{H} where $[\hat{H}, \hat{U}(G)] = 0$, each group of eigenstates transforming according to a representation Γ is d_Γ -fold degenerate. Any degeneracies not associated with the group symmetry are said to be accidental.

Accidental degeneracies can be removed by varying parameters in the Hamiltonian without breaking the underlying symmetry. As an example, consider the case of a Hilbert space with six states, labeled $\{|u_1\rangle, |v_1\rangle, |u_2\rangle, |v_2\rangle, |u_3\rangle, |v_3\rangle\}$ and the Hamiltonian

$$\hat{H} = - \sum_{n=1}^3 \left[t_0 \left(|u_n\rangle\langle u_{n+1}| + |u_{n+1}\rangle\langle u_n| + |v_n\rangle\langle v_{n+1}| + |v_{n+1}\rangle\langle v_n| \right) + t_1 \left(|u_n\rangle\langle v_n| + |v_n\rangle\langle u_n| \right) \right] \quad (3.5)$$

where $|u_4\rangle \equiv |u_1\rangle$ and $|v_4\rangle \equiv |v_1\rangle$. The geometry is sketched in Fig. 3.1.

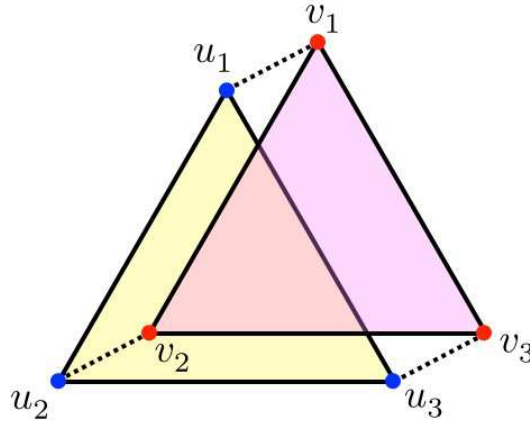


Figure 3.1: Six site cluster with D_{3h} symmetry. Solid bonds between orbitals signify matrix element $-t_0$, while dashed bonds signify matrix element $-t_1$.

The Hamiltonian is symmetric under the symmetry group C_{3v} , which has six elements, corresponding to the symmetries of the equilateral triangle. In fact, this model has an enlarged symmetry, since it is also symmetric under a reflection σ_h in the horizontal plane, which interchanges the orbitals $|u_n\rangle \leftrightarrow |v_n\rangle$, corresponding to the group D_{3h} . The group D_{nh} has $4n$ elements and is generated by three elements: a $\frac{2\pi}{n}$ rotation r , a vertical reflection σ_v , and a horizontal reflection σ_h . Its presentation is

$$D_{nh} : \langle r, \sigma_v, \sigma_h | r^n, \sigma_v^2, \sigma_h^2, (\sigma_v r)^2, (\sigma_v \sigma_h)^2, \sigma_h r \sigma_h r^{n-1} \rangle \quad (3.6)$$

The character table for D_{3h} is given in Tab. 3.1.

The Hamiltonian \hat{H} in Eqn. 3.5 is known as a "tight binding model" and its diagonalization is sufficiently simple that those with a rudimentary background in solid state physics can do so by inspection.

Explicitly, define the states

$$|\hat{u}_j\rangle = \frac{1}{\sqrt{3}} \sum_{n=1}^3 e^{-2\pi i j n/3} |u_n\rangle \quad , \quad |\hat{v}_j\rangle = \frac{1}{\sqrt{3}} \sum_{n=1}^3 e^{-2\pi i j n/3} |v_n\rangle \quad . \quad (3.7)$$

with $j \in \{-1, 0, +1\}$. This is a simple discrete Fourier transform whose inverse is

$$|u_n\rangle = \frac{1}{\sqrt{3}} \sum_{j=-1}^1 e^{2\pi i j n/3} |\hat{u}_j\rangle \quad , \quad |v_n\rangle = \frac{1}{\sqrt{3}} \sum_{j=-1}^1 e^{2\pi i j n/3} |\hat{v}_j\rangle \quad . \quad (3.8)$$

One then has

$$\hat{H} = - \sum_{j=-1}^1 \left[2t_0 \cos(2\pi j/3) \left(|\hat{u}_j\rangle\langle \hat{u}_j| + |\hat{v}_j\rangle\langle \hat{v}_j| \right) + t_1 \left(|\hat{u}_j\rangle\langle \hat{v}_j| + |\hat{v}_j\rangle\langle \hat{u}_j| \right) \right] \quad . \quad (3.9)$$

Next, define

$$|\hat{\psi}_{j,\pm}\rangle = \frac{1}{\sqrt{2}} \left(|\hat{u}_j\rangle \pm |\hat{v}_j\rangle \right) \quad , \quad (3.10)$$

in which case

$$\hat{H} = \sum_{j=-1}^1 \left(\varepsilon_{j,+} |\hat{\psi}_{j,+}\rangle\langle \hat{\psi}_{j,+}| + \varepsilon_{j,-} |\hat{\psi}_{j,-}\rangle\langle \hat{\psi}_{j,-}| \right) \quad , \quad (3.11)$$

where the six eigenvalues of H are given by

$$\varepsilon_{j,\pm} = -2t_0 \cos(2\pi j/3) \mp t_1 \quad . \quad (3.12)$$

For generic t_0 and t_1 , we have that the eigenstates $|\hat{\psi}_{0,\pm}\rangle$ are each singly degenerate with energies $\varepsilon_{0,\pm} = -2t_0 \mp t_1$, respectively. They transform according to the A_1 and A'_2 representations of D_{3h} , respectively. The eigenstates $|\hat{\psi}_{\pm 1,+}\rangle$ are doubly degenerate, with energy $\varepsilon_{\pm 1,+} = t_0 - t_1$, and transform according to the E representation. Finally, the states $|\hat{\psi}_{\pm 1,-}\rangle$ are also doubly degenerate, with energy $\varepsilon_{\pm 1,-} = t_0 + t_1$, and transform according to E' (see Tab. 3.1).

To elicit an accidental degeneracy, we set $\varepsilon_{0,-} = -2t_0 + t_1$ equal to $\varepsilon_{\pm 1,+} = t_0 - t_1$, i.e. $t_1 = \frac{3}{2}t_0$. For this special ratio of t_1/t_0 , there is a threefold degeneracy, due to a crossing of A'_2 and E levels. The multiplicity of this degeneracy is therefore $d_{A'_2} + d_E = 3$, which corresponds to none of the dimensions of the IRREPS of D_{3h} . The degeneracy is accidental and is removed whenever $t_1 \neq \frac{3}{2}t_0$.

Finally, we can break the D_{3h} symmetry back down to C_{3v} by choosing different matrix elements $t_{0,u}$ and $t_{0,v}$ for the two triangles³. *Mutatis mutandis*⁴, one finds that the degeneracy structure is the same, and the eigenspectrum is given by

$$\varepsilon_{j,\pm} = -(t_{0,u} + t_{0,v}) \cos(2\pi j/3) \mp \sqrt{(t_{0,u} - t_{0,v})^2 \cos^2(2\pi j/3) + t_1^2} \quad . \quad (3.13)$$

³Here we should recall the careful discussion at the end of §1.2.4 regarding the difference between D_n and C_{nv} .

⁴Vah! Denuone Latine loquebar?

D_{3h}	E	$2C_3$	$3C'_2$	σ_h	$2S_3$	$3\sigma_v$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E	2	-1	0	2	-1	0
A'_1	1	1	1	-1	-1	-1
A'_2	1	1	-1	-1	-1	1
E'	2	-1	0	-2	1	0

Table 3.1: Character table for the group D_{3h} . The upper left 3×3 block is the character table for D_3 . Take care not to confuse the identity element E and its class with the two-dimensional IRREP also labeled E .

The eigenstates are now classified in terms of representations of $C_{3v} \cong D_3$. The two nondegenerate levels each transform according to A_1 , and the two sets of doubly degenerate levels each transform according to E .

In general, identical IRREPs cannot be coaxed into degeneracy by terms in the Hamiltonian which preserve the full symmetry group G . This is due to level repulsion. Accidental degeneracy, when it occurs, is in general between distinct IRREPs, and therefore the size of the resulting *supermultiplet* is given by $d_{\Gamma_a} + d_{\Gamma_b}$, where $\Gamma_a \not\cong \Gamma_b$. We note that this sort of degeneracy requires the fine tuning of one parameter in the Hamiltonian, such as t_1 (or the dimensionless ratio t_1/t_0) in our above example.

Can we tune further for even greater degeneracy? Yes we can! Mathematically, if $\hat{H} = \hat{H}(\boldsymbol{\lambda})$, where $\boldsymbol{\lambda} = \{\lambda_1, \dots, \lambda_K\}$ is a set of parameters living in some parameter space manifold \mathcal{M} , and $[\hat{H}(\boldsymbol{\lambda}), \hat{U}(g)] = 0$ for all $\boldsymbol{\lambda} \in \mathcal{M}$ and all $g \in G$, then requiring that the multiplets for $p > 1$ distinct IRREPs are simultaneously degenerate imposes $p - 1$ equations of the form

$$E_{\Gamma_a, t_a}(\lambda_1, \dots, \lambda_K) = E_{\Gamma_b, t_b}(\lambda_1, \dots, \lambda_K) \quad , \quad (3.14)$$

and therefore such a degeneracy, whose multiplicity is $d = \sum_{j=1}^p \dim(\Gamma_{a_j})$, has *codimension* $p - 1$, meaning that the solution set in \mathcal{M} is of dimension $K - p + 1$. It may be that this value of d corresponds to d_Γ for some other IRREP Γ , but this is not necessarily the case. And of course, it may be that there are no solutions at all. In the above example with symmetry group D_{3h} , we had $\hat{H} = \hat{H}(t_0, t_1)$, so $K = 2$, and degeneracy of the $p (= 2)$ multiplets A'_2 and E imposed $p - 1 (= 1)$ conditions on $\{t_1, t_2\}$, with a one-dimensional solution set of the form $t_1 = \frac{3}{2}t_0$.

Accidental degeneracy in the C_{60} molecule

Mathematical appetizer : There is a marvelous result in graph theory, due to Euler, which says that for any connected graph on a surface of genus g , the number of faces f , edges e , and vertices v are related according to

$$f - e + v = 2 - 2g \quad . \quad (3.15)$$

The genus g is the number of holes, hence a sphere has genus $g = 0$, a torus $g = 1$, *etc.* It turns out that for the plane we should take $g = \frac{1}{2}$, which we can understand identifying the points at infinity and

thereby compactifying the plane to a sphere. Then the area outside the original graph counts as an extra face. Try sketching some connected graphs on a sheet of paper and see if Euler's theorem holds.

Consider now a threefold coordinated graph on the sphere S^2 . Every site is linked to three neighboring sites. Furthermore, let's assume that every face is either a pentagon or a hexagon. The number of faces is then $f = p + h$, where p is the number of pentagons and h the number of hexagons. If we add $5p$ to $6h$, we count every edge twice, so $5p + 6h = 2e$. Similarly, $5p + 6h = 3v$ because the same calculation counts each vertex three times. Thus $e = \frac{5}{2}p + 3h$ and $v = \frac{5}{3}p + 2h$. Now apply Euler's theorem and find that h drops out completely and we are left with $p = 12$. *Any three-fold coordinated graph on the sphere with pentagonal and hexagonal faces will always have twelve pentagons.* Amazing! Take a close look at a soccer ball sometime and you will notice it has 12 pentagonal faces and 20 hexagonal ones, for a total of $f = 32$ faces to go along with $e = 90$ edges and $v = 60$ vertices.

Physics entree : There is a marvelous molecule with chemical formula C_{60} , also known as *Buckminsterfullerene*⁵ (colloquially a *buckyball*) which consists of 60 carbon atoms arranged in a soccer ball pattern⁶. See the left panel of Fig. 3.2. Each atom is threefold coordinated, meaning it has three nearest neighbors. As you know, carbon has the electronic structure $1s^2 2s^2 2p^2$. In the planar form graphene, which has the structure of a honeycomb lattice, the $2s$ and $2p_{x,y}$ orbitals engage in sp^2 hybridization. For each carbon atom, three electrons in each atom's sp^2 orbitals are distributed along bonds connecting to its neighbors⁷. Thus each bond gets two electrons (of opposite spin), one from each carbon atom at its ends, which form what chemists call a σ -bond. The $1s$ orbitals are of course filled, so this leaves one remaining electron from each p_z orbital (the π orbital to our chemist friends) to roam about. The situation is much the same with the buckyball, although unlike graphene it is curved. The single (π) orbital tight binding model is

$$\hat{H} = - \sum_{\langle ij \rangle} \left(t_{ij} | \pi_i \rangle \langle \pi_j | + t_{ij}^* | \pi_j \rangle \langle \pi_i | \right) , \quad (3.16)$$

where $\langle ij \rangle$ denotes a nearest neighbor bond on the lattice between sites i and j and t_{ij} is the *hopping integral*, which may be complex so long as \hat{H} itself is Hermitian⁸.

The eigenspectrum of \hat{H} will be arranged in multiplets whose sizes are given by the dimensions of the IRREPS of the symmetry group of the buckyball. The discrete rotational symmetries of C_{60} belong to the *icosahedral group*, I . You can look up the character table for I and see that it is a nonabelian group with 60 elements, five classes, and five IRREPS A , T_1 , T_2 , G , and H , with dimensions 1, 3, 3, 4, and 5, respectively. Note that $60 = 1^2 + 3^2 + 3^2 + 4^2 + 5^2$. The icosahedron also has an inversion symmetry, so its full symmetry group, including the improper rotations, has 120 elements and is called I_h .⁹ The group I_h has ten classes and ten IRREPS, such that each of the five IRREPS in I is doubled within I_h into

⁵After Buckminster Fuller, the American architect who invented the geodesic dome.

⁶"The icosahedral group ... has no physical interest, since for crystals 5-fold axes cannot occur, and no examples of molecules with this symmetry are known." - M. Hamermesh, *Group Theory and its Application to Physical Problems* (1962), p. 51.

⁷In diamond, the carbon atoms are fourfold coordinated, and the orbitals are sp^3 hybridized.

⁸A local gauge transformation of the orbitals $|\pi_i\rangle \rightarrow e^{i\theta_i} |\pi_i\rangle$ is equivalent to replacing t_{ij} by $t_{ij} e^{i(\theta_i - \theta_j)}$. The product $\prod_{(ij) \in \kappa} t_{ij}$ of the t_{ij} around a plaquette κ is therefore gauge invariant, and the phase of the product is equal to the total magnetic flux through κ in units of $\hbar c/e$.

⁹Recall that D_n has $2n$ elements, but adding a horizontal reflection plane yields D_{nh} with $4n$ elements. The icosahedron has 15 reflection planes, appearing as class σ in its character tables. Each such reflection can be written as the product of an inversion and a proper rotation. *Fun facts* : $I \cong A_5$ and $I_h \cong \mathbb{Z}_2 \times A_5$, where A_5 is the alternating group with five symbols.

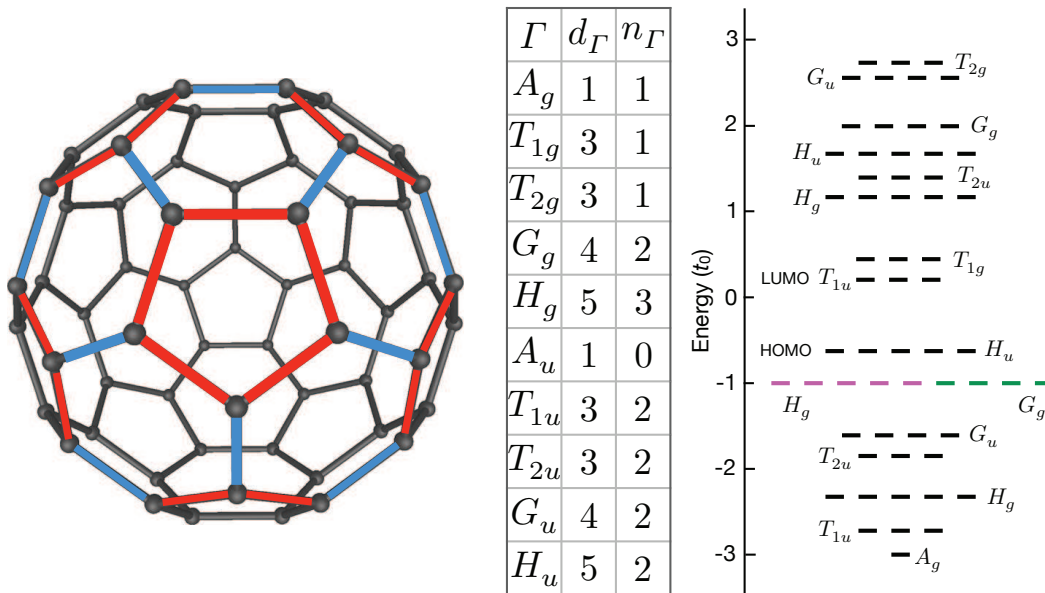


Figure 3.2: Electronic structure of the C_{60} molecule. Left: C_{60} molecule, showing inequivalent bonds. All red bonds lie along pentagons, while all blue bonds do not. Middle: Irreducible representations of the icosahedral group I_h and their dimensions. Right: Tight binding energy spectrum when all bonds have hopping amplitude t_0 . Note the accidental degeneracy between G_g and H_g levels, at $E = -t_0$, resulting in a nine-fold degenerate supermultiplet. When the hopping amplitudes along the blue and red bonds differ, icosahedral symmetry is maintained, but the accidental degeneracy is resolved.

an even and an odd version with respect to the inversion¹⁰, sort of like the good and evil versions of Mr. Spock in the original *Star Trek* series episode entitled “*Mirror, Mirror*”. The IRREPS of I_h are labeled with subscripts g and u , for *gerade* and *ungerade*, respectively (from the German for “even” and “odd”).

The eigenvalues for the C_{60} tight binding Hamiltonian are shown in Fig. 3.2 for the case $t_{ij} = t_0$ for all nearest neighbor bonds $\langle ij \rangle$. Each of the energy levels accommodates two electrons (spin \uparrow and \downarrow), so in the ground state the sixty π electrons fill the lowest 30 levels. HOMO and LUMO respectively refer to “highest occupied molecular orbital” and “lowest unoccupied molecular orbital”. The multiplicities of the different energy states correspond to the dimension of the IRREPS, except for a ninefold degenerate level at $E = -t_0$. This is an accidental degeneracy between G_g and H_g IRREPS, whose dimensions are four and five, respectively.

In order for the degeneracy to be accidental, we should be able to remove it by modifying the Hamiltonian while still preserving the I_h symmetry. One physical way to do this is to note that there are actually two inequivalent sets of bonds (edges) on the buckyball: bonds that lie along pentagons (marked red in Fig. 3.2, called 6:5 bonds, 60 in total), and bonds that do not lie along pentagons (marked blue, 6:6 bonds, 30 total). Clearly no symmetry operation can transform a red bond into a blue one, so why should their hopping amplitudes be the same? The answer is that they are not the same. Indeed, the 6:6 bonds are slightly shorter than the 6:5 bonds, and they have a slightly larger value of t_{ij} . By distinguishing

¹⁰See the discussion in §2.4.7.

$t_0 \equiv t_{(6:6)}$ and $t_1 \equiv t_{(6:5)}$, one retains the I_h symmetry, but the aforementioned degeneracy occurs only for $t_1 = t_0$, precisely in analogy to what we found in our D_{3h} example.

Note that in the tight binding eigenspectrum some IRREPs occur several times. There are three H_g levels, for example, and A_u isn't present anywhere in the spectrum. The eigenfunctions form a reducible 60-dimensional representation of the group I_h whose decomposition is

$$\Gamma^{\text{elec}} = A_g \oplus T_{1g} \oplus T_{2g} \oplus 2G_g \oplus 3H_g \oplus 2T_{1u} \oplus 2T_{2u} \oplus 2G_u \oplus 2H_u \quad . \quad (3.17)$$

The number of times the IRREP Γ appears, n_Γ , is also listed in the table in Fig. 3.2. For singly degenerate atomic orbitals such as the π orbitals of C_{60} , the representation matrices $D^{\text{elec}}(g)$ are *permutation matrices* of the site labels i , with

$$D_{ij}^{\text{elec}}(g) = \langle i | g | j \rangle \equiv \begin{cases} 1 & \text{if } g \text{ takes } j \text{ to } i \\ 0 & \text{otherwise} \end{cases} \quad . \quad (3.18)$$

The character $\chi^{\text{elec}}(g)$ is then simply the number of sites i left invariant by the operation g . We can then find n_Γ using the representation decomposition formula. This will be discussed more fully in §6.4.

3.1.3 Operators and wavefunctions

Here we consider the transformation properties of the Hilbert space vectors $|\Gamma\mu, l\rangle$ for fixed l . Accordingly we suppress these indices throughout this discussion. Recall that

$$\hat{U}(g) |\Gamma\nu\rangle = |\Gamma\mu\rangle \langle \Gamma\mu | \hat{U}(g) | \Gamma\nu \rangle = |\Gamma\mu\rangle D_{\mu\nu}^\Gamma(g) \quad . \quad (3.19)$$

Taking the Hermitian conjugate, one has $\langle \Gamma\nu | U^\dagger(g) = D_{\mu\nu}^{\Gamma*}(g) \langle \Gamma\mu |$. Thus,

$$D_{\mu\nu}^\Gamma(g) = \langle \Gamma\mu | \hat{U}(g) | \Gamma\nu \rangle \quad , \quad D_{\mu\nu}^{\Gamma*}(g) = \langle \Gamma\mu | \hat{U}(g) | \Gamma\nu \rangle^* = \langle \Gamma\nu | \hat{U}^\dagger(g) | \Gamma\mu \rangle \quad . \quad (3.20)$$

Note that the matrix representation is a group homomorphism:

$$\hat{U}(g_a) \hat{U}(g_b) | \Gamma\nu \rangle = \hat{U}(g_a) | \Gamma\rho \rangle D_{\rho\nu}^\Gamma(g_b) = |\Gamma\mu\rangle D_{\mu\rho}^\Gamma(g_a) D_{\rho\nu}^\Gamma(g_b) = |\Gamma\mu\rangle D_{\mu\nu}^\Gamma(g_a g_b) \quad . \quad (3.21)$$

Acting on the state $|\mathbf{r}\rangle$, one has $\hat{U}(g) |\mathbf{r}\rangle = |g\mathbf{r}\rangle$, and therefore $\langle \mathbf{r} | U(g) = \langle g^{-1}\mathbf{r} |$. Therefore, with $\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle$, we then have

$$\hat{U}(g) \psi(\mathbf{r}) \equiv \langle \mathbf{r} | \hat{U}(g) | \psi \rangle = \psi(g^{-1}\mathbf{r}) \quad . \quad (3.22)$$

We also have

$$\hat{U}(gh) \psi(\mathbf{r}) = \hat{U}(g) \hat{U}(h) \psi(\mathbf{r}) = \hat{U}(g) \psi(h^{-1}\mathbf{r}) = \psi(h^{-1}g^{-1}\mathbf{r}) = \psi((gh)^{-1}\mathbf{r}) \quad . \quad (3.23)$$

Acting on a basis function $\psi_\nu^\Gamma(\mathbf{r}) = \langle \mathbf{r} | \Gamma\nu \rangle$, we have

$$\psi_\nu^\Gamma(g^{-1}\mathbf{r}) = \hat{U}(g) \psi_\nu^\Gamma(\mathbf{r}) = \langle \mathbf{r} | \hat{U}(g) | \Gamma\nu \rangle = \langle \mathbf{r} | \Gamma\mu \rangle D_{\mu\nu}^\Gamma(g) = \psi_\mu^\Gamma(\mathbf{r}) D_{\mu\nu}^\Gamma(g) \quad . \quad (3.24)$$

Multiplying by $D_{\nu\alpha}^{\Gamma*}(g)$ and contracting on the index ν , this result entails $\psi_\alpha^\Gamma(\mathbf{r}) = D_{\alpha\nu}^{\Gamma*}(g) \psi_\nu^\Gamma(g^{-1}\mathbf{r})$.

Fun fact about bras and kets:

◇ While the ket $|\Gamma\mu, l\rangle$ transforms according to Γ , the bra $\langle\Gamma\mu, l|$ transforms according to Γ^* .

Recall also that the product of IRREPS $\Gamma \times \Gamma'$ contains the identity representation if and only if $\Gamma' = \Gamma^*$, with $D_{\mu\nu}^{\Gamma^*}(g) = [D_{\nu\mu}^{\Gamma}(g)]^*$.

3.1.4 Projection operators

This section recapitulates the results of §2.4.2, now expressed in the form of abstract operators rather than matrices. Consider a unitary representation $D^{\Gamma}(G)$ and define the operators

$$\hat{H}_{\mu\nu}^{\Gamma} \equiv \frac{d_{\Gamma}}{N_G} \sum_{g \in G} D_{\mu\nu}^{\Gamma^*}(g) \hat{U}(g) \quad . \quad (3.25)$$

which project onto the μ basis vector of the Γ representation. They satisfy the following three conditions. First: $\hat{H}_{\mu\nu}^{\Gamma} \hat{H}_{\mu'\nu'}^{\Gamma} = \delta_{\Gamma\Gamma'} \delta_{\nu\mu'} \hat{H}_{\mu\nu}^{\Gamma}$. Second: $(\hat{H}_{\mu\nu}^{\Gamma})^{\dagger} = \hat{H}_{\nu\mu}^{\Gamma}$. Third: $\sum_{\Gamma} \sum_{\mu=1}^{d_{\Gamma}} \hat{H}_{\mu\mu}^{\Gamma} = \mathbb{1}$. The proof of these relations is left as an exercise to the student.

Starting with an arbitrary collection of initial states $\{|\psi_l\rangle\}$, one can form the states

$$|\Gamma\mu, l\rangle = \hat{H}_{\mu\nu}^{\Gamma} |\psi_l\rangle \quad , \quad (3.26)$$

where the index ν is held fixed for each l . One then has $\hat{H}_{\mu\nu}^{\Gamma} |\Gamma'\rho, l\rangle = \delta_{\Gamma\Gamma'} \delta_{\nu\rho} |\Gamma\mu, l\rangle$. Note that

$$\begin{aligned} \hat{U}(g) \hat{H}_{\mu\nu}^{\Gamma} &= \frac{d_{\Gamma}}{N_G} \sum_{h \in G} D_{\mu\nu}^{\Gamma^*}(h) \hat{U}(g) \hat{U}(h) = \frac{d_{\Gamma}}{N_G} \sum_{h \in G} D_{\mu\nu}^{\Gamma^*}(g^{-1}gh) \hat{U}(gh) \\ &= D_{\mu\rho}^{\Gamma^*}(g^{-1}) \underbrace{\frac{d_{\Gamma}}{N_G} \sum_{h \in G} D_{\rho\nu}^{\Gamma^*}(gh) \hat{U}(gh)}_{\hat{H}_{\rho\nu}^{\Gamma} \text{ (rearrangement)}} = D_{\mu\rho}^{\Gamma^*}(g^{-1}) \hat{H}_{\rho\nu}^{\Gamma} = \hat{H}_{\rho\mu}^{\Gamma} D_{\rho\nu}^{\Gamma}(g) \quad . \end{aligned} \quad (3.27)$$

Applying this to $|\psi_l\rangle$, we have

$$\hat{U}(g) |\Gamma\mu, l\rangle = |\Gamma\rho, l\rangle D_{\rho\mu}^{\Gamma}(g) \quad , \quad (3.28)$$

which says that the states $\{|\Gamma\mu, l\rangle\}$ transform as the Γ IRREP of G . Note further that

$$\begin{aligned} \langle\Gamma\mu, l | \Gamma'\mu', l'\rangle &= \langle\psi_l | (\hat{H}_{\mu\nu}^{\Gamma})^{\dagger} \hat{H}_{\mu'\nu'}^{\Gamma'} | \psi_{l'}\rangle = \langle\psi_l | \hat{H}_{\nu\mu}^{\Gamma} \hat{H}_{\mu'\nu'}^{\Gamma'} | \psi_{l'}\rangle \\ &= \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} \langle\psi_l | \hat{H}_{\nu\nu'}^{\Gamma} | \psi_{l'}\rangle \equiv \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} O_{ll'}^{\Gamma} \quad , \end{aligned} \quad (3.29)$$

where $O_{ll'}^{\Gamma} = \langle\psi_l | \hat{H}_{\nu\nu'}^{\Gamma} | \psi_{l'}\rangle$. Recall that the column indices are held fixed for each choice of (Γ, l) , independent of the row indices. If the choice of ν for each (Γ, l) is considered implicit, we may suppress the indices ν and ν' in the overlap matrix $O_{ll'}^{\Gamma}$. At any rate, we see that the states constructed by projection in eqn. 3.26 are orthogonal only in their representation labels (Γ and Γ') and row labels (μ and μ'), but not in the multiplicity labels l and l' .

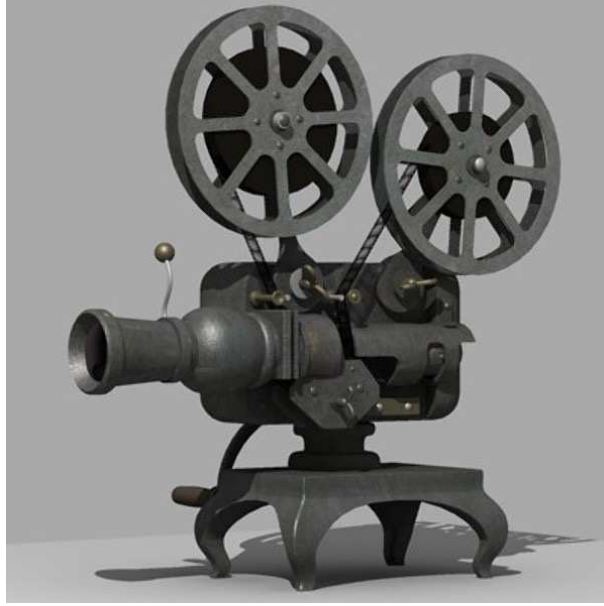


Figure 3.3: A projector from the early days of group theory. This projector belonged to Eugene Wigner.

Taking the trace of $\hat{\Pi}_{\mu\nu}^{\Gamma}$, we obtain, for unitary representations, the projection operator

$$\hat{\Pi}^{\Gamma} \equiv \sum_{\mu=1}^{d_{\Gamma}} \hat{\Pi}_{\mu\mu}^{\Gamma} = \frac{d_{\Gamma}}{N_G} \sum_{g \in G} \chi^{\Gamma*}(g) \hat{U}(g) \quad . \quad (3.30)$$

If $|\psi\rangle = \sum_{\Gamma} \sum_l \sum_{\mu=1}^{d_{\Gamma}} C_{\Gamma\mu}^l |\Gamma\mu, l\rangle$ is a general sum over Hilbert space basis vectors, then

$$\hat{\Pi}^{\Gamma_a} |\psi\rangle = \sum_l \sum_{\mu=1}^{d_{\Gamma}} C_{\Gamma_a\mu}^l |\Gamma_a\mu, l\rangle \quad (3.31)$$

projects $|\psi\rangle$ onto the IRREP Γ_a .

3.1.5 Projecting arbitrary functions onto IRREPs

Here we describe a straightforward generalization of the method in §2.3.4 of projecting vectors, now applied to functions. For any function $\psi(\mathbf{r})$, define

$$\psi_{\mu}^{(\Gamma\nu)}(\mathbf{r}) \equiv \hat{\Pi}_{\mu\nu}^{\Gamma} \psi(\mathbf{r}) = \frac{d_{\Gamma}}{N_G} \sum_{g \in G} D_{\mu\nu}^{\Gamma*}(g) \psi(g^{-1}\mathbf{r}) \quad . \quad (3.32)$$

Here the representation label Γ as well as the column index ν serve as labels for a set of functions with $\mu \in \{1, \dots, d_{\Gamma}\}$. Invoking Eqn. 3.27, we find

$$\hat{U}(g) \hat{\Pi}_{\mu\nu}^{\Gamma} = \hat{\Pi}_{\rho\nu}^{\Gamma} D_{\rho\mu}^{\Gamma}(g) \quad (3.33)$$

and therefore

$$\hat{U}(g) \psi_{\mu}^{(\Gamma\nu)}(\mathbf{r}) = \psi_{\rho}^{(\Gamma\nu)}(\mathbf{r}) D_{\rho\mu}^{\Gamma}(g) \quad . \quad (3.34)$$

In other words, suppressing the $(\Gamma\nu)$ label, we have that the functions $\psi_{\mu}(\mathbf{r})$ transform according to the Γ representation of the group. Thus, we have succeeded in projecting an arbitrary function $\psi(\mathbf{r})$ onto any IRREP Γ of G we please. This deserves a celebration with some unusual L^AT_EX symbols: ☺ 🚲 🌀 🍷 .

Example: \mathbb{Z}_2

Let's see how this marvelous projection machinery works with two examples. The first is rather trivial, from the group $G = \mathbb{Z}_2$, with elements $\{E, P\}$, where $P^2 = E$. We take P to correspond to parity, with $Px = -x$. Thus for any function $\psi(x)$,

$$\hat{U}(E) \psi(x) = \psi(x) \quad , \quad \hat{U}(P) \psi(x) = \psi(P^{-1}x) = \psi(Px) = \psi(-x) \quad . \quad (3.35)$$

\mathbb{Z}_2 has two IRREPs, both of which are one-dimensional. In the identity representation Γ_1 , the 1×1 matrices are $\hat{U}^{\Gamma_1}(E) = \hat{U}^{\Gamma_1}(P) = 1$. In the sign representation Γ_2 , and $\hat{U}^{\Gamma_2}(E) = 1$ while $\hat{U}^{\Gamma_2}(P) = -1$. The projectors are then

$$\hat{\Pi}^{\Gamma_1} = \frac{1}{2} [\hat{U}(E) + \hat{U}(P)] \quad , \quad \hat{\Pi}^{\Gamma_2} = \frac{1}{2} [\hat{U}(E) - \hat{U}(P)] \quad . \quad (3.36)$$

Now for the projection:

$$\hat{\Pi}^{\Gamma_1} \psi(x) = \frac{1}{2} [\psi(x) + \psi(-x)] \quad , \quad \hat{\Pi}^{\Gamma_2} \psi(x) = \frac{1}{2} [\psi(x) - \psi(-x)] \quad . \quad (3.37)$$

Example: C_{3v}

Let's now see how the projection onto basis functions works for a higher-dimensional representation of a nonabelian group. We turn to our old and trusted friend, C_{3v} , which has a two-dimensional representation, E .

Before we project onto E , let's warm up by projecting onto the two one-dimensional representations A_1 and A_2 . We have

$$\begin{aligned} \hat{\Pi}^{A_1} &= \frac{1}{6} \left\{ \hat{U}(E) + \hat{U}(R) + \hat{U}(W) + \hat{U}(\sigma) + \hat{U}(\sigma') + \hat{U}(\sigma'') \right\} \\ \hat{\Pi}^{A_2} &= \frac{1}{6} \left\{ \hat{U}(E) + \hat{U}(R) + \hat{U}(W) - \hat{U}(\sigma) - \hat{U}(\sigma') - \hat{U}(\sigma'') \right\} \quad . \end{aligned} \quad (3.38)$$

Thus the projection of an arbitrary initial function $\psi(x, y)$ onto A_1 will, according to Eqn. 3.32, be

$$\begin{aligned} \psi^{(A_1)}(x, y) &= \frac{1}{6} \left\{ \psi(x, y) + \psi\left(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y, -\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) + \psi\left(-\frac{1}{2}x - \frac{\sqrt{3}}{2}y, \frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) \right. \\ &\quad \left. + \psi(-x, y) + \psi\left(\frac{1}{2}x + \frac{\sqrt{3}}{2}y, \frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) + \psi\left(\frac{1}{2}x - \frac{\sqrt{3}}{2}y, -\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) \right\} . \end{aligned} \quad (3.39)$$

Similarly, projecting onto A_2 yields

$$\begin{aligned} \psi^{(A_2)}(x, y) = \frac{1}{6} \left\{ \psi(x, y) + \psi\left(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y, -\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) + \psi\left(-\frac{1}{2}x - \frac{\sqrt{3}}{2}y, \frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) \right. \\ \left. - \psi(-x, y) + \psi\left(\frac{1}{2}x - \frac{\sqrt{3}}{2}y, \frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) - \psi\left(\frac{1}{2}x + \frac{\sqrt{3}}{2}y, -\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) \right\}. \end{aligned} \quad (3.40)$$

Note that \hat{I}^{A_1} preserves all constant functions (e.g. $\psi = 1$) but annihilates all linear functions of the form $\psi(x, y) = ax + by$.¹¹ What happens if we take $\psi(x, y) = x^2$? Then we find $\psi^{(A_1)}(x, y) = \frac{1}{2}(x^2 + y^2)$, which does indeed transform like the identity, but $\psi^{(A_2)}(x, y) = 0$. What do we need to do to get a nontrivial representation of A_2 ? Let's try starting with $\psi(x, y) = x^3$. Now we find $\psi^{(A_1)}(x, y) = 0$ but $\psi^{(A_2)}(x, y) = \frac{1}{4}x^3 - \frac{3}{4}xy^2$. Eureka! Note that we may write $\psi^{(A_2)}(x, y) = x\left(\frac{1}{2}x + \frac{\sqrt{3}}{2}y\right)\left(\frac{1}{2}x - \frac{\sqrt{3}}{2}y\right)$, which renders its transformation properties more apparent.

Now let's roll up our sleeves and do the projection onto E . Recall the matrices for E :

$$\begin{aligned} D^E(E) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & D^E(R) &= \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} & D^E(W) &= \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \\ D^E(\sigma) &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} & D^E(\sigma') &= \frac{1}{2} \begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} & D^E(\sigma'') &= \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \end{aligned} \quad (3.41)$$

We now select an arbitrary function $\psi(\mathbf{r})$ which itself may have no special symmetry properties. According to Eqn. 3.32, the projection of $\psi(\mathbf{r})$ onto the μ row of the E representation is given by

$$\begin{aligned} \psi_\mu^{(E\nu)}(\mathbf{r}) = \frac{1}{3} \left\{ D_{\mu\nu}^E(E) \psi(\mathbf{r}) + D_{\mu\nu}^E(R) \psi(R^{-1}\mathbf{r}) + D_{\mu\nu}^E(W) \psi(W^{-1}\mathbf{r}) \right. \\ \left. + D_{\mu\nu}^E(\sigma) \psi(\sigma^{-1}\mathbf{r}) + D_{\mu\nu}^E(\sigma') \psi(\sigma'^{-1}\mathbf{r}) + D_{\mu\nu}^E(\sigma'') \psi(\sigma''^{-1}\mathbf{r}) \right\}. \end{aligned} \quad (3.42)$$

Thus,

$$\begin{aligned} \psi_\mu^{(E\nu)}(\mathbf{r}) = \frac{1}{3} \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \psi(x, y) + \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \psi\left(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y, -\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) \right. \\ \left. + \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \psi\left(-\frac{1}{2}x - \frac{\sqrt{3}}{2}y, \frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) + \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \psi(-x, y) \right. \\ \left. + \frac{1}{2} \begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \psi\left(\frac{1}{2}x + \frac{\sqrt{3}}{2}y, \frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) + \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \psi\left(\frac{1}{2}x - \frac{\sqrt{3}}{2}y, -\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) \right\}_{\mu\nu}. \end{aligned} \quad (3.43)$$

Let's take $\nu = 1$, which means we only use the first column of each of the matrices in the above expression. Starting with $\psi(x, y) = x$, we obtain $\psi_1^{(E,1)}(x, y) = x$ and $\psi_2^{(E,1)}(x, y) = y$. Had we chosen instead $\psi(x, y) = y$, we would have found $\psi_1^{(E,1)}(x, y) = \psi_2^{(E,1)}(x, y) = 0$, i.e. the projection annihilates the initial state. Generically this will not occur – our choices here have been simple and nongeneric.

Had we chosen instead $\nu = 2$, then taking the second column above we find that $\psi(x, y) = x$ is annihilated by the projection, while for $\psi(x, y) = y$ we obtain $\psi_1^{(E,2)}(x, y) = x$ and $\psi_2^{(E,2)}(x, y) = y$. At any rate, the upshot of this analysis is that $\psi_1(x, y) = x$ and $\psi_2(x, y) = y$ are appropriate basis functions for the E representation of C_{3v} .

¹¹Nasty stuff, these projectors.

3.1.6 Partial diagonalization of H

Suppose we have a set of appropriately transforming basis vectors $|\Gamma\mu\rangle$. One way to obtain such a set is to start with an arbitrary function $f(\mathbf{r})$ and then perform the projection onto row μ of representation Γ , forming $f_\mu^{(\Gamma\kappa)}(\mathbf{r}) = \hat{\Pi}_{\mu\kappa}^\Gamma f(\mathbf{r})$, and then defining

$$|\Gamma\mu\rangle = \mathcal{N}_\mu^\Gamma \int d^d r f_\mu^{(\Gamma\kappa)}(\mathbf{r}) |\mathbf{r}\rangle \quad , \quad (3.44)$$

where \mathcal{N}_μ^Γ is a normalization constant. The column index κ is fixed for each Γ and is suppressed. We assume that the projection of $f(\mathbf{r})$ onto $f_\mu^{(\Gamma\kappa)}(\mathbf{r})$ does not annihilate $f(\mathbf{r})$ (else we try again with a different $f(\mathbf{r})$ function). We then have¹²

$$\begin{aligned} \langle \Gamma\mu | \Gamma'\mu' \rangle &= \mathcal{N}_\mu^{\Gamma*} \mathcal{N}_{\mu'}^{\Gamma'} \int d^d r [f_\mu^{(\Gamma\kappa)}(\mathbf{r})]^* f_{\mu'}^{(\Gamma'\kappa')}(\mathbf{r}) = \mathcal{N}_\mu^{\Gamma*} \mathcal{N}_{\mu'}^{\Gamma'} \int d^d r f^*(\mathbf{r}) (\hat{\Pi}_{\mu\kappa}^\Gamma)^\dagger \hat{\Pi}_{\mu'\kappa'}^{\Gamma'} f(\mathbf{r}) \\ &= \mathcal{N}_\mu^{\Gamma*} \mathcal{N}_{\mu'}^{\Gamma'} \int d^d r f^*(\mathbf{r}) \hat{\Pi}_{\kappa\mu}^\Gamma \hat{\Pi}_{\mu'\kappa'}^{\Gamma'} f(\mathbf{r}) = \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} |\mathcal{N}_\mu^\Gamma|^2 \int d^d r f^*(\mathbf{r}) \hat{\Pi}_{\kappa\mu}^\Gamma f(\mathbf{r}) \quad , \end{aligned} \quad (3.45)$$

which confirms that the basis vectors are orthogonal unless their representations (Γ, Γ') and basis indices (μ, μ') agree. We can therefore enforce the normalization $\langle \Gamma\mu | \Gamma'\mu' \rangle = \delta_{\Gamma\Gamma'} \delta_{\mu\mu'}$.

Now assuming $[\hat{H}, \hat{U}(G)] = 0$, we may write $\hat{H} = \hat{U}(g)^\dagger \hat{H} \hat{U}(g)$, and therefore

$$\begin{aligned} \langle \Gamma\mu | H | \Gamma'\mu' \rangle &= \frac{1}{N_G} \sum_{g \in G} \langle \Gamma\mu | \hat{U}(g)^\dagger \hat{H} \hat{U}(g) | \Gamma'\mu' \rangle \\ &= \frac{1}{N_G} \sum_{g \in G} D_{\nu\mu}^{\Gamma*}(g) \langle \Gamma\nu | \hat{H} | \Gamma'\nu' \rangle D_{\nu'\mu'}^{\Gamma'}(g) \\ &= \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} \frac{1}{d_\Gamma} \sum_{\nu=1}^{d_\Gamma} \langle \Gamma\nu | \hat{H} | \Gamma\nu \rangle \quad , \end{aligned} \quad (3.46)$$

where we have invoked the Great Orthogonality Theorem to collapse the sum over the group elements. Thus we see that if we choose our basis functions accordingly, *i.e.* as transforming appropriately under the group operations, the Hamiltonian will automatically be diagonal in the $\Gamma\mu$ indices. Of course this isn't the entire Hilbert space, since in the eigenspectrum of \hat{H} , a given representation Γ may occur many times – perhaps even infinitely many. We could, for example, have started by projecting an entire family of arbitrary initial functions, $\{f_l(\mathbf{r})\}$, indexed by l , and create their corresponding basis states, which we would label $|\Gamma\mu, l\rangle$. The overlaps and the Hamiltonian matrix elements between these two different sectors will in general be nonzero provided the representations and the basis indices agree:

$$\begin{aligned} \langle \Gamma\mu, l | \Gamma'\mu', l' \rangle &= \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} \frac{1}{d_\Gamma} \sum_{\nu=1}^{d_\Gamma} \langle \Gamma\nu, l | \Gamma\nu, l' \rangle \equiv O_{ll'}^\Gamma \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} \\ \langle \Gamma\mu, l | \hat{H} | \Gamma'\mu', l' \rangle &= \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} \frac{1}{d_\Gamma} \sum_{\nu=1}^{d_\Gamma} \langle \Gamma\nu, l | \hat{H} | \Gamma\nu, l' \rangle \equiv H_{ll'}^\Gamma \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} \quad , \end{aligned} \quad (3.47)$$

¹²No sum on μ or μ' in Eqn. 3.45.

with no sum on Γ or μ . The first of these comes from the generalized version of Eqn. 3.46 upon replacing \hat{H} by 1. Here $O_{ll'}^{\Gamma}$ and $H_{ll'}^{\Gamma}$ are the overlap matrix and Hamiltonian matrix, respectively; note that neither depends on the basis index μ . Our task is then to simultaneously diagonalize these two Hermitian matrices, *i.e.* to solve the linear system $H_{ll'}^{\Gamma} \phi_{l'}^{\Gamma s} = E_{\Gamma s} O_{ll'}^{\Gamma} \phi_{l'}^{\Gamma s}$, where a labels the eigenvalue and corresponding eigenfunctions of the s^{th} occurrence of the IRREP Γ . In systems with an infinite number of degrees of freedom, both O^{Γ} and H^{Γ} will in general be of infinite rank for each IRREP Γ , *i.e.* each IRREP will in general appear an infinite number of times in the eigenspectrum. Still, we have achieved a substantial simplification by organizing the basis vectors in terms of group symmetry.

3.2 Product Representations

3.2.1 Direct product of two representations

In chapter 2 we discussed the direct product of IRREPS $\Gamma_a \times \Gamma_b$. Recall the action of the group element g on the direct product space $\mathcal{V}_a \otimes \mathcal{V}_b$ is defined in terms of its action on the basis vectors,

$$\hat{U}(g) |e_{\alpha\beta}^{\Gamma_a \times \Gamma_b}\rangle = |e_{\alpha'\beta'}^{\Gamma_a \times \Gamma_b}\rangle D_{\alpha'\alpha}^{\Gamma_a}(g) D_{\beta'\beta}^{\Gamma_b}(g) \quad , \quad (3.48)$$

where $|e_{\alpha\beta}^{\Gamma_a \times \Gamma_b}\rangle \equiv |e_{\alpha}^{\Gamma_a}\rangle \otimes |e_{\beta}^{\Gamma_b}\rangle$, where $|e_{\mu}^{\Gamma}\rangle = |\Gamma\mu\rangle$ in our previous notation¹³. Thus the matrix of g in the direct product representation $\Gamma_a \times \Gamma_b$ is given by

$$D_{\alpha'\beta', \alpha\beta}^{\Gamma_a \times \Gamma_b}(g) = D_{\alpha'\alpha}^{\Gamma_a}(g) D_{\beta'\beta}^{\Gamma_b}(g) \quad , \quad (3.49)$$

where $\alpha\beta$ and $\alpha'\beta'$ on the LHS are composite indices, each taking $d_{\Gamma_a} \times d_{\Gamma_b}$ possible values. The characters in the product representation are given by the product of the individual characters, *viz.*

$$\chi^{\Gamma_a \times \Gamma_b}(g) = \chi^{\Gamma_a}(g) \chi^{\Gamma_b}(g) \quad . \quad (3.50)$$

3.2.2 Products of identical representations

Here we discuss three ways of taking the product of identical representations. Since we will be assuming the same representation Γ throughout, might as well suppress the Γ label.

- *Direct product* : This is also called the simple product. Consider an IRREP Γ of a finite group G and construct the tensor product basis $|e_{\mu\nu}\rangle = |e_{\mu}\rangle \otimes |e_{\nu}\rangle$, where $\mu, \nu \in \{1, \dots, d_{\Gamma}\}$. There are d_{Γ}^2 linearly independent basis states in the tensor product space $\mathcal{V} \times \mathcal{V}$. In the direct product representation $\Gamma \times \Gamma$, one has

$$\hat{U}(g) |e_{\mu\nu}\rangle = |e_{\mu'\nu'}\rangle D_{\mu'\mu}(g) D_{\nu'\nu}(g) \equiv |e_{\mu'\nu'}\rangle D_{\mu'\nu', \mu\nu}^{\text{D}}(g) \quad . \quad (3.51)$$

¹³When there are multiple occurrences of the IRREP Γ , we will use $|e_{\mu}^{\Gamma, l}\rangle$ to always denote an orthonormal basis, with $\langle e_{\mu}^{\Gamma, l} | e_{\mu'}^{\Gamma, l'} \rangle = \delta_{\Gamma\Gamma'} \delta_{ll'} \delta_{\mu\mu'}$.

Therefore the character of g in the direct product representation $\Gamma \times \Gamma$ is

$$\chi^D(g) = [\chi^\Gamma(g)]^2 \quad , \quad (3.52)$$

which is the square of the character in the Γ representation.

- *Symmetrized product*: Consider now the symmetrized basis states,

$$|e_{\mu\nu}^S\rangle = \frac{1}{\sqrt{2}} \left(|e_\mu\rangle \otimes |e_\nu\rangle + |e_\nu\rangle \otimes |e_\mu\rangle \right) \quad . \quad (3.53)$$

Clearly $|e_{\mu\nu}^S\rangle = |e_{\nu\mu}^S\rangle$, so there are $\frac{1}{2}d_\Gamma(d_\Gamma + 1)$ linearly independent basis states in the symmetric product space $(\mathcal{V} \otimes \mathcal{V})^S$. You might worry about the normalization, since

$$\langle e_{\mu\nu}^S | e_{\mu'\nu'}^S \rangle = \delta_{\mu\mu'} \delta_{\nu\nu'} + \delta_{\mu\nu'} \delta_{\nu\mu'} \quad , \quad (3.54)$$

and thus the diagonal basis vectors $|e_{\mu\mu}^S\rangle$ (no sum on μ) have norm $\sqrt{2}$. It turns out that this doesn't matter, and we can always impose a proper normalization later on. Now let's apply the operator $\hat{U}(g)$:

$$\begin{aligned} \hat{U}(g) |e_{\mu\nu}^S\rangle &= \frac{1}{\sqrt{2}} \left(|e_{\mu'}\rangle \otimes |e_{\nu'}\rangle D_{\mu'\mu}(g) D_{\nu'\nu}(g) + |e_{\nu'}\rangle \otimes |e_{\mu'}\rangle D_{\nu'\mu}(g) D_{\mu'\nu}(g) \right) \\ &= |e_{\mu'\nu'}^S\rangle \cdot \frac{1}{2} \left(D_{\mu'\mu}(g) D_{\nu'\nu}(g) + D_{\nu'\mu}(g) D_{\mu'\nu}(g) \right) \equiv |e_{\mu'\nu'}^S\rangle D_{\mu'\nu',\mu\nu}^S(g) \quad . \end{aligned} \quad (3.55)$$

The character of g in this representation is then

$$\chi^S(g) = D_{\mu\nu,\mu\nu}^S(g) = \frac{1}{2} \left([\chi^\Gamma(g)]^2 + \chi^\Gamma(g^2) \right) \quad . \quad (3.56)$$

- *Antisymmetrized product*: Consider now the antisymmetrized basis states,

$$|e_{\mu\nu}^A\rangle = \frac{1}{\sqrt{2}} \left(|e_\mu\rangle \otimes |e_\nu\rangle - |e_\nu\rangle \otimes |e_\mu\rangle \right) \quad . \quad (3.57)$$

Now we have $|e_{\mu\nu}^A\rangle = -|e_{\nu\mu}^A\rangle$, so there are $\frac{1}{2}d_\Gamma(d_\Gamma - 1)$ linearly independent basis states in the antisymmetric product space $(\mathcal{V} \otimes \mathcal{V})^A$. We then have

$$\langle e_{\mu\nu}^A | e_{\mu'\nu'}^A \rangle = \delta_{\mu\mu'} \delta_{\nu\nu'} - \delta_{\mu\nu'} \delta_{\nu\mu'} \quad . \quad (3.58)$$

Note that the diagonal basis vectors $|e_{\mu\mu}^A\rangle = 0$ (no sum on μ) vanish identically. Now let's apply the operator $\hat{U}(g)$:

$$\begin{aligned} \hat{U}(g) |e_{\mu\nu}^A\rangle &= \frac{1}{\sqrt{2}} \left(|e_{\mu'}\rangle \otimes |e_{\nu'}\rangle D_{\mu'\mu}(g) D_{\nu'\nu}(g) - |e_{\nu'}\rangle \otimes |e_{\mu'}\rangle D_{\nu'\mu}(g) D_{\mu'\nu}(g) \right) \\ &= |e_{\mu'\nu'}^A\rangle \cdot \frac{1}{2} \left(D_{\mu'\mu}(g) D_{\nu'\nu}(g) - D_{\nu'\mu}(g) D_{\mu'\nu}(g) \right) \equiv |e_{\mu'\nu'}^A\rangle D_{\mu'\nu',\mu\nu}^A(g) \quad . \end{aligned} \quad (3.59)$$

The character of g in this representation is then

$$\chi^A(g) = D_{\mu\nu,\mu\nu}^A(g) = \frac{1}{2} \left([\chi^\Gamma(g)]^2 - \chi^\Gamma(g^2) \right) \quad . \quad (3.60)$$

Note that this vanishes whenever Γ is a one-dimensional IRREP, because one-dimensional representations cannot be antisymmetrized!

Note that $\chi(g^2) = \chi((h^{-1}gh)^2)$, and so the class structure is the same. In other words, if g and g' belong to the same class, then g^2 and g'^2 also belong to the same class. Let's now use the equation

$$n_{\Gamma}(\Psi) = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}} \chi^{\Gamma}(\mathcal{C})^* \chi^{\Psi}(\mathcal{C}) \quad (3.61)$$

to decompose some of these product representations. We'll choose the group D_3 , the character table for which is the upper left 3×3 block of the character table for D_{3h} provided in Tab. 3.1. We first work out the direct product $E \times E$, for which $\chi^D(E) = 4$, $\chi^D(C_3) = 1$, and $\chi^D(C'_2) = 0$. Applying the decomposition formula, we obtain $E \times E = A_1 \oplus A_2 \oplus E$. This is consistent with a naïve counting of dimensions, since $2^2 = 1 + 1 + 2$.

In order to decompose the symmetrized and antisymmetrized product representations $(E \times E)^{S,A}$, we must compute the characters $\chi^{\Gamma}(g^2)$, and for this we need to invoke class relations $[E]^2 = E$, $[C_3]^2 = C_3$, and $[C'_2]^2 = E$. These are easy to see, since C_3 contains the rotations R and W , which satisfy $R^2 = W$ and $W^2 = R$. The class C'_2 consists of the three two-fold rotations (or mirrors, for C_{3v} elements), each of which squares to the identity. We then have¹⁴

$$\chi^E([E]^2) = \chi^E(E) = 2 \quad , \quad \chi^E([C_3]^2) = \chi^E(C_3) = -1 \quad , \quad \chi^E([C'_2]^2) = \chi^E(E) = 2 \quad . \quad (3.62)$$

According to Eqns. 3.56 and 3.60, we then have

$$\chi^S(E) = 3 \qquad \chi^S(C_3) = 0 \qquad \chi^S(C'_2) = 1 \quad (3.63)$$

$$\chi^A(E) = 1 \qquad \chi^A(C_3) = 1 \qquad \chi^A(C'_2) = -1 \quad . \quad (3.64)$$

We therefore conclude $(E \times E)^S = A_1 \oplus E$ and $(E \times E)^A = A_2$. Can you make sense of the dimensions?

3.2.3 Clebsch-Gordan Coefficients

Recall the decomposition formulae for the product representation $\Gamma_a \times \Gamma_b$ for any finite group G :

$$\Gamma_a \times \Gamma_b = \bigoplus_{\Gamma} n_{\Gamma}^{ab} \Gamma \quad (3.65)$$

where

$$n_{\Gamma}^{ab} = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}} \chi^{\Gamma*}(\mathcal{C}) \chi^{\Gamma_a}(\mathcal{C}) \chi^{\Gamma_b}(\mathcal{C}) \quad . \quad (3.66)$$

We may express the direct product of orthonormal basis states $|e_{\alpha}^{\Gamma_a}\rangle$ and $|e_{\beta}^{\Gamma_b}\rangle$, with $1 \leq \alpha \leq d_{\Gamma_a}$ and $1 \leq \beta \leq d_{\Gamma_b}$, in terms of the new orthonormal basis set $|e_{\gamma}^{\Gamma,s}\rangle$, viz.

$$|e_{\alpha}^{\Gamma_a}\rangle \otimes |e_{\beta}^{\Gamma_b}\rangle = \sum_{\Gamma} \sum_{s=1}^{n_{\Gamma}^{ab}} \sum_{\gamma=1}^{d_{\Gamma}} \left(\begin{matrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{matrix} \middle| \begin{matrix} \Gamma & s \\ \gamma \end{matrix} \right) |e_{\gamma}^{\Gamma,s}\rangle \quad . \quad (3.67)$$

¹⁴Remember that E labels the identity element and its class, as well as the two-dimensional representation. Take care not to confuse the meaning of E in its appropriate context!

Here, the label s indexes possible multiple appearances of the representation Γ in the decomposition of the product $\Gamma_a \times \Gamma_b$. The quantities $\left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma \end{smallmatrix} \right)$, known as *Clebsch-Gordan coefficients* (CGCs), are unitary matrices relating the two orthonormal sets of basis vectors. Orthonormality of the bases means

$$\left\langle e_{\alpha}^{\Gamma_a} \middle| e_{\alpha'}^{\Gamma_a} \right\rangle = \delta_{\alpha\alpha'} \quad , \quad \left\langle e_{\beta}^{\Gamma_b} \middle| e_{\beta'}^{\Gamma_b} \right\rangle = \delta_{\beta\beta'} \quad , \quad \left\langle e_{\gamma}^{\Gamma, s} \middle| e_{\gamma'}^{\Gamma', s'} \right\rangle = \delta_{\Gamma\Gamma'} \delta_{ss'} \delta_{\gamma\gamma'} \quad . \quad (3.68)$$

The inverse basis transformation is

$$\left| e_{\gamma}^{\Gamma, s} \right\rangle = \sum_{\alpha=1}^{d_a} \sum_{\beta=1}^{d_b} \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma \end{smallmatrix} \right)^* \left| e_{\alpha}^{\Gamma_a} \right\rangle \otimes \left| e_{\beta}^{\Gamma_b} \right\rangle \quad , \quad (3.69)$$

where we abbreviate $d_a \equiv d_{\Gamma_a}$ and $d_b \equiv d_{\Gamma_b}$. Note that the component IRREPs Γ_a and Γ_b are fixed throughout this discussion.

Relations satisfied by CGCs

Orthonormality and completeness of the CGCs require

$$\sum_{\alpha=1}^{d_a} \sum_{\beta=1}^{d_b} \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma \end{smallmatrix} \right)^* \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma', s' \\ \gamma' \end{smallmatrix} \right) = \delta_{\Gamma\Gamma'} \delta_{ss'} \delta_{\gamma\gamma'} \quad (3.70)$$

and

$$\sum_{\Gamma} \sum_{s=1}^{n_{\Gamma}^{ab}} \sum_{\gamma=1}^{d_{\Gamma}} \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma \end{smallmatrix} \right)^* \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma \end{smallmatrix} \right) = \delta_{\alpha\alpha'} \delta_{\beta\beta'} \quad . \quad (3.71)$$

Applying the unitary operators $\hat{U}(g)$ to the basis vectors in their respective representations, one then obtains the relations

$$\sum_{\Gamma} \sum_{s=1}^{n_{\Gamma}^{ab}} \sum_{\gamma=1}^{d_{\Gamma}} \sum_{\gamma'=1}^{d_{\Gamma}} \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma \end{smallmatrix} \right)^* D_{\gamma\gamma'}^{\Gamma}(g) \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma' \end{smallmatrix} \right) = D_{\alpha\alpha'}^{\Gamma_a}(g) D_{\beta\beta'}^{\Gamma_b}(g) \quad (3.72)$$

and

$$\sum_{\alpha=1}^{d_a} \sum_{\alpha'=1}^{d_a} \sum_{\beta=1}^{d_b} \sum_{\beta'=1}^{d_b} \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma \end{smallmatrix} \right) D_{\alpha\alpha'}^{\Gamma_a}(g) D_{\beta\beta'}^{\Gamma_b}(g) \left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s' \\ \gamma' \end{smallmatrix} \right)^* = D_{\gamma\gamma'}^{\Gamma}(g) \delta_{\Gamma\Gamma'} \delta_{ss'} \quad . \quad (3.73)$$

3.2.4 Simply reducible groups

A group G is *simply reducible* if the multiplicities n_{Γ}^{ab} in its IRREP product decompositions are all either $n_{\Gamma}^{ab} = 0$ or $n_{\Gamma}^{ab} = 1$. In this case, we may drop the multiplicity index s . For simply reducible groups, we

can obtain an explicit expression for the CGCs, courtesy of the Great Orthogonality Theorem :

$$\begin{aligned} \frac{d_\Gamma}{N_G} \sum_{g \in G} D_{\alpha\alpha'}^{\Gamma_a}(g) D_{\beta\beta'}^{\Gamma_b}(g) D_{\gamma\gamma'}^{\Gamma^*}(g) &= \sum_{\Gamma'} \sum_{\sigma, \sigma'} \left(\begin{array}{c|c} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{array} \middle| \begin{array}{c} \Gamma' \\ \sigma \end{array} \right)^* \left(\begin{array}{c|c} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{array} \middle| \begin{array}{c} \Gamma' \\ \sigma' \end{array} \right) \overbrace{\frac{d_\Gamma}{N_G} \sum_{g \in G} D_{\sigma\sigma'}^{\Gamma'}(g) D_{\gamma\gamma'}^{\Gamma^*}(g)}^{= \delta_{\Gamma\Gamma'} \delta_{\sigma\gamma} \delta_{\sigma'\gamma'}} \\ &= \left(\begin{array}{c|c} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{array} \middle| \begin{array}{c} \Gamma \\ \gamma \end{array} \right)^* \left(\begin{array}{c|c} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{array} \middle| \begin{array}{c} \Gamma \\ \gamma' \end{array} \right) . \end{aligned} \quad (3.74)$$

We now set $\alpha = \alpha' \equiv \alpha_0$, $\beta = \beta' \equiv \beta_0$, and $\gamma = \gamma' \equiv \gamma_0$ in such a way that the LHS of the above equation is nonvanishing¹⁵ to obtain

$$\left(\begin{array}{c|c} \Gamma_a & \Gamma_b \\ \alpha_0 & \beta_0 \end{array} \middle| \begin{array}{c} \Gamma \\ \gamma_0 \end{array} \right) = \sqrt{\frac{d_\Gamma}{N_G} \sum_{g \in G} D_{\alpha_0\alpha_0}^{\Gamma_a}(g) D_{\beta_0\beta_0}^{\Gamma_b}(g) D_{\gamma_0\gamma_0}^{\Gamma^*}(g)}}, \quad (3.75)$$

with no sum on the repeated indices α_0 , β_0 , and γ_0 . We can choose $\left(\begin{array}{c|c} \Gamma_a & \Gamma_b \\ \alpha_0 & \beta_0 \end{array} \middle| \begin{array}{c} \Gamma \\ \gamma_0 \end{array} \right)$ to be real and positive, which amounts to a phase convention for the CGCs. The general CGC is then given by

$$\left(\begin{array}{c|c} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{array} \middle| \begin{array}{c} \Gamma \\ \gamma \end{array} \right) = \frac{1}{\left(\begin{array}{c|c} \Gamma_a & \Gamma_b \\ \alpha_0 & \beta_0 \end{array} \middle| \begin{array}{c} \Gamma \\ \gamma_0 \end{array} \right)} \frac{d_\Gamma}{N_G} \sum_{g \in G} D_{\alpha\alpha_0}^{\Gamma_a}(g) D_{\beta\beta_0}^{\Gamma_b}(g) D_{\gamma\gamma_0}^{\Gamma^*}(g) \quad (3.76)$$

When G is not simply reducible and there are multiple appearances of the same representation in the decomposition of the product $\Gamma_a \times \Gamma_b$, the situation is more complicated. Tables of CGCs for physically useful groups are listed in, e.g., Koster *et al.* (1963).

Example : C_{3v}

As an example, consider the case of C_{3v} , with representations A_1 , A_2 , and E . $A_{1,2}$ are one-dimensional and can be read off from the character table. For the two-dimensional IRREP E , we use the representation matrices in Eqn. 3.41. Since $A_1 \times A_1 = A_2 \times A_2 = A_1$ and $A_1 \times A_2 = A_2$, we have

$$\left(\begin{array}{c|c} A_1 & A_1 \\ 1 & 1 \end{array} \middle| \begin{array}{c} A_1 \\ 1 \end{array} \right) = \left(\begin{array}{c|c} A_1 & A_2 \\ 1 & 1 \end{array} \middle| \begin{array}{c} A_2 \\ 1 \end{array} \right) = \left(\begin{array}{c|c} A_2 & A_2 \\ 1 & 1 \end{array} \middle| \begin{array}{c} A_1 \\ 1 \end{array} \right) = 1 . \quad (3.77)$$

Recall $A_1 \times E = A_2 \times E = E$. We then have

$$\left(\begin{array}{c|c} A_1 & E \\ 1 & \nu \end{array} \middle| \begin{array}{c} E \\ \xi \end{array} \right) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_{\nu\xi}, \quad \left(\begin{array}{c|c} A_2 & E \\ 1 & \nu \end{array} \middle| \begin{array}{c} E \\ \xi \end{array} \right) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}_{\nu\xi} . \quad (3.78)$$

Finally, $E \times E = A_1 \oplus A_2 \oplus E$, and we have

$$\left(\begin{array}{c|c} E & E \\ \mu & \nu \end{array} \middle| \begin{array}{c} A_1 \\ 1 \end{array} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_{\mu\nu}, \quad \left(\begin{array}{c|c} E & E \\ \mu & \nu \end{array} \middle| \begin{array}{c} A_2 \\ 1 \end{array} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}_{\mu\nu} \quad (3.79)$$

and

$$\left(\begin{array}{c|c} E & E \\ \mu & \nu \end{array} \middle| \begin{array}{c} E \\ 1 \end{array} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_{\mu\nu}, \quad \left(\begin{array}{c|c} E & E \\ \mu & \nu \end{array} \middle| \begin{array}{c} E \\ 2 \end{array} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_{\mu\nu} . \quad (3.80)$$

¹⁵See R. Winkler, *Introduction to Group Theory* (2015), p. 84.

Online at <http://www.niu.edu/rwinkler/teaching/group-11/g-lecture.pdf>

3.2.5 Wigner-Eckart theorem

The transformation properties of basis vectors were defined in Eqn. 3.19: $\hat{U}(g) |\Gamma\mu\rangle = |\Gamma\nu\rangle D_{\nu\mu}^\Gamma(g)$. Operators, too, may be classified by their transformation properties under group actions. Since we would like $\langle\phi'|\hat{Q}'|\psi'\rangle = \langle\phi|\hat{Q}|\psi\rangle$, where, dropping representation and basis indices, the primes denote the transformed Hilbert space vectors and operators, the action of a group operation $g \in G$ on a general operator \hat{Q} is $\hat{Q}' = \hat{U}(g)\hat{Q}\hat{U}^\dagger(g)$. We now consider the case of *tensor operators*, which form families which transform among themselves under group operations.

DEFINITION : A *tensor operator* \hat{Q}_μ^Γ is a Hilbert space operator which transforms according to an IRREP of some group G . Tensor operators carry representation and basis indices.

The tensor operator \hat{Q}_μ^Γ transforms as

$$\hat{U}(g)\hat{Q}_\mu^\Gamma\hat{U}^\dagger(g) = \hat{Q}_\nu^\Gamma D_{\nu\mu}^\Gamma(g) \quad . \quad (3.81)$$

We can think of families of tensor operators as invariant subspaces in operator space, $\text{End}(\mathcal{H})$.

Now consider the action of tensor operators on basis vectors, such as $\hat{Q}_\alpha^{F_a} |e_\beta^{F_b}\rangle$. We ask how such an object transforms under group operations. We have

$$\begin{aligned} \hat{U}(g)\hat{Q}_\alpha^{F_a} |e_\beta^{F_b}\rangle &= \hat{U}(g)\hat{Q}_\alpha^{F_a}\hat{U}^\dagger(g)\hat{U}(g)|e_\beta^{F_b}\rangle \\ &= \hat{Q}_{\alpha'}^{F_a} |e_{\beta'}^{F_b}\rangle D_{\alpha'\alpha}^{F_a}(g) D_{\beta'\beta}^{F_b}(g) = \hat{Q}_{\alpha'}^{F_a} |e_{\beta'}^{F_b}\rangle D_{\alpha'\beta',\alpha\beta}^{F_a \times F_b}(g) \quad . \end{aligned} \quad (3.82)$$

This tells us that $\hat{Q}_\alpha^{F_a} |e_\beta^{F_b}\rangle$ transforms according to the product representation $F_a \times F_b$. This means that we can expand $\hat{Q}_\alpha^{F_a} |e_\beta^{F_b}\rangle$ as a sum over its irreducible components, *viz.*

$$\hat{Q}_\alpha^{F_a} |e_\beta^{F_b}\rangle = \sum_{\Gamma,s,\gamma} \left(\begin{array}{cc|c} F_a & F_b & \Gamma, s \\ \alpha & \beta & \gamma \end{array} \right) |\Psi_\gamma^{\Gamma,s}\rangle \quad , \quad (3.83)$$

where $|\Psi_\gamma^{\Gamma,s}\rangle$ transforms according to the Γ IRREP of the symmetry group G , meaning

$$\hat{U}(g)|\Psi_\gamma^{\Gamma,s}\rangle = |\Psi_{\gamma'}^{\Gamma,s}\rangle D_{\gamma'\gamma}^\Gamma(g) \quad . \quad (3.84)$$

This will be explicitly demonstrated at the end of this section. Note that, upon invoking orthogonality of the CGCs,

$$|\Psi_\gamma^{\Gamma,s}\rangle = \sum_{\alpha,\beta} \left(\begin{array}{cc|c} F_a & F_b & \Gamma, s \\ \alpha & \beta & \gamma \end{array} \right)^* \hat{Q}_\alpha^{F_a} |e_\beta^{F_b}\rangle \quad . \quad (3.85)$$

Since states which transform according to different IRREPs are orthogonal, we must have

$$\langle e_\gamma^{F_c} | \Psi_\sigma^{\Gamma,s} \rangle = \langle \Gamma_c || Q^{F_a} || \Gamma_b \rangle_s \delta_{\Gamma\Gamma_c} \delta_{\gamma\sigma} \quad , \quad (3.86)$$

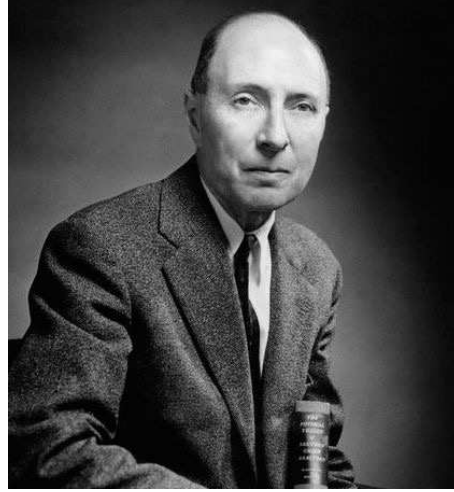


Figure 3.4: Eugene P. Wigner, the Ph.D. thesis supervisor of the Ph.D. thesis supervisor of my Ph.D. thesis supervisor.

where the *reduced matrix element* $\langle \Gamma_c \| Q^{F_a} \| \Gamma_b \rangle_s$ is independent of the basis indices γ and σ . We therefore have

$$\langle e_{\gamma}^{\Gamma_c} | \hat{Q}_{\alpha}^{\Gamma_a} | e_{\beta}^{\Gamma_b} \rangle = \sum_s \begin{pmatrix} \Gamma_a & \Gamma_b & \Gamma_c, s \\ \alpha & \beta & \gamma \end{pmatrix} \langle \Gamma_c \| Q^{F_a} \| \Gamma_b \rangle_s \quad (3.87)$$

a result known as the *Wigner-Eckart theorem*. Note that we have assumed that the ket vector $|e_{\mu}^{\Gamma}\rangle$ is conjugate to the bra vector $\langle e_{\mu}^{\Gamma}|$. In fact, they can come from different copies of each representation corresponding to different quantum numbers¹⁶. A more general expression of the Wigner-Eckart theorem is then

$$\langle e_{\gamma}^{\Gamma_c, l_c} | \hat{Q}_{\alpha}^{\Gamma_a} | e_{\beta}^{\Gamma_b, l_b} \rangle = \sum_s \begin{pmatrix} \Gamma_a & \Gamma_b & \Gamma_c, s \\ \alpha & \beta & \gamma \end{pmatrix} \langle \Gamma_c, l_c \| Q^{F_a} \| \Gamma_b, l_b \rangle_s \quad (3.88)$$

Appealing once again to the orthogonality of the CGCs, we obtain the following expression for the Wigner-Eckart reduced matrix elements:

$$\langle \Gamma_c, l_c \| Q^{F_a} \| \Gamma_b, l_b \rangle_s \delta_{\Gamma\Gamma_c} \delta_{\sigma\gamma} = \sum_{\alpha, \beta} \begin{pmatrix} \Gamma_a & \Gamma_b & \Gamma_c, s \\ \alpha & \beta & \sigma \end{pmatrix}^* \langle e_{\gamma}^{\Gamma_c, l_c} | \hat{Q}_{\alpha}^{\Gamma_a} | e_{\beta}^{\Gamma_b, l_b} \rangle \quad (3.89)$$

¹⁶Note that the multiplicity index s is not the same sort of animal as the index l in the state $|e_{\mu}^{\Gamma, l}\rangle$. The essential difference is that l labels states according to quantum numbers not associated with the group symmetry. The multiplicity index s , by contrast, knows nothing of the other quantum numbers and arises purely from a group theoretic analysis of the product representations.

If different appearances of the same IRREP are not orthogonal, we still have

$$\begin{aligned}
\langle \Gamma_c \gamma, l_c | \Gamma_b \beta, l_b \rangle &= \frac{1}{N_G} \sum_{g \in G} \langle \Gamma_c \gamma, l_c | U^\dagger(g) U(g) | \Gamma_b \beta, l_b \rangle \\
&= \frac{1}{N_G} \sum_{g \in G} D_{\gamma' \gamma}^{\Gamma_c}(g)^* \langle \Gamma_c \gamma', l_c | \Gamma_b \beta', l_b \rangle D_{\beta' \beta}^{\Gamma_b}(g) \\
&= \frac{1}{d_{\Gamma_c}} \sum_{\mu=1}^{d_{\Gamma_b}} \langle \Gamma_c \mu, l_c | \Gamma_b \mu, l_b \rangle \delta_{\Gamma_b \Gamma_c} \delta_{\alpha \beta} \equiv \langle \Gamma_c, l_c || \Gamma_b, l_b \rangle \delta_{\Gamma_b \Gamma_c} \delta_{\alpha \beta} .
\end{aligned} \tag{3.90}$$

The quantity $\langle \Gamma, l_a || \Gamma, l_b \rangle$ is called the *reduced overlap*, or the overlap matrix $O_{l_a l_b}^\Gamma$. Note that it does not depend on the basis indices α and β . By the same token, we also have

$$\langle \Gamma_c \gamma, l_c | \Psi_\sigma^{\Gamma, s} \rangle = \frac{1}{d_\Gamma} \sum_{\mu=1}^{d_\Gamma} \langle \Gamma_c \mu, l_c | \Psi_\mu^{\Gamma, s} \rangle \delta_{\Gamma \Gamma_c} \delta_{\gamma \sigma} . \tag{3.91}$$

Wigner-Eckart theorem for simply reducible groups

For simply reducible groups, there is no representation multiplicity index s for the direct products, and we have the simpler expression

$$\langle e_\gamma^{\Gamma_c, l_c} | \hat{Q}_\alpha^{\Gamma_a} | e_\beta^{\Gamma_b, l_b} \rangle = \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c \\ \alpha & \beta & \gamma \end{array} \right) \langle \Gamma_c, l_c || Q^{\Gamma_a} || \Gamma_b, l_b \rangle . \tag{3.92}$$

In this case, the ratios of matrix elements

$$\frac{\langle e_{\gamma'}^{\Gamma_c, l_c} | \hat{Q}_{\alpha'}^{\Gamma_a} | e_{\beta'}^{\Gamma_b, l_b} \rangle}{\langle e_\gamma^{\Gamma_c, l_c} | \hat{Q}_\alpha^{\Gamma_a} | e_\beta^{\Gamma_b, l_b} \rangle} = \frac{\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c \\ \alpha' & \beta' & \gamma' \end{array} \right)}{\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c \\ \alpha & \beta & \gamma \end{array} \right)} \tag{3.93}$$

are *independent* of all details of the operators $\hat{Q}_\alpha^{\Gamma_a}$ other than the representation by which it transforms.

Proof that $|\Psi_\gamma^{\Gamma, l}\rangle$ transforms as advertised

Start with Eqn. 3.83 and apply $\hat{U}(g)$ to both sides. The LHS transforms

$$\hat{U}(g) \hat{Q}_\alpha^{\Gamma_a} | e_\beta^{\Gamma_b} \rangle = \sum_{\alpha', \beta'} \hat{Q}_{\alpha'}^{\Gamma_a} | e_{\beta'}^{\Gamma_b} \rangle D_{\alpha' \alpha}^{\Gamma_a}(g) D_{\beta' \beta}^{\Gamma_b}(g) = \sum_{\Gamma', l', \gamma'} \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c \\ \alpha & \beta & \gamma \end{array} \right) \hat{U}(g) | \Psi_\gamma^{\Gamma, l} \rangle . \tag{3.94}$$

Now multiply by $\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma' \\ \alpha & \beta & \gamma' \end{array} \right)^*$ and sum on α and β . Using orthogonality of the CGCs, and dropping primes on the Γ', l' , and γ' indices, we obtain

$$\sum_{\alpha, \beta} \sum_{\alpha', \beta'} \hat{Q}_{\alpha'}^{\Gamma_a} | e_{\beta'}^{\Gamma_b} \rangle D_{\alpha' \alpha}^{\Gamma_a}(g) D_{\beta' \beta}^{\Gamma_b}(g) \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c \\ \alpha & \beta & \gamma \end{array} \right)^* = \hat{U}(g) | \Psi_\gamma^{\Gamma, l} \rangle . \tag{3.95}$$

Finally, reexpress $\hat{Q}_{\alpha'}^{\Gamma_a} |e_{\beta'}^{\Gamma_b}\rangle$ on the LHS above in terms of the $|\Psi_{\gamma}^{\Gamma, l}\rangle$, to find

$$\begin{aligned} \hat{U}(g) |\Psi_{\gamma}^{\Gamma, l}\rangle &= \sum_{\Gamma', l', \gamma'} \sum_{\alpha, \beta} \sum_{\alpha', \beta'} \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{pmatrix} \begin{pmatrix} \Gamma' & l' \\ \gamma' \end{pmatrix} D_{\alpha'\alpha}^{\Gamma_a}(g) D_{\beta'\beta}^{\Gamma_b}(g) \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{pmatrix} \begin{pmatrix} \Gamma & l \\ \gamma \end{pmatrix}^* |\Psi_{\gamma'}^{\Gamma', l'}\rangle \\ &= \sum_{\Gamma', l', \gamma'} |\Psi_{\gamma'}^{\Gamma', l'}\rangle D_{\gamma'\gamma}^{\Gamma'}(g) \quad , \end{aligned} \quad (3.96)$$

after invoking the CGC relation Eqn. 3.73.

3.2.6 Level repulsion and degeneracies

Consider a Hamiltonian \hat{H}_0 with $[\hat{H}_0, \hat{U}(G)] = 0$ whose eigenstates are labeled $|\Gamma\mu, l\rangle \equiv |e_{\mu}^{\Gamma, l}\rangle$. Suppose two multiplets $|\Gamma_a \alpha, l_a\rangle$ and $|\Gamma_b \beta, l_b\rangle$ are in close proximity, with energies E_a and E_b , respectively. Can they be made degenerate by varying the Hamiltonian in a way which preserves the full symmetry of G ? Let's write $\hat{H}(\lambda) = \hat{H}_0 + \lambda\hat{V}$, where $[\hat{V}, \hat{U}(G)] = 0$, and, neglecting all other multiplets which by assumption lie much further away in energy than the gap $|E_a - E_b|$, we compute the Hamiltonian matrix elements in the a, b multiplet basis. Since \hat{V} transforms as the Γ_1 identity IRREP, we have $\Gamma_1 \times \Gamma_b = \Gamma_b$, and therefore

$$\langle \Gamma_a \alpha, l_a | \hat{V} | \Gamma_b \beta, l_b \rangle = \overbrace{\begin{pmatrix} \Gamma_b & \Gamma_1 \\ \beta & 1 \end{pmatrix} \begin{pmatrix} \Gamma_a \\ \alpha \end{pmatrix}}^{= \delta_{\Gamma_a \Gamma_b} \delta_{\alpha\beta}} \langle \Gamma_a, l_a | \hat{V} | \Gamma_b, l_b \rangle \quad (3.97)$$

vanishes unless $\Gamma_a = \Gamma_b$, although we may have $l_a \neq l_b$. When $\Gamma_a = \Gamma_b$,

$$\langle \Gamma_a, l_a | \hat{V} | \Gamma_a, l_b \rangle = \frac{1}{d_{\Gamma_a}} \sum_{\mu=1}^{d_{\Gamma_a}} \langle \Gamma_a \mu, l_a | \hat{V} | \Gamma_a \mu, l_b \rangle \equiv V_{ab} \quad . \quad (3.98)$$

Consider first the case $\Gamma_a \not\cong \Gamma_b$. Then there are no off-diagonal matrix elements in our basis, and the energy shifts are given by

$$\begin{aligned} E_a(\lambda) &= E_a + \lambda V_{aa} \\ E_b(\lambda) &= E_b + \lambda V_{bb} \end{aligned} \quad (3.99)$$

Setting $E_a(\lambda) = E_b(\lambda)$, we obtain a degeneracy of the two multiplets when $\lambda = \lambda_*$, with

$$\lambda_* = \frac{E_b - E_a}{V_{aa} - V_{bb}} \quad . \quad (3.100)$$

The resulting supermultiplet has degeneracy $d = d_{\Gamma_a} + d_{\Gamma_b}$.

When $\Gamma_a = \Gamma_b$, we have nonzero off-diagonal elements. The reduced basis Hamiltonian is given by

$$\hat{H}_{\text{red}} = \begin{pmatrix} E_a + \lambda V_{aa} & \lambda V_{ab} \\ \lambda V_{ab}^* & E_b + \lambda V_{bb} \end{pmatrix} \otimes \mathbb{1}_{d_{\Gamma_a} \times d_{\Gamma_a}} \quad . \quad (3.101)$$

Note that we still must distinguish the a and b multiplets, because while they belong to the same representations, they are not identical multiplets, *i.e.* their wavefunctions are different¹⁷. There are then two d_{Γ_a} -fold degenerate sets of states, with energies

$$E_{ab,\pm} = \frac{1}{2}(E_a + \lambda V_{aa} + E_b + \lambda V_{bb}) \pm \frac{1}{2}\sqrt{(E_a + \lambda V_{aa} - E_b - \lambda V_{bb})^2 + 4\lambda^2|V_{ab}|^2} . \quad (3.102)$$

The only way for these multiplets to become degenerate is for the radical to vanish. But there is no choice for λ which will make that happen. Therefore we have an avoided crossing. The best we can do is to minimize the energy difference.

My personal advice: if you are ever caught being degenerate, say that it was an accident.

3.2.7 Example: C_{4v}

Consider the problem of a particle in a two-dimensional $L \times L$ square box, with $\hat{H}_0 = \frac{p^2}{2m} + V(x, y)$ with

$$V(x, y) = \begin{cases} 0 & \text{if } |x| < \frac{1}{2}L \text{ and } |y| < \frac{1}{2}L \\ \infty & \text{otherwise} \end{cases} . \quad (3.103)$$

This problem has a C_{4v} symmetry. Recall $C_{4v} \cong D_4$ is the symmetry group of the square, and is generated by two elements, *i.e.* a counterclockwise rotation through $\frac{1}{2}\pi$ (r) and a reflection in the x -axis (σ). One has $r^4 = \sigma^2 = (r\sigma)^2 = 1$. There are five conjugacyclasses: $\{E\}$, $\{r, r^3\}$, $\{r^2\}$, $\{r\sigma, \sigma r\}$ (diagonal reflections), and $\{\sigma, \sigma r^2\}$ (reflections in the x and y axes). The character table is given in Tab. 3.2.

Note that

$$r \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -y \\ x \end{pmatrix} , \quad \sigma \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ -y \end{pmatrix} , \quad r^2 \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ -y \end{pmatrix} , \quad r\sigma \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} y \\ x \end{pmatrix} . \quad (3.104)$$

And recall that $\hat{U}(g)\Psi(x, y) = \Psi(g^{-1}x, g^{-1}y)$. We define the functions

$$\begin{aligned} \phi_n(u) &= \sqrt{\frac{2}{L}} \cos\left(\frac{2(n - \frac{1}{2})\pi u}{L}\right) \\ \chi_n(u) &= \sqrt{\frac{2}{L}} \sin\left(\frac{2n\pi u}{L}\right) , \end{aligned} \quad (3.105)$$

where $n \in \mathbb{Z}_{>0}$ is a positive integer in either case. Note that the $\{\phi_n(u)\}$ are even under $u \rightarrow -u$ whereas the $\{\chi_n(u)\}$ are odd, and that $\phi_n(\pm\frac{1}{2}L) = \chi_n(\pm\frac{1}{2}L) = 0$. We will find it convenient to define the energy unit $\varepsilon_0 \equiv 2\pi^2\hbar^2/mL^2$.

Let's now write down all the possible wavefunctions for this problem. We'll find there are basically five different forms to consider:

¹⁷Think of the tower of even and odd states for the one-dimensional particle in a symmetric potential. All even states belong to the same Γ_1 representation, but have different wavefunctions.

C_{4v}	E	$\{r, r^3\}$	$\{r^2\}$	$\{r\sigma, \sigma r\}$	$\{\sigma, \sigma r^2\}$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

Table 3.2: Character table for the group C_{4v} .

- (i) $\Psi_{nn}^{(i)}(x, y) = \phi_n(x)\phi_n(y)$: The energy is $E_{nn}^{(i)} = 2n^2\varepsilon_0$. The wavefunction is invariant under all group operations, *i.e.*

$$\hat{U}(r)\Psi = \hat{U}(r^2)\Psi = \hat{U}(r\sigma)\Psi = \hat{U}(\sigma)\Psi = \Psi \quad , \quad (3.106)$$

and thus corresponds to the A_1 IRREP.

- (ii) $\Psi_{nn}^{(ii)}(x, y) = \chi_n(x)\chi_n(y)$: The energy is $E_{nn}^{(ii)} = 2(n - \frac{1}{2})^2\varepsilon_0$. We find

$$\hat{U}(r)\Psi = \hat{U}(\sigma)\Psi = -\Psi \quad , \quad \hat{U}(r^2)\Psi = \hat{U}(r\sigma)\Psi = \Psi \quad , \quad (3.107)$$

corresponding to the B_1 IRREP.

- (iii) $\Psi_{mn,\pm}^{(iii)}(x, y) = \frac{1}{\sqrt{2}}[\phi_m(x)\phi_n(y) \pm \phi_m(y)\phi_n(x)]$ with $m < n$. The energy for both states is given by $E_{mn}^{(iii)} = (m^2 + n^2)\varepsilon_0$. Is this a two-dimensional representation? We have

$$\hat{U}(r)\Psi_{\pm} = \hat{U}(r\sigma)\Psi_{\pm} = \pm\Psi_{\pm} \quad , \quad \hat{U}(r^2)\Psi_{\pm} = \hat{U}(\sigma)\Psi_{\pm} = \Psi_{\pm} \quad , \quad (3.108)$$

which tells us that Ψ_+ transforms according to A_1 and Ψ_- according to B_2 . So we have two one-dimensional IRREPs and no sign of the two-dimensional E IRREP yet.

- (iv) $\Psi_{mn,\pm}^{(iv)}(x, y) = \frac{1}{\sqrt{2}}[\chi_m(x)\chi_n(y) \pm \chi_m(y)\chi_n(x)]$ with $m < n$. The energy for both states is given by $E_{mn}^{(iv)} = ((m - \frac{1}{2})^2 + (n - \frac{1}{2})^2)\varepsilon_0$. We find

$$\hat{U}(r)\Psi_{\pm} = \mp\Psi_{\pm} \quad , \quad \hat{U}(r^2)\Psi_{\pm} = \Psi_{\pm} \quad , \quad \hat{U}(r\sigma)\Psi_{\pm} = \pm\Psi_{\pm} \quad , \quad \hat{U}(\sigma)\Psi_{\pm} = -\Psi_{\pm} \quad . \quad (3.109)$$

which tells us that Ψ_+ transforms as B_1 according and Ψ_- according to A_2 . So again two one-dimensional IRREPs and still no sign of the elusive E .

- (v) $\Psi_{mn,\pm}^{(v)}(x, y) = \frac{1}{\sqrt{2}}[\phi_m(x)\chi_n(y) \pm \phi_m(y)\chi_n(x)]$ with $m \leq n$. The energy for both states is given by $E_{mn}^{(v)} = (m^2 + (n - \frac{1}{2})^2)\varepsilon_0$. We find

$$\hat{U}(r)\Psi_{\pm} = \pm\Psi_{\mp} \quad , \quad \hat{U}(r^2)\Psi_{\pm} = -\Psi_{\pm} \quad , \quad \hat{U}(r\sigma)\Psi_{\pm} = \pm\Psi_{\pm} \quad , \quad \hat{U}(\sigma)\Psi_{\pm} = -\Psi_{\mp} \quad . \quad (3.110)$$

At long last, the E representation has shown itself! Note how in this basis,

$$D^E(r) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad , \quad D^E(r^2) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad D^E(r\sigma) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad D^E(\sigma) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \quad . \quad (3.111)$$

Now suppose we add a perturbation which transforms as the identity IRREP Γ_1 . For example, we could take $\hat{H} = \hat{H}_0 + \hat{V}$ with $\hat{V}(x, y) = \lambda x^2 y^2$. According to the Wigner-Eckart theorem, this won't split any of the E multiplets, but rather will simply lead to an equal energy shift for both E states. One only need compute one matrix element, per Eqn. 3.97.

3.3 Appendix : Random True Facts About Linear Algebra

Normal matrices and eigenspectra : Quantum mechanical Hamiltonians can be represented as Hermitian matrices. In elementary school linear algebra class, we all learned that any Hermitian matrix H is diagonalizable by a unitary transformation, its eigenvalues are real, and eigenvectors corresponding to different eigenvalues are necessarily orthogonal. In the case of degenerate eigenvalues, their associated eigenvectors may be chosen to be mutually orthogonal via the Gram-Schmidt process. In the following discussion, we will assume our matrices are in general complex, but we can of course restrict to the real case, as is appropriate for real linear dynamical systems.

Any complex square matrix A which satisfies $A^\dagger A = AA^\dagger$ is called *normal*. Hermitian matrices are normal, but so are antihermitian and unitary matrices¹⁸. Real symmetric, antisymmetric, and orthogonal matrices satisfy $A^T A = AA^T$. The *Schur decomposition theorem* guarantees that any $n \times n$ matrix A may be decomposed as $A = VTV^\dagger$, where $V \in U(n)$ and T is upper triangular. Now if A is normal, $[A, A^\dagger] = V [T, T^\dagger] V^\dagger = 0$, hence T is normal. However, it is easy to show that any normal upper triangular matrix must be diagonal¹⁹, so $A = VDV^\dagger$, which means $D = V^\dagger A V$ is the diagonal matrix of eigenvalues of A . Conversely, if $A = VDV^\dagger$ is unitarily equivalent to a diagonal matrix, it is trivial to show that A is normal. Thus *any $n \times n$ matrix A is diagonalizable by a unitary transformation if and only if A is normal.*

There is a real version of Schur decomposition whereby a real matrix B satisfying $B^T B = B B^T$ may be decomposed as $B = R S R^T$, where R is a real orthogonal matrix, and S is *block upper triangular*. The diagonal blocks of S are either 1×1 , corresponding to real eigenvalues, or 2×2 , corresponding to complex eigenvalues. One eventually concludes that real symmetric matrices have real eigenvalues, real antisymmetric matrices have pure imaginary (or zero) eigenvalues, and real orthogonal matrices have unimodular complex eigenvalues.

Now let's set $A = VDV^\dagger$ and consider different classes of matrix A . If A is Hermitian, $A = A^\dagger$ immediately yields $D = D^\dagger$, which says that all the eigenvalues of A must be real. If $A^\dagger = -A$, then $D^\dagger = -D$ and all the eigenvalues are purely imaginary. And if $A^\dagger = A^{-1}$, then $D^\dagger = D^{-1}$ and we conclude that all the eigenvalues are unimodular, *i.e.* of the form $e^{i\omega_j}$. This analysis also tells us that any unitary matrix U can be written in the form $U = \exp(iH)$ for some Hermitian matrix H .

Jordan blocks : What happens when an $n \times n$ matrix A is not normal? In this case A is not diagonalizable

¹⁸There are many examples of normal matrices which are neither Hermitian, antihermitian, nor unitary. For example, any diagonal matrix with arbitrary complex diagonal entries is normal.

¹⁹ $T^\dagger T = T T^\dagger$ says that $\sum_j |T_{ij}|^2 = \sum_j |T_{ji}|^2$, *i.e.* the sum of the square moduli of the elements in the i^{th} row is the same as that for the i^{th} column. Starting with $i = 1$, the only possible nonzero entry in the first column is $T_{1,1}$, hence all the remaining entries in the first row must vanish. Filling in all these zeros, proceed to $i = 2$. Since we just showed $T_{1,2} = 0$, we conclude that the only possible nonzero entry in the second column is $T_{2,2}$, hence all remaining entries in the second row must vanish. Continuing in this manner, we conclude that T is diagonal if it is both normal and upper triangular.

by a unitary transformation, and while the sum of the dimensions of its eigenspaces is generically equal to the matrix dimension $\dim(A) = n$, this is not guaranteed; it may be less than n . For example, consider the matrix

$$A = \begin{pmatrix} a & 1 \\ 0 & a \end{pmatrix} . \quad (3.112)$$

The eigenvalues are solutions to $\det(\lambda I - A) = 0$, hence $\lambda = a$, but there is only one eigenvector, $\psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. What is always true for any complex matrix A is that it can be brought to *Jordan canonical form* by a similarity transformation $J = P^{-1}AP$, where P is invertible, and

$$J = \begin{pmatrix} J^{(1)} & & \\ & \ddots & \\ & & J^{(b)} \end{pmatrix} , \quad (3.113)$$

where b is the number of *Jordan blocks* and where each block $J^{(r)}$ is an $n_r \times n_r$ matrix of the form

$$J^{(r)} = \begin{pmatrix} \lambda_r & 1 & & \\ & \lambda_r & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_r \end{pmatrix} . \quad (3.114)$$

Thus each $J^{(r)}$ is tridiagonal, with diagonal elements all given by λ_r and each element directly above the diagonal equal to one. Clearly $J^{(r)}$ has only one eigenvalue, λ_r , and writing the corresponding *right* eigenvector as $\vec{R}^{(r)}$, the condition $J^{(r)} \vec{R}^{(r)} = \lambda^{(r)} \vec{R}^{(r)}$ yields the equations

$$\lambda_r R_1^{(r)} + R_2^{(r)} = \lambda_r R_1^{(r)} \quad , \quad \lambda_r R_2^{(r)} + R_3^{(r)} = \lambda_r R_2^{(r)} \quad \dots \quad \lambda_r R_{n_r-1}^{(r)} + R_{n_r}^{(r)} = \lambda_r R_{n_r-1}^{(r)} \quad , \quad (3.115)$$

where $n_r = \dim(J^{(r)})$. These equations entail $R_2^{(r)} = R_3^{(r)} = \dots = R_{n_r}^{(r)} = 0$, which says that there is only one such eigenvector, whose components are $R_j^{(r)} = \delta_{j,1}$. Note that the corresponding *left* eigenvector $\vec{L}^{(r)}$ then has components $L_j^{(r)} = \delta_{j,n_r}$. If $n_r > 1$ we then have $\langle L^{(r)} | R^{(r)} \rangle \equiv \vec{L}^{(r)} \cdot \vec{R}^{(r)} = 0$, which means that the left and right eigenvectors of A which correspond to the Jordan blocks with $n_r > 1$ are orthogonal. *Nota bene*: It may be the case that there are degeneracies among the eigenvalues $\{\lambda_r\}$.

To summarize²⁰, for every general complex $n \times n$ matrix A ,

- A may be brought to Jordan canonical form by a similarity transformation $J = P^{-1}AP$, where $J = \text{bdiag}(J^{(1)}, \dots, J^{(b)})$ is block diagonal, with each $(J^{(r)})_{ij} = \lambda_r \delta_{i,j} + \delta_{i,j-1}$ with $\dim(J^{(r)}) = n_r$, for $r \in \{1, \dots, b\}$.
- There are $b \leq n$ eigenvalues $\{\lambda_1, \dots, \lambda_b\}$ (again, not necessarily all distinct) and b corresponding eigenvectors $\{\vec{R}^{(1)}, \dots, \vec{R}^{(b)}\}$. If $b = n$ then the matrix is diagonalizable.
- The dimension n of the matrix A satisfies $n = n_1 + \dots + n_b$, *i.e.* it is the sum of the dimensions of all its Jordan blocks.

²⁰See https://en.wikipedia.org/wiki/Jordan_normal_form.

- Let $\lambda \in \{\lambda_1, \dots, \lambda_b\}$ be an eigenvalue, and define

$$\mathfrak{t}_k(\lambda) = \dim \ker(A - \lambda)^k \quad , \quad (3.116)$$

which is the *dimension of the null space* of the matrix $A - \lambda I$. Then

- ◊ $\mathfrak{t}_k(\lambda)$ is the number of Jordan blocks corresponding to the eigenvalue λ .
- ◊ The number of Jordan blocks of size greater than k is $\mathfrak{t}_{k+1}(\lambda) - \mathfrak{t}_k(\lambda)$. Thus the number of Jordan blocks of size k for the eigenvalue λ is

$$N_k(\lambda) = 2\mathfrak{t}_k(\lambda) - \mathfrak{t}_{k+1}(\lambda) - \mathfrak{t}_{k-1}(\lambda) \quad . \quad (3.117)$$

Singular value decomposition : Note the difference between the decomposition into Jordan canonical form and singular value decomposition (SVD), in which we write an $m \times n$ matrix A as $A = USV^\dagger$, where U is $m \times k$, V is $n \times k$ (hence V^\dagger is $k \times n$), $U^\dagger U = V^\dagger V = \mathbb{I}_{k \times k}$, and $S = \text{diag}(s_1, \dots, s_k)$ is a $k \times k$ real matrix with $k \leq \min(m, n)$ and each $s_j > 0$. The elements s_j are the singular values and the rows of U and V are the singular vectors. Note that $A^\dagger A = VS^2V^\dagger$ is $n \times n$ and $AA^\dagger = US^2U^\dagger$ is $m \times m$. If we define

$$F(\lambda) = \prod_{j=1}^k (\lambda - s_j^2) \quad , \quad (3.118)$$

Then

$$P(\lambda) \equiv \det(\lambda - A^\dagger A) = \lambda^{n-k} F(\lambda) \quad , \quad Q(\lambda) \equiv \det(\lambda - AA^\dagger) = \lambda^{m-k} F(\lambda) \quad . \quad (3.119)$$

Some comments:

- When $A \in \mathbb{R}$ is real, then both U and V may be chosen to be real, and we may write $A = USV^\top$.
- We may also adopt a convention where U is $m \times m$, V is $n \times n$, and S to be $m \times n$, where only the first k diagonal elements S_{ii} are the (nonzero and real) singular values. In this case, $U^\dagger U = \mathbb{I}_{m \times m}$ and $V^\dagger V = \mathbb{I}_{n \times n}$.
- For any square $n \times n$ complex matrix A we therefore have two decompositions, via JCF and SVD, viz.

$$A = PJP^{-1} = USV^\dagger \quad , \quad (3.120)$$

where J is the Jordan canonical form of A . When A is normal, $k = n$ and $U = V = P$, which says that the two decompositions are equivalent.

Example : As an example highlighting the difference between eigenvalues and singular values, consider

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} = RDL^\top = USV^\top \quad , \quad (3.121)$$

where

$$L^T = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}, \quad D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad R = \begin{pmatrix} 1 & 1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix} \quad (3.122)$$

and

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \\ 0 & 0 \end{pmatrix}, \quad S = \begin{pmatrix} \sqrt{3} & 0 \\ 0 & 1 \end{pmatrix}, \quad V^T = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 1 & 2 \\ -\sqrt{3} & \sqrt{3} & 0 \end{pmatrix}. \quad (3.123)$$

Note that U and V^T are both chosen to be real, which is a consequence of the fact that A itself is real. One can check that R is the matrix of right column eigenvectors, L^T is the matrix of left row eigenvectors, and D is the matrix of eigenvalues. Thus, the three eigenvalues are $\{\lambda_1, \lambda_2, \lambda_3\} = \{1, 1, 0\}$. One also has $L^T R = \mathbb{I}$, *i.e.* $L^T = R^{-1}$, which says that $L_i^{(a)} R_i^{(b)} = \delta^{ab}$ – the row and column eigenvectors satisfy orthonormality. Thus $R^{-1} A R = D$ and A is diagonalizable by R , which is a consequence of there being no Jordan blocks. Note that there are only two singular values, $\{s_1, s_2\} = \{\sqrt{3}, 1\}$, and that U has dimensions 3×2 while V^T has dimensions 2×3 . One can further check that $U^T U = V^T V = \mathbb{I}_{2 \times 2}$.

Had we adopted the convention where both U and V are square, we would have

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}, \quad S = \begin{pmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad V^T = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 1 & 2 \\ -\sqrt{3} & \sqrt{3} & 0 \\ -\sqrt{2} & -\sqrt{2} & \sqrt{2} \end{pmatrix}, \quad (3.124)$$

for which $U^T U = V^T V = \mathbb{I}_{3 \times 3}$. The extra zeroes in the matrix S are padding, and there are only two singular values, $\sqrt{3}$ and 1.

For this example, both the set of eigenvalues and the set of singular values are distinct. Furthermore,

$$A^\dagger A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 2 \end{pmatrix} = V S^2 V^T, \quad A A^\dagger = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix} = U S^2 U^\dagger. \quad (3.125)$$

The singular values of A are thus the positive square roots of the eigenvalues of the nonnegative definite Hermitian matrix $A^\dagger A$ (or, equivalently, of $A A^\dagger$). In general, the eigenvalues λ_j of a non-normal matrix A may not be real, even if $A \in \text{GL}(n, \mathbb{R})$ is itself real. (In this case the eigenvalues are either real or come in complex conjugate pairs.) The singular values, however, are always real and positive.

As a second example, consider the matrix

$$B = \begin{pmatrix} 1 & 1 \\ -3 & 3 \end{pmatrix} = R D L^T = U S V^T, \quad (3.126)$$

where

$$L^T = \frac{i}{2\sqrt{2}} \begin{pmatrix} +\sqrt{3} e^{-i\phi} & -1 \\ -\sqrt{3} e^{+i\phi} & 1 \end{pmatrix}, \quad D = \begin{pmatrix} 2 + i\sqrt{2} & 0 \\ 0 & 2 - i\sqrt{2} \end{pmatrix}, \quad R = \begin{pmatrix} 1 & 1 \\ \sqrt{3} e^{+i\phi} & \sqrt{3} e^{-i\phi} \end{pmatrix} \quad (3.127)$$

with $e^{i\phi} = \frac{1}{\sqrt{3}}(1 + i\sqrt{2})$ and

$$U = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad S = \begin{pmatrix} 3\sqrt{2} & 0 \\ 0 & \sqrt{2} \end{pmatrix}, \quad V^T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \quad (3.128)$$

Note that the two right eigenvectors form a complex conjugate pair, as do the two left eigenvectors. This situation pertains for every complex eigenvalue, since if $\lambda_r \in \mathbb{C}$ is an eigenvalue then so is λ_r^* . Again, since $B \in \text{GL}(2, \mathbb{R})$, the U and V matrices may be chosen real. There are two singular values $\{s_1, s_2\} = \{3\sqrt{2}, \sqrt{2}\}$. But unlike the matrix A in the previous example, B has complex eigenvalues $\lambda_{\pm} = 2 \pm i\sqrt{2}$, and the matrices L^T and R of the left (row) and right (column) eigenvectors are complex. As in the previous case, $L^T = R^{-1}$, hence $R^{-1}BR = D$, i.e. B is diagonalized by the matrix R , which is possible because there are no nontrivial Jordan blocks when it is brought to canonical form.

Selection rules : Suppose $[H, A] = 0$ where $H = H^\dagger$ and A is general. Then in the basis of H eigenstates, $\langle n|A|n \rangle = 0$ if $E_m \neq E_n$. The proof is elementary. In the eigenbasis of H ,

$$0 = \langle m|[H, A]|n \rangle = (E_m - E_n) \langle m|A|n \rangle \quad . \quad (3.129)$$

This result helps us establish that H and A can be simultaneously diagonalized, for expressed in the eigenbasis of H , the operator A must be block diagonal, where the sizes of each of the blocks correspond to the degrees of degeneracy in the eigenspectrum of H . But then a separate unitary transformation can be applied to each of these blocks in order to bring each to diagonal form, without any effect on H .

Degeneracies and nonabelian symmetries : Suppose $[H, A] = [H, B] = 0$ but $[A, B] \neq 0$, where H is a Hamiltonian, and A, B are general operators. A and B might represent different generators of a nonabelian symmetry, for example, such as the components of the total spin operator S , which satisfy $[S^\alpha, S^\beta] = i\epsilon_{\alpha\beta\gamma} S^\gamma$. We conclude that the spectrum of H must be degenerate. The reason is that in the eigenbasis of H , both A and B are block diagonal, with the dimensions of the blocks corresponding to the degree of degeneracy in the spectrum of H . If H had a nondegenerate spectrum, then A and B would also be diagonal in the H eigenbasis, which would contradict the fact that $[A, B] \neq 0$. When degeneracies are present, the A blocks and B blocks occur in the same locations, and cannot in general be simultaneously diagonalized. So nonabelian symmetries entail degenerate energy eigenvalues. We will study this in great detail in subsequent chapters.

Polar decomposition : Any matrix A may be decomposed in the form $A = HU$, where H is Hermitian and U is unitary. This is reminiscent of writing any complex number z as $z = r e^{i\theta}$. The proof is surprisingly simple. First, note that the matrix AA^\dagger is nonnegative definite. Therefore one can write $AA^\dagger = VD^2V^\dagger$ where D is a real diagonal matrix and V is unitary. Now define $H \equiv VDV^\dagger$, in which case $AA^\dagger = H^2$. This must mean $U = H^{-1}A$. We just need to check that U is unitary: $UU^\dagger = H^{-1}AA^\dagger H^{-1} = H^{-1}H^2H^{-1} = E$, so we are done.

Matrix direct product : Given the $n \times n$ matrix A and the $r \times r$ matrix Θ , the direct product matrix $M \equiv A \otimes \Theta$ is defined by its matrix elements $M_{ia,jb} = A_{ij} \Theta_{ab}$. Multiplication is a snap:

$$(A \otimes \Theta)(A' \otimes \Theta') = AA' \otimes \Theta\Theta' \quad . \quad (3.130)$$

Expressed as a single matrix, we can write the composite indices ia and jb as $\mu \equiv (i-1)r + a$ and $\nu \equiv (j-1)r + b$. Note $\mu, \nu \in \{1, \dots, nr\}$ as i, j, a, b range over their allowed values. Thus i, j refer to the

larger block structure and a, b to the structure within the blocks. The general structure is then

$$A \otimes \Theta = \begin{pmatrix} A_{11} \Theta & \cdots & A_{1n} \Theta \\ \vdots & \ddots & \vdots \\ A_{n1} \Theta & \cdots & A_{nn} \Theta \end{pmatrix}, \quad (3.131)$$

where each Θ is an $r \times r$ matrix.

As an example, consider the matrices

$$\Gamma^1 = \sigma^x \otimes E, \quad \Gamma^2 = \sigma^y \otimes E, \quad \Gamma^3 = \sigma^z \otimes \sigma^x, \quad \Gamma^4 = \sigma^z \otimes \sigma^y, \quad \Gamma^5 = \sigma^z \otimes \sigma^z. \quad (3.132)$$

We can express these in 4×4 form as

$$\Gamma^1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \Gamma^2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad \Gamma^3 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \quad (3.133)$$

and

$$\Gamma^4 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}, \quad \Gamma^5 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (3.134)$$

These matrices form a *Clifford algebra*, defined by the anticommutator $\{\Gamma^a, \Gamma^b\} = 2\delta^{ab}$. Note that for any Hamiltonian $H = \sum_a d_a \Gamma^a$ that $H^2 = \sum_a d_a^2 \mathbb{1}$. If H is of rank $2k$, then its eigenspectrum consists of two k -fold degenerate levels with $\lambda = \pm|\mathbf{d}|$.

3.4 Jokes for Chapter Three

I feel I am running out of math/physics-related jokes, and soon I may have to draw upon my inexhaustible supply of rabbi jokes.

PHILOSOPHER JOKE : Jean-Paul Sartre is sitting in a coffeeshop. A waitress comes by and asks, "What can I get for you today, Professor Sartre?" "Coffee. Black. No cream," comes the reply. A few minutes later the waitress returns. "I'm very sorry, Professor, but we are all out of cream," she says, "Can I bring your coffee with no milk instead?"

RABBI JOKE : (Actually this is something of a math riddle appropriate for children and, sadly, certain undergraduates, but it happens to involve a rabbi.) An old Jew named Shmuel died in the *shtetl* and his will gave his estate to his three sons. It specified that the eldest son should get one half, the middle son one third, and the youngest one ninth. The problem was that Shmuel's entire estate consisted of seventeen chickens, and, well, seventeen is a prime number.

So the sons met to discuss what they should do and the eldest says, "let's ask the rabbi - he is very wise and he will tell us how best to proceed." So they go to the rabbi, who starts to think and think and finally he says, "this is a very difficult problem. But I'll tell you what. Your father was a very good man who always helped out at the *shul*²¹, and it just so happens that I have an extra chicken which I am willing to donate to his estate. Now you have eighteen chickens and can execute his will properly. *Zei gezunt!*²²"

The sons were overjoyed and agreed that the rabbi was indeed wise, and generous as well. So they divided the eighteen chickens. The eldest got half, or nine chickens. The middle got a third, which is six. And the youngest got a ninth, which is two. But nine plus six plus two is seventeen, so they had a chicken left over.

So they gave it back to the rabbi.

²¹*I.e.* the local synagogue.

²²A Yiddish benediction meaning "be healthy".