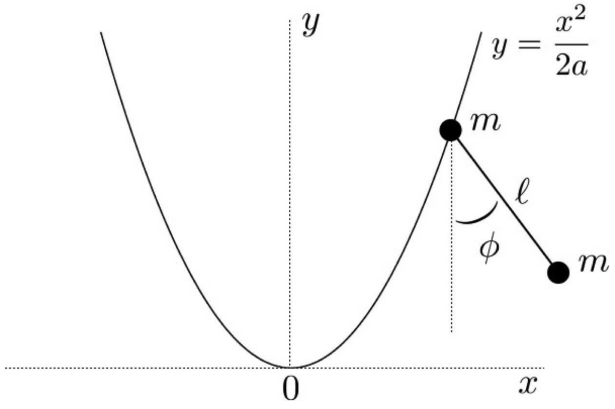
PHYSICS 200A : CLASSICAL MECHANICS
PROBLEM SET #4

[1] A mass m moves frictionlessly under the influence of gravity along the curve $y = x^2/2a$. Attached to the mass is a massless rigid rod of length ℓ, at the end of which is an identical mass m. The rod is constrained to swing in the (x, y) plane, as depicted in the figure below.



(a) Choose as generalized coordinates x and ϕ, where x is the horizontal coordinate of the upper mass. Find the kinetic energy T and potential energy U.

(b) For small oscillations, find the T and V matrices. It may be convenient to define $\Omega_1 \equiv \sqrt{g/a}$ and $\Omega_2 \equiv \sqrt{g/\ell}$.

(c) Find the eigenfrequencies of the normal modes of oscillation.

(d) Suppose $\Omega_1 = \sqrt{3}\,\Omega_0$ and $\Omega_2 = 2\,\Omega_0$, where Ω_0 has dimensions of frequency. Find the modal matrix. *Nota bene: Because the coordinates x and ϕ have different dimensions, the dimensions of the elements of $A_{\sigma i}$ may differ depending on the row index σ.*

[2] Two blocks and three springs are configured as in Fig. 1. All motion is horizontal. When the blocks are at rest, all springs are unstretched.

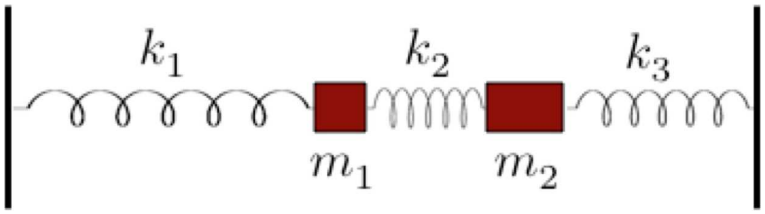


Figure 1: A system of masses and springs.

(a) Choose as generalized coordinates the displacement of each block from its equilibrium position, and write the Lagrangian.

(b) Find the T and V matrices.

(c) Suppose

$$m_1 = 2m \quad , \quad m_2 = m \quad , \quad k_1 = 4k \quad , \quad k_2 = k \quad , \quad k_3 = 2k \quad ,$$

Find the frequencies of small oscillations.

(d) Find the normal modes of oscillation.

(e) At time $t = 0$, mass #1 is displaced by a distance b relative to its equilibrium position. *I.e.* $x_1(0) = b$. The other initial conditions are $x_2(0) = 0$, $\dot{x}_1(0) = 0$, and $\dot{x}_2(0) = 0$. Find t^*, the next time at which x_2 vanishes.

[3] Investigate the small amplitude oscillations of $N + 1$ identical point masses m, labeled by $\sigma \in \{0, \ldots, N\}$, joined by N identical springs of spring constant k.

(a) Let $\{u_\sigma\}$ be the deviations of each mass from its equilibrium position. Introduce the quantities $u_{-1}(t)$ and $u_{N+1}(t)$ and the constraints $u_{-1}(t) = u_0(t)$ and $u_{N+1}(t) = u_N(t)$. Since these are holonomic they may be substituted directly into the Lagrangian. Show that the equations of motion are then given by

$$m\ddot{u}_\sigma = -k\big(2u_\sigma - u_{\sigma+1} - u_{\sigma-1}\big) \quad ,$$

where $\sigma \in \{0, \ldots, N\}$.

(b) Show that

$$u_\sigma(t) = \big(A\, e^{iq\sigma} + B\, e^{-iq\sigma}\big)\, e^{-i\omega t}$$

is a solution to the equations of motion provided that $\omega = \omega(q)$ satisfies a particular dispersion relation. Find $\omega(q)$.

(c) Now apply the boundary conditions, *i.e.* the constraint equations $u_{-1} = u_0$ and $u_N = u_{N+1}$. They should provide you with a *mode quantization condition* on the quantity q. Show that this condition is $e^{2(N+1)iq} = 1$. Then find the eigenvalues and eigenfunctions of the normal mode problem, labeled by the discrete mode index arising from the mode quantization.

(d) Show that the normal mode solutions are either even or odd under the reflection operation $u_\sigma(t) \leftrightarrow u_{N-\sigma}(t)$.

(e) Identify the zero eigenmode resulting from overall translational invariance.

[4] Consider a linear chain of $N + 2$ mass points connected by springs and subject to fixed end boundary conditions: $u_0 = u_{N+1} = 0$. The allowed motion is one-dimensional, along the direction of the chain.

(a) Following the method used in problem **[3]**, verify the normal modes are of the form

$$u_\sigma^{(j)}(t) = C_j\, \sin\Big(\frac{\pi j \sigma}{N+1}\Big)\, \cos(\omega_j t + \delta_j)$$

where

$$\omega_j = 2\sqrt{\frac{k}{m}}\,\left|\sin\Big(\frac{j\pi}{2N+2}\Big)\right|$$

and $j \in \{1, \ldots, N\}$.

(b) Verify the orthonormality of the normal modes,

$$\psi^{(j)}_\sigma = \sqrt{\frac{2}{(N+1)\,m}}\,\sin\Big(\frac{\pi j \sigma}{N+1}\Big) \quad .$$

(c) Let $z_\ell = \exp\big(2\pi i \ell/M\big)$ with $\ell \in \{0, \ldots, M-1\}$ be the complex $M^{\rm th}$ roots of unity. Verify, for any integer p, that

$$\sum_{\ell=0}^{M-1} z_\ell^p = M\,\delta_{p\,,\,0\,\mathsf{mod}\,M} \quad .$$

(d) Compare the eigenspectrum with that from problem **[3]** and comment on the differences.

[5] *For the brave only! I will be impressed if you can solve this. (50 quatloos extra credit)* In equilibrium, a collection of six identical springs k and four identical masses m are arranged in a perfect tetrahedron. One way to identify the vertices of a tetrahedron is to inscribe it in a cube of side length $2a$. With the origin at the center, the coordinates of the vertices may be taken as $(-a, a, a)$, $(a, -a, a)$, $(a, a, -a)$, and $(-a, -a, -a)$. The side length of the tetrahedron is then $b = 2\sqrt{2}a$.

(a) Find all the zero modes and provide explicit expressions for their eigenvectors $\psi^{(i)}_\sigma$. How many zero modes should there be?

(b) Find numerically or analytically all the remaining normal modes and their eigenfrequencies.

(c) The tetrahedral group T_d, *i.e.* the discrete group of symmetry operations acting on a tetrahedron, has 24 elements (arranged among five conjugacy classes) and five irreducible representations ('irreps'). The A_1 and A_2 irreps are each one-dimensional, the E irrep is two-dimensional, and the T_1 and T_2 irreps are each three-dimensional. (If you sum the squares of the dimensions of the irreps, you always get the order of the group, *i.e.* the number of group elements. Lo and behold: $1^2 + 1^2 + 2^2 + 3^2 + 3^2 = 24$.) Based on the degeneracy of your finite frequency normal modes, identify what possible irreps they might belong to. (See appendices for some notes on the discrete group theory involved.)

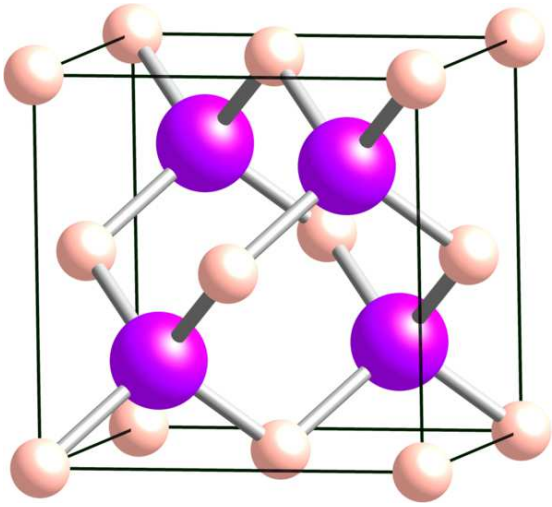


Figure 2: The zincblende structure is two interpenetrating FCC lattices separated by $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$, where a is the side length of the cube.

0.1 Appendix I : The Tetrahedral Group, T_d

Many III-V semiconductors, such as GaAs, have a zincblende crystal structure, shown in fig. 2. The zincblende structure AB consists of two interpenetrating FCC lattices A and B, separated by $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$, where a is the side length of the cube. As fig. 2 shows, the B sublattice sites within the cube form a tetrahedron. The crystallographic point group for this structure is T_d, the tetrahedral group. A noteworthy feature is that the zincblende structure has no center of inversion symmetry.

If all the atoms are identical, *i.e.* A = B, then we get the diamond structure, which is the structure of silicon and of course carbon diamond. The diamond lattice is inversion symmetric, with the point of inversion halfway between the A and B sublattice sites. The point group for diamond is the cubic group O_h. This might be surprising upon staring at the structure for a time, because it doesn't possess a cubic symmetry. However, the space group for diamond is *non-symmorphic*, which means that the certain point group operations must be combined with a *glide plane* or *screw axis* operation in order to leave the structure invariant. A glide plane operation is a reflection in a plane, followed by a translation parallel to that plane. A screw axis operation is a rotation about an axis followed by translation along that axis. The diamond structure has a glide plane.

The group T_d has 24 elements; these are listed in table 1. These are arranged in five group *classes*. One class is the identity, E. Another class consists of three 180° rotations about the $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$ axes, respectively. A third classs, with eight elements, consists of rotations by $\pm 120°$ about each of the four body diagonals. This amounts to 12 group operations, all of which are proper rotations. The remaining 12 elements involve the inversion operator, I, which takes (x, y, z) to $(-x, -y, -z)$, and are therefore improper rotations, with determinant -1. These elements fall into two classes, one of which consists of 180° rotations about

diagonals parallel to one of the sides of the cube (*e.g.* the line $y = x$, $z = 0$), followed by inversion. The last class consists of rotations by $\pm 90°$ about $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$, also followed by an inversion.

0.1.1 Tetrahedral *vs.* Octahedral Symmetry

In the case of the octahedral group, O, the inversion operation is not included in the last two classes, and they are written as $6C_2$ and $6C_4$, respectively. The symmetry operations of O are depicted in fig. 4. The groups O and T_d are isomorphic. Completing either of them by adding in the inversion operator I results in the full cubic group, O_h, which has 48 elements.

While the groups T_d and O are isomorphic, the symmetry of particular basis functions may differ between the two groups. Consider, for example, the function $\varphi = xyz$. It is easy to see from table 1 that every element of T_d leaves φ invariant. Within O, however, the classes $6\sigma_d$ and $6S_4$ are replaced by $6C_2$ and $6C_4$ when the inversion operation is removed. Each element of these classes then takes φ to $-\varphi$. Thus, within T_d, the function $\varphi = xyz$ is indistinguishable from unity, and it transforms according to the trivial A_1 representation. Within O, however, φ is distinguishable from 1 because φ reverses sign under the operation of all group elements in classes $6C_2$ and $6C_4$.

In O, the triplets of basis functions $\{x, y, z\}$ and $\{yz, zx, xy\}$ belong to different representations (T_1 and T_2, respectively). In T_d, however, they must belong to the same representation, since one set of functions is obtained from the other by dividing into xyz:

Table 1: Table of elements and classes for T_d

class	x	y	z	$g \in \mathrm{O}(3)$	class	x	y	z	$g \in \mathrm{O}(3)$
E	x	y	z	1	$6\sigma_\mathrm{d}$	$-y$	$-x$	z	$IR_{[110]}(\pi)$
$3C_2$	x	$-y$	$-z$	$R_{[100]}(\pi)$	$(6IC_2)$	y	x	z	$IR_{[1\bar{1}0]}(\pi)$
	$-x$	y	$-z$	$R_{[010]}(\pi)$		$-z$	y	$-x$	$IR_{[101]}(\pi)$
	$-x$	$-y$	z	$R_{[001]}(\pi)$		z	y	x	$IR_{[\bar{1}01]}(\pi)$
$8C_3$	z	x	y	$R_{[111]}(+\frac{2\pi}{3})$		x	$-z$	$-y$	$IR_{[011]}(\pi)$
	y	z	x	$R_{[111]}(-\frac{2\pi}{3})$		x	z	y	$IR_{[01\bar{1}]}(\pi)$
	z	$-x$	$-y$	$R_{[1\bar{1}1]}(+\frac{2\pi}{3})$	$6S_4$	$-x$	z	$-y$	$IR_{[100]}(+\frac{\pi}{2})$
	$-y$	$-z$	x	$R_{[1\bar{1}1]}(-\frac{2\pi}{3})$	$(6IC_4)$	$-x$	$-z$	y	$IR_{[100]}(-\frac{\pi}{2})$
	$-z$	x	$-y$	$R_{[11\bar{1}]}(+\frac{2\pi}{3})$		$-z$	$-y$	x	$IR_{[010]}(+\frac{\pi}{2})$
	y	$-z$	$-x$	$R_{[11\bar{1}]}(-\frac{2\pi}{3})$		z	$-y$	$-x$	$IR_{[010]}(-\frac{\pi}{2})$
	$-z$	$-x$	y	$R_{[1\bar{1}\bar{1}]}(+\frac{2\pi}{3})$		y	$-x$	$-z$	$IR_{[001]}(+\frac{\pi}{2})$
	$-y$	z	$-x$	$R_{[1\bar{1}\bar{1}]}(-\frac{2\pi}{3})$		$-y$	x	$-z$	$IR_{[001]}(-\frac{\pi}{2})$

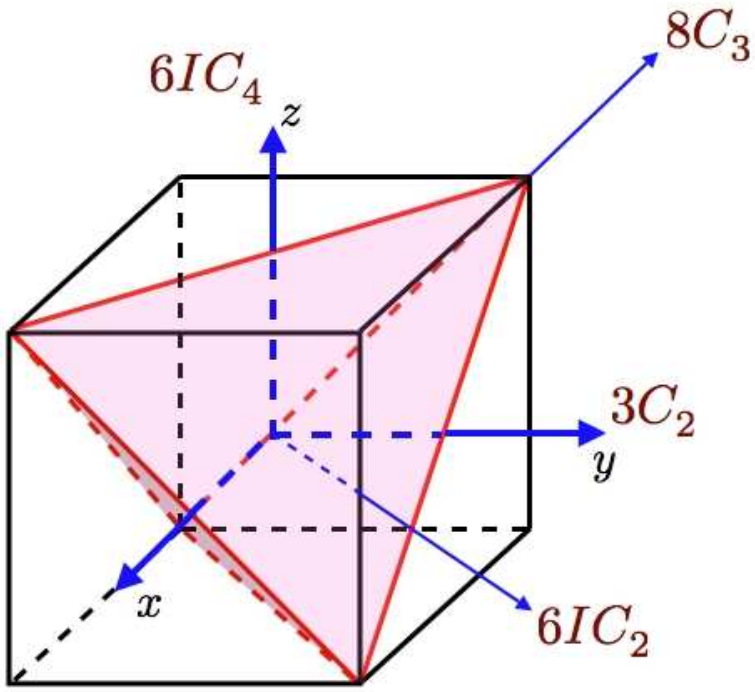


Figure 3: Symmetry operations of the tetrahedral group, T_d. The group conjugacy classes C_2, C_3, IC_2, and IC_4 are defined in the appendix.

Table 2: Irreducible representations and basis functions for T_d and O

$\Gamma^{(i)}$	d	basis functions φ^i_μ for T_d	basis functions φ^i_μ for O
$\Gamma^{(1)} = \mathrm{A}_1$	1	1 or xyz	1
$\Gamma^{(2)} = \mathrm{A}_2$	1	$x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)$	xyz
$\Gamma^{(3)} = \mathrm{E}$	2	$\left\{\sqrt{3}\,(x^2-y^2)\,,\, 2z^2-x^2-y^2\right\}$	$\left\{\sqrt{3}\,(x^2-y^2)\,,\, 2z^2-x^2-y^2\right\}$
$\Gamma^{(4)} = \mathrm{T}_1$	3	$\left\{x\,(y^2-z^2)\,,\, y\,(z^2-x^2)\,,\, z\,(x^2-y^2)\right\}$	$\left\{x,\ y,\ z\right\}$
$\Gamma^{(5)} = \mathrm{T}_2$	3	$\left\{x\,,\, y\,,\, z\right\}$ or $\left\{yz\,,\, zx\,,\, xy\right\}$	$\left\{yz\,,\, zx\,,\, xy\right\}$

$x = (xyz)/(yz)$, *et cyc.* But xyz transforms as the identity, so 'polar' and 'axial' vectors belong to the same representation of T_d.

Finally, let's think about how O differs from O_h. Consider the function

$$\varphi = xyz \cdot \left(x^4\,(y^2-z^2) + y^4\,(z^2-x^2) + z^4\,(x^2-y^2)\right) \quad . \tag{1}$$

One can check that this function is left invariant by every element of O. It therefore transforms according to the A_1 representation of O. But it reverses sign under parity, so within the full cubic group O_h, it transforms according to separate one-dimensional representation. Note that φ transforms according to the A_2 representation of T_d.

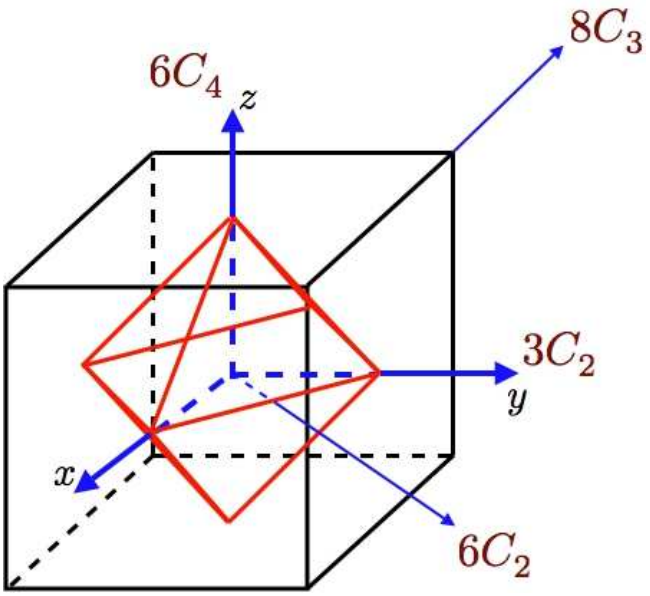


Figure 4: Symmetry operations of the octahedral group, O.

0.2 Appendix II : Elements of Discrete Group Theory

We are concerned with representations of crystallographic point groups. A representation Γ of a discrete group G is a mapping

$$\Gamma\colon G \longrightarrow \mathrm{GL}(n, \boldsymbol{C}) \quad . \tag{2}$$

i.e. the group G is mapped onto the space of complex matrices, such that the group multiplication table is preserved. Typically we shall be concerned with *unitary* representations since the context here is quantum mechanics. A representation is *reducible* if it can be brought to block diagonal form by a similarity transformation. We label the *irreducible* representations with superscripts on Γ. Thus, $\Gamma^{(i)}(g)_{\mu\nu}$ is the $(\mu\nu)$ element of the matrix which represents the group element g in the i^{th} irreducible representation.

0.3 Great Orthogonality Theorem

The Great Orthogonality Theorem states that

$$\sum_g \Gamma^{(i)}(g)^*_{\mu\nu}\, \Gamma^{(j)}(g)_{\alpha\beta} = \frac{h}{d_i}\, \delta_{ij}\, \delta_{\mu\alpha}\, \delta_{\nu\beta} \tag{3}$$

where the $\Gamma^{(i)}$ are inequivalent, irreducible, unitary representations of a group, and d_i is the dimension (rank) of $\Gamma^{(i)}$ and h is the order (number of elements) of the group. The sum of

Table 3: Character table for the tetrahedral group, T_d

T_d	E	$8C_3$	$3C_2$	$6\sigma_{\rm d}$	$6S_4$
Γ_1 (A_1)	1	1	1	1	1
Γ_2 (A_2)	1	1	1	−1	−1
Γ_3 (E)	2	−1	2	0	0
Γ_4 (T_1)	3	0	−1	−1	1
Γ_5 (T_2)	3	0	−1	1	−1

the squares of the dimensions of the irreducible representations is equal to the number of elements in the group:

$$\sum_i d_i^2 = h \quad . \tag{4}$$

0.4 Group Characters

Two group elements g_1 and g_2 are said to be *conjugate* if there exists another group element g_3 such that $g_1 = g_3^{-1}\, g_2\, g_3$. Conjugacy is a transitive relation. The collection of all mutually conjugate elements is a *conjugacy class*, $\mathcal{C}$.

The character of a group element g in the representation $\Gamma^{(i)}$ is

$$\chi^{(i)}(g) = {\rm Tr}\,\Gamma^{(i)}(g) = \sum_{\mu=1}^{d_i} \Gamma^{(i)}(g)_{\mu\mu} \quad . \tag{5}$$

As the trace is invariant under a similarity transformation, the character is the same for all elements within a given class.

The number of conjugacy classes of a group is equal to the number of irreducible representations. Thus, the *character table* of a group, where the rows correspond to irreducible representations and the columns to conjugacy classes, is a square matrix. The columns of this matrix are mutually orthogonal, satisfying

$$\sum_{\mathcal{C}} N_{\mathcal{C}}\, \chi^{(i)}(\mathcal{C})^*\, \chi^{(j)}(\mathcal{C}') = h\, \delta_{ij} \quad , \tag{6}$$

where $N_{\mathcal{C}}$ is the number of elements in class $\mathcal{C}$. The columns are also orthogonal:

$$\sum_i \chi^{(i)}(\mathcal{C})^*\, \chi^{(i)}(\mathcal{C}') = \frac{h}{N_{\mathcal{C}}}\, \delta_{\mathcal{C}\mathcal{C}'} \quad . \tag{7}$$

As an exercise, one can verify these relations for the character table of T_d, given in table 3.

0.5 Decomposition of Reducible Representations

A reducible representation may be brought to block diagonal form, where each irreducible $d_i \times d_i$ block occurs a_i times. Clearly

$$\chi(g) = \sum_j a_j \, \chi^{(j)}(g) \quad , \tag{8}$$

which, using the row orthogonality of the character table, yields

$$a_j = h^{-1} \sum_g \chi(g)^* \, \chi^{(j)}(g) \quad . \tag{9}$$

Suppose we take a product of two irreducible representations, $\Gamma^{(i)}$ and $\Gamma^{(j)}$. The matrix corresponding to a group element g then has a composite form,

$$\Gamma^{(i\times j)}(g)_{\mu\alpha,\nu\beta} = \Gamma^{(i)}(g)_{\mu\nu} \, \Gamma^{(j)}(g)_{\alpha\beta} \quad . \tag{10}$$

and therefore

$$\chi^{(i\times j)}(g) = \chi^{(i)}(g) \, \chi^{(j)}(g) \quad . \tag{11}$$

Thus, we can decompose the product representation, using the orthogonality of the rows of the character table:

$$\begin{aligned} \Gamma^{(i)} \times \Gamma^{(j)} &= \sum_k a_{ijk} \, \Gamma^{(k)} \\ a_{ijk} &= h^{-1} \sum_{\mathcal{C}} N_{\mathcal{C}} \, \chi^{(i)}(\mathcal{C}) \, \chi^{(j)}(\mathcal{C}) \, \chi^{(k)}(\mathcal{C})^* \end{aligned} \tag{12}$$

0.5.1 Example

As an example, consider the tensor product $\Gamma_4 \times \Gamma_4$. We have

$$\Gamma_4 \times \Gamma_4 = \sum_k a_{44k} \, \Gamma^{(k)} \quad , \tag{13}$$

where

$$a_{44k} = \frac{1}{24} \Big\{ 9 \, \chi^{(k)}(E) + 3 \, \chi^{(k)}(C_2) + 6 \, \chi^{(k)}(\sigma_{\rm d}) + 6 \, \chi^{(k)}(S_4) \Big\} \quad . \tag{14}$$

Using Table 3,

$$\begin{aligned} a_{441} &= \tfrac{1}{24}\big(9 + 3 + 6 + 6\big) = 1 \\ a_{442} &= \tfrac{1}{24}\big(9 + 3 - 6 - 6\big) = 0 \\ a_{443} &= \tfrac{1}{24}\big(9 \cdot 2 + 3 \cdot 2 + 6 \cdot 0 + 6 \cdot 0\big) = 1 \\ a_{444} &= \tfrac{1}{24}\big(9 \cdot 3 - 3 - 6 + 6\big) = 1 \\ a_{445} &= \tfrac{1}{24}\big(9 \cdot 3 - 3 + 6 - 6\big) = 1 \end{aligned} \tag{15}$$

and we conclude

$$\Gamma_4 \times \Gamma_4 = \Gamma_1 \oplus \Gamma_3 \oplus \Gamma_4 \oplus \Gamma_5 \quad . \tag{16}$$

Note that the dimension of the LHS is $3^2 = 9$ and that of the RHS is $1 + 2 + 3 + 3 = 9$.

0.6 Projection Operators

Let P_g be an operator which effects the group operation g, and let $\varphi_\nu^{(i)}$ be a basis function belonging to the $\nu^{\rm th}$ row of the $i^{\rm th}$ irreducible representation. By definition,

$$P_g\,\varphi_\nu^{(i)} = \sum_{\mu=1}^{d_i} \varphi_\mu^{(i)}\,\Gamma^{(i)}(g)_{\mu\nu} \quad . \tag{17}$$

Using the Great Orthogonality Theorem, we obtain

$$\begin{aligned} \sum_g \Gamma^{(j)}(g)^*_{\alpha\beta}\,P_g\,\varphi_\nu^{(i)} &= \sum_{\mu=1}^{d_i} \varphi_\mu^{(i)} \sum_g \Gamma^{(i)}(g)_{\mu\nu}\,\Gamma^{(j)}(g)^*_{\alpha\beta} \\ &= \frac{h}{d_j}\,\delta_{ij}\,\delta_{\nu\beta}\,\varphi_\alpha^{(i)} \quad . \end{aligned} \tag{18}$$

Therefore we can define a projection operator,

$$\Pi^{(j)}_{\alpha\beta} = \frac{d_i}{h} \sum_g \Gamma^{(j)}(g)^*_{\alpha\beta}\,P_g \quad , \tag{19}$$

which annihilates any basis function $\varphi_\nu^{(i)}$ unless $i = j$ and $\nu = \beta$, *i.e.* unless the basis function belongs to the $\beta^{\rm th}$ row of $\Gamma^{(j)}$. Taking the trace, we obtain the projector onto $\Gamma^{(j)}$:

$$\Pi^{(j)} = \sum_{\alpha=1}^{d_j} \Pi^{(j)}_{\alpha\alpha} = \frac{d_j}{h} \sum_g \chi^{(j)}(g)^*\,P_g \quad . \tag{20}$$

As an example, let us evaluate the projection of a function $\psi(x, y, z)$ onto the Γ_3 representation of T_d, using the Tables 1 and 3. We find

$$\begin{aligned} \Pi^{(3)}\psi(x,y,z) =& \tfrac{1}{6}\Big[\psi(x,y,z) + \psi(x,-y,-z) + \psi(-x,y,-z) + \psi(-x,-y,z)\Big] \\ &- \tfrac{1}{12}\Big[\psi(z,x,y) + \psi(y,z,x) + \psi(z,-x,-y) + \psi(-y,-z,x) \\ &+ \psi(-z,x,-y) + \psi(y,-z,-x) + \psi(-z,-x,y) + \psi(-y,z,-x)\Big] \end{aligned} \tag{21}$$

We then find

$$\begin{aligned} \Pi^{(3)}x^2 &= \tfrac{1}{3}(2x^2 - y^2 - z^2) \\ \Pi^{(3)}(x^2 - y^2) &= x^2 - y^2 \\ \Pi^{(3)}xy &= 0 \quad , \end{aligned} \tag{22}$$

etc.

Table 4: Standard Notation for Point Group Operations

Operation	Description
E	identity
C_n	rotation through $2\pi/n$ about some axis $\hat{\boldsymbol{n}}$; operator equivalent: $e^{2\pi i \hat{\boldsymbol{n}}\cdot\boldsymbol{J}/\hbar}$ where $\boldsymbol{J} = \boldsymbol{F} + \boldsymbol{S}$
I	inversion ($\boldsymbol{r} \to -\boldsymbol{r}$) ; leaves spinor coordinates invariant
σ	C_2 rotation followed by reflection in plane perpendicular to the axis of rotation ; equivalent to IC_2 or $C_2\,I$
$\sigma_{\rm h}$	reflection in a 'horizontal' plane perpendicular to a principal axis of symmetry
$\sigma_{\rm v}$	reflection in a 'vertical' plane which contains a principal axis of symmetry
$\sigma_{\rm d}$	reflection in a 'diagonal' plane containing a principal axis of symmetry and which bisects the angle between two twofold axes perpendicular to a principal axis
S_n	improper rotation through $2\pi/n$, *i.e.* a C_n rotation followed by reflection in the plane perpendicular to the rotation axis ($I = S_2$)
$\bar{E}$	spinor rotation through 2π ; $\bar{E} = e^{2\pi i \hat{\boldsymbol{n}}\cdot\boldsymbol{S}}$ ($S = \frac{1}{2}$) ; leaves spatial coordinates (x, y, z) invariant
$\bar{g}$	any point group operation g followed by $\bar{E}$

Table 5: Character table for the double group of T_d

$T_d \times \{E, \bar{E}\}$	E	$\bar{E}$	$8C_3$	$8\bar{E}C_3$	$3C_2+$ $3\bar{E}C_2$	$6\sigma_{\rm d}+$ $6\bar{E}\sigma_{\rm d}$	$6S_4$	$6\bar{E}S_4$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	−1	−1	−1
Γ_3	2	2	−1	−1	2	0	0	0
Γ_4	3	3	0	0	−1	−1	1	1
Γ_5	3	3	0	0	−1	1	−1	−1
Γ_6	2	−2	1	−1	0	0	$\sqrt{2}$	$-\sqrt{2}$
Γ_7	2	−2	1	−1	0	0	$-\sqrt{2}$	$\sqrt{2}$
Γ_8	4	−4	−1	1	0	0	0	0

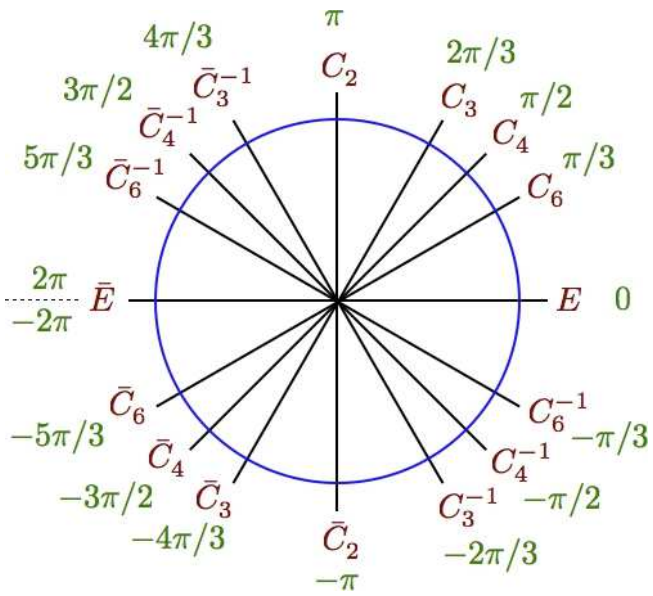


Figure 5: Schematic diagram of (common axis) double group rotation operators. The operation of C_2, for example, amounts to a 90° counterclockwise rotation on the diagram. Taken from Fig. 1 of Koster *et al.* (1963).

0.7 Crystallographic Point Groups

Table 4 lists the standard abbreviations for elements of crystallographic point groups. The group operations act on electron wavefunctions, which are spinor functions of the spatial coordinates $\boldsymbol{r} = (x, y, z)$:

$$\vec{\psi}(\boldsymbol{r}) = \begin{pmatrix} \psi_\uparrow(\boldsymbol{r}) \\ \psi_\downarrow(\boldsymbol{r}) \end{pmatrix} \quad . \tag{23}$$

Rotations by an angle θ about an axis $\hat{\boldsymbol{n}}$ are represented by the unitary operator

$$U(\theta; \hat{\boldsymbol{n}}) = e^{i\theta \hat{\boldsymbol{n}} \cdot \boldsymbol{J}/\hbar} \quad , \tag{24}$$

where $\boldsymbol{J} = \boldsymbol{F} + \boldsymbol{S}$ is the sum of orbital ($\boldsymbol{F}$) and intrinsic spin ($\boldsymbol{S}$) angular momenta. For crystallographic point groups, $\theta = 2\pi/n$ where $n = 1$, 2, 3, 4, or 6.

When spin is neglected, the group is the usual point group. With spin, we must include the operation $\bar{E}$ which reverses the sign of the spinor but leaves $\boldsymbol{r}$ unchanged. For $S = \frac{1}{2}$ this is equivalent to a rotation by 2π about any axis; $\bar{E}^2 = E$. The resulting group is called the *double group*. A schematic description of proper rotations within a double group is shown in Fig. 5. If g is an element of the point group, then we define $\bar{g} = \bar{E}g$, which is an element of the double group. Note that, for rotations about the same axis,

$$\begin{aligned} C_2\, C_2 &= C_1 = \bar{E} \\ \sigma_{\rm h}\, \sigma_{\rm h} &= \bar{E} \\ \bar{\sigma}_{\rm h}\, \sigma_{\rm h} &= E \quad , \end{aligned} \tag{25}$$

et cetera. Thus, $\sigma_{\mathrm{h}}^{-1} = \bar{\sigma}_{\mathrm{h}}$.

Most of the time, for each class C of a point group there will be a unique corresponding class $\bar{C}$ of the double group. The exception is when $n = 2$. In that case, C and $\bar{C}$ can be joined to form a single class $C + \bar{C}$ if any twofold axis in C is bilateral. A bilateral axis is one for which there exists a twofold rotation about an axis in the plane perpendicular to the first axis. The same exception holds for improper rotations. In such cases, the number of classes of the double group is less than twice the number of classes for the point group. As an example, consider the tetrahedral group T_d. There are three twofold axis: $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$. All are bilateral because a rotation by π about $\hat{\boldsymbol{x}}$ reverses the direction of both $\hat{\boldsymbol{y}}$ and $\hat{\boldsymbol{z}}$, *etc.* Accordingly, in the character table for the double group of T_d, given in Table 5, the classes C_2 and $\bar{C}_2$ are adjoined, as are σ_d and $\bar{\sigma}_d$.

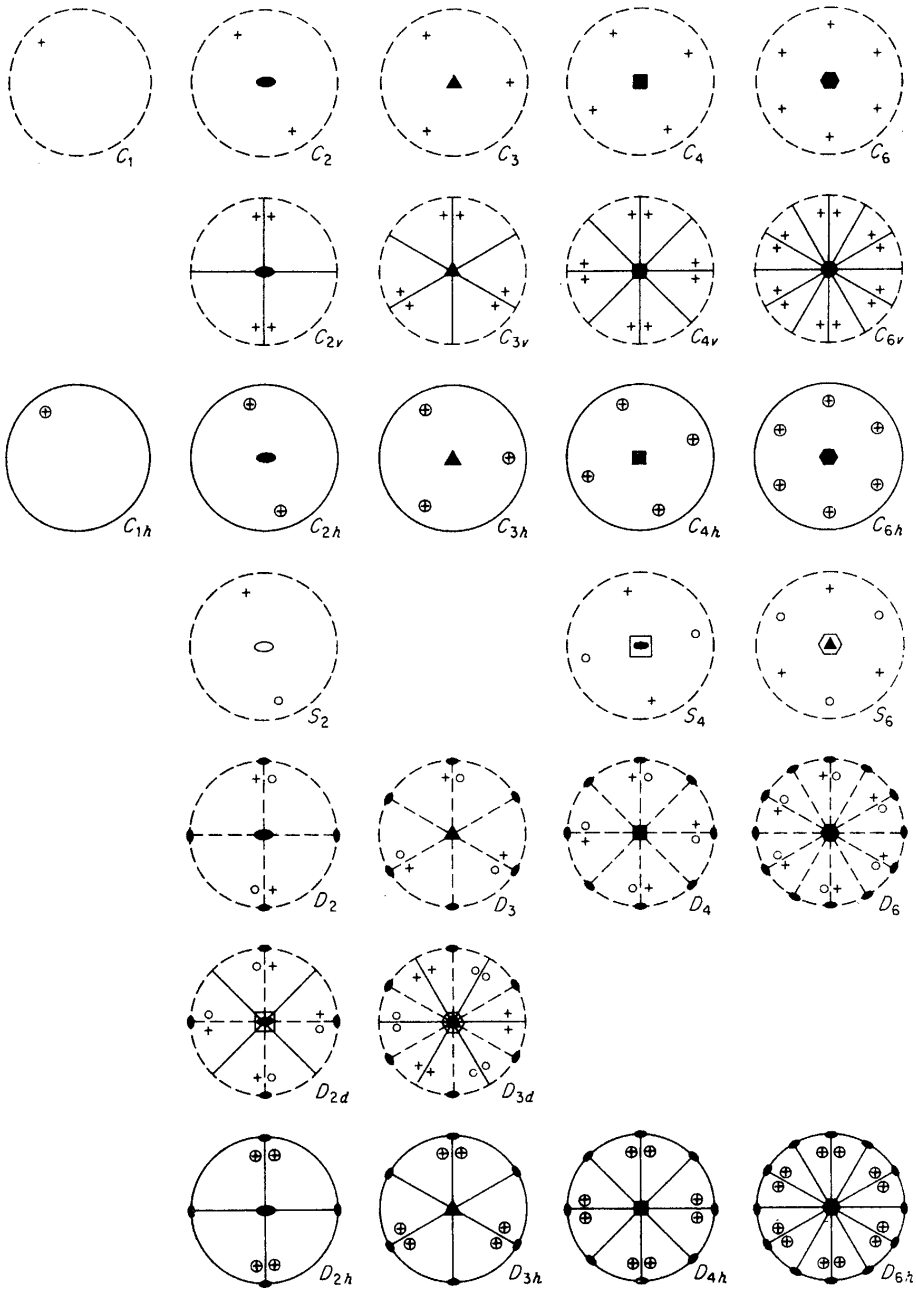


Figure 6: Stereographic projections of simple point groups. Copied from Table 4.2 of M. Tinkham, *Group Theory and Quantum Mechanics*.