Last time we did all the orthogonality and completeness relations for matrix elements of irreps and for the characters of irreps, except for the inverse orthogonality (column orthogonality) of character tables. For this see p. 16, notes of 3/12/03.

For reference, the character table of $C_{3v}$:

<table>
<thead>
<tr>
<th></th>
<th>${E}$</th>
<th>${R_1, R_2}$</th>
<th>${R_3, R_4, R_5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>-1</td>
<td>0</td>
</tr>
</tbody>
</table>

Here I have labelled the irreps by their standard designations $A_1, A_2, E$ instead of $\tau = 1, 2, 3$. (A irreps are 1D, E are 2D.)

There are quite a few more topics in Ch. 4 of the book on general aspects of representation theory, including:

1. Projection operators
2. Direct product representations
3. Clebsch-Gordan coefficients
4. Irreducible tensor operators and the Wigner-Eckart theorem
5. Reduction upon restriction to a subgroup.
Homework problem 2 for this week: Find character table of $D_4$.

Since $\# \text{irreps} = \# \text{classes}$, let's first find the number of classes.

Remind you, the group elements. $D_4$ = group of proper covering rotations of a square.

\[
\begin{align*}
\hat{n}_1 & \quad \hat{n}_5 \\
\hat{n}_2 & \quad \hat{n}_7 \\
\hat{n}_3 & \quad \hat{n}_4
\end{align*}
\]

$E$ = identity

$R_1 = R(\hat{x}, \pi/2)$

$R_2 = R(\hat{x}, \pi)$

$R_3 = R(\hat{x}, 3\pi/2)$

$R_4 = R(\hat{y}_4, \pi)$

$R_5 = R(\hat{y}_5, \pi)$

$R_6 = R(\hat{y}_6, \pi)$

$R_7 = R(\hat{y}_7, \pi)$

\[\begin{align*}
\text{Use} & \\
R_0 \cdot R(\hat{x}, 0) R_0^{-1} = R(R_0 \hat{x}, 0) & \text{valid for } R_0, R \in \text{SO}(3).
\end{align*}\]

\{E\} is a class by itself.

\{R_2\} is a class by itself; there are other notio with the same angle $\pi$ ($R_4, R_5, R_6, R_7$) but there is no rotation in $D_4$ that maps the axis of $R_2$ ($\hat{x}$) into the axis of one of the others ($\hat{y}_4, \hat{y}_5, \hat{y}_6, \hat{y}_7$).

\{R_1, R_3\} are in same class, since $R_3 = R(-\hat{x}, \pi/2)$, and any of $R_4 - R_7$ map $\hat{x}$ into $-\hat{x}$.

\{R_4, R_6\} are in same class because angles the same and because $R_1 \hat{y}_4 = \hat{y}_6$.

But $R_5$ does not belong to this class because no rotation (in $D_4$) maps $\hat{y}_4$ into $\hat{y}_5$ or $\hat{y}_6$ into $\hat{y}_5$.

However, \{R_5, R_7\} do belong to same class.

Hence, 5 classes $\Rightarrow$ 5 irreps.
Label the columns of the char. table by classes, the rows by irreps. The trivial irrep is $r=1$, it has $d_r=1$.

<table>
<thead>
<tr>
<th></th>
<th>${E}$</th>
<th>${R_2}$</th>
<th>${R_1, R_3}$</th>
<th>${R_4, R_6}$</th>
<th>${R_5, R_7}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
</tbody>
</table>

Now we know $\sum_{r=1}^{5} d_r^2 = 1 + \sum_{r=2}^{5} d_r^2 = 8$, or $d_2^2 + d_3^2 + d_4^2 + d_5^2 = 7$.

The only solution in integers is $d_2 = d_3 = d_4 = 1$, $d_5 = 2$. $1^2 + 1^2 + 1^2 + 2^2 = 7$.

Note also, $d_r = tr E^{(r)}$, so we get the first column.

Now let $x = x(R_2)$
$y = x(R_1, R_3)$ running across some row of the char. table
$z = x(R_4, R_6)$ of one of the $1D$ irreps ($r=2, 3, 4$).
$t = x(R_5, R_7)$

This row must be orthogonal to the 1st row (weighting the scalar product by #c). Thus, we must have...

$$\sum_{c} (hc) x^{(c)} x^{(c)} = 1 \cdot 1 \cdot 1 + 1 \cdot 1 \cdot x + 2 \cdot 1 \cdot y + 2 \cdot 1 \cdot z + 2 \cdot 1 \cdot t, \quad r=2, 3, 4$$

= $0$ (demand), i.e.

$$1 + x + 2y + 2z + 2t = 0.$$

We also know $x = \pm 1$,
$y = \pm 1, \pm i$,
$z = \pm 1$,
$t = \pm 1$.

Since if $n = \text{order of } g \in G$, then for a 1-D irrep, $X(g) = n$-th root of 1.
Thus there are $2 \times 4 \times 2 \times 2 = 32$ choices for $x,y,z,t$.

But we can show that the imaginary choices for $y$ are impossible, since the other terms in the expression $1 + x + 2(y+z+t)$ are purely real and the sum must be zero. So there are only 16 choices. List them all, and form the (weighted) scalar product with the trivial rep.

<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>t</th>
<th>scalar prod. = $1 + x + 2(y+z+t)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>8 \leftarrow \text{trivial rep.}</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>4 \leftarrow 0 \leftarrow</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>4 \leftarrow 0 \leftarrow</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0 \leftarrow 0 \leftarrow</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-2 \leftarrow 2 \leftarrow</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-2 \leftarrow 2 \leftarrow</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-2 \leftarrow 2 \leftarrow</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-2 \leftarrow 2 \leftarrow</td>
</tr>
</tbody>
</table>

There are only 3 cases where the scalar product is 0. These must be rows for $r = 2, 3, 4$. Thus we have all the 1D reps.

<table>
<thead>
<tr>
<th></th>
<th>{E}</th>
<th>{R_2}</th>
<th>{R_1,R_3}</th>
<th>{R_4,R_5}</th>
<th>{R_6,R_7}</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Now the last row has to be orthogonal to the first four, i.e., if we write

\[ 2 \ x \ y \ z \ t \]

for last row, then

\[ 2 + x + 2(y+z+t) = 0 \]
\[ 2 + x + 2(y-z-t) = 0 \]
\[ 2 + x + 2(-y+z-t) = 0 \]
\[ 2 + x + 2(-y-z+t) = 0 \]

The equations imply \( y = z = t = 0, \ x = -2 \). Last row is

\[ 2 \ -2 \ 0 \ 0 \ 0 \]

Can check the table, must have \[ \sum_C (\#C) |X''(C)|^2 = \#G \].

Now let's do a physical application. We're not through with the general theory, but we'll come back to it and develop it as we need it. We'd like to do a problem in molecular vibrations, but that's too hard for now so let's take a simpler problem.

---

\[ \text{mass shown in equilibrium position.} \]

---

\[ \text{mass shown in equilibrium position.} \]
This system is 2D only, we ignore motion in the z-direction.
(That's so we can use \( c_{3y} \) instead of \( D_{3y} \).)

All vectors are 2D, e.g. \( \vec{r} = (x, y) = (x_1, x_2) \).

The mass \( m \) is attached by 3 identical springs to the vertices of an equilateral triangle. Pegs or nails are at the vertices, at locations

\[
\begin{align*}
\vec{c}_1 &= a(0, 1) & \text{a = distance from origin to one of the vertices.} \\
\vec{c}_2 &= a\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \\
\vec{c}_3 &= a\left(+\frac{\sqrt{3}}{2}, -\frac{1}{2}\right).
\end{align*}
\]

Let \( \vec{x} = (x, y) \) be the position of the mass. Problem: find \( \vec{x}(t) \) for small displacements.

This system has 2 degrees of freedom, the configuration space is \((x, y)\)-space, \( = \mathbb{R}^2 \). (the plane, although we're only interested in small \( x, y \)).

The Lagrangian is \( L = T - V \),

\[
T = \text{kinetic energy} = \frac{m}{2} \sum_{i=1}^{2} \dot{x}_i^2 \\
V = \text{some function } V(\vec{x}).
\]

Let \( V = V(\vec{x}) \) = the potential energy of a spring \( k = k_f \).

Now it's intuitively obvious that the potential energy is invariant under \( C_{3y} \), that is, if \( R_n \in C_{3y}, n = 0, 1, \ldots, 5, \) \( (R_0 = E) \) then

\[
(\tilde{R}_n V)(\vec{x}) = V(R_n^{-1} \vec{x}) = V(\vec{x})
\]

\( \uparrow \) induced transformation \( \uparrow \) because we "see" that \( \uparrow \) defn of induced transformation \( V \) is invariant.
Here $R_n$ stands for the 2x2 representation of $C_{3v}$ acting on the $x,y$ plane. See p.1, 315/03 for the matrices. This rep. is irreducible (the $E$ irrep.)

How to actually prove that $\mathcal{V}$ is invariant. Let 

$$\mathcal{V}(l) = \text{potential energy of one spring, as a function of length } l. \quad (\text{Don't necessarily assume Hooke's law})$$

Then 

$$\mathcal{V}(\vec{r}) = \sum_{k=1}^{3} \mathcal{V}(l_k), \quad l_k = |\vec{r} - \vec{C}_k|.$$ 

Then 

$$(R_n \mathcal{V})(\vec{r}) = \mathcal{V}(R_n^{-1} \vec{r}) = \sum_{k=1}^{3} \mathcal{V}(1 - R_n^{-1} \vec{r} - \vec{C}_k) .$$

But 

$$|R_n^{-1} \vec{r} - \vec{C}_k| = |\vec{r} - R_n \vec{C}_k|$$

since rotations don't change lengths.

$$\Rightarrow \quad \mathcal{V}(1 - R_n^{-1} \vec{r} - \vec{C}_k) = \sum_{k=1}^{3} \mathcal{V}(1 - \vec{r} - R_n \vec{C}_k) .$$

But all the $R_n$'s, when acting on $(\vec{C}_1, \vec{C}_2, \vec{C}_3)$, just permute them, so they just rearrange the terms of the sum without changing the total. So...

$$\Rightarrow \quad \sum_{k=1}^{3} \mathcal{V}(1 - \vec{r} - R_n \vec{C}_k) = \mathcal{V}(\vec{r}) .$$

We say $\mathcal{V}(\vec{r})$ transforms as a scalar under the group.

Now expand $\mathcal{V}$ out to 2nd order:

$$\mathcal{V}(\vec{r}) = \mathcal{V}(0) + \sum_{i=1}^{2} \frac{\partial \mathcal{V}(0) \vec{r}_i}{\partial \vec{r}_i} + \frac{1}{2} \sum_{i,j} \frac{\partial^2 \mathcal{V}(0) \vec{r}_i \vec{r}_j}{\partial \vec{r}_i \partial \vec{r}_j} + \text{h.o.t.} .$$

\[\uparrow\text{const drop it.}\]
\[\uparrow\text{vanishes, see.}\]
\[\vec{r}=0 \text{ is equil.}\]
Define \( V''_{ij} = \frac{\partial^2 V}{\partial x_i \partial x_j} \) \((0)\), so

\[
V(\mathbf{x}) = \frac{1}{2} \sum_{i,j} V''_{ij} x_i x_j = \frac{1}{2} \mathbf{\dot{x}}^T \cdot V'' \cdot \mathbf{\dot{x}}
\]

This gives a Lagrangian,

\[
L = \frac{m}{2} \left( \dot{\mathbf{x}}^2 \right) - \frac{1}{2} \mathbf{\dot{x}}^T \cdot V'' \cdot \mathbf{\dot{x}}.
\]

To find the normal modes of the system we have to find a linear transformation that diagonalizes \( V'' \). (The normal modes are linear combinations of the \( x_i \) that evolve at a single frequency.) \( V'' \) is only a 2x2 matrix so it's easy to diagonalize, but before doing that let's look at what group theory tells us.

Since \( V(\mathbf{x}) \) is invariant under \( C_{3v} \), we have

\[
(\mathbf{R}_n V)(\mathbf{x}) = V(\mathbf{R}_n^{-1} \mathbf{x}) = V(\mathbf{R}_n^T \mathbf{x}) = \frac{1}{2} \mathbf{\dot{x}}^T \cdot R_n V'' R_n^T \cdot \mathbf{\dot{x}}
\]

\[
= V(\mathbf{x}) = \frac{1}{2} \mathbf{\dot{x}}^T \cdot V'' \cdot \mathbf{\dot{x}}.
\]

Therefore

\[
R_n V'' R_n^T = V''
\]

or

\[
R_n V'' = V'' R_n \quad \text{all} \ R_n \in C_{3v}.
\]

But since \( \{R_n\} \) is an irrep of the group, we have

\[
V'' = \lambda \mathbf{I} \quad \text{(Schur's lemma #1)}.
\]

or

\[
V''_{ij} = \lambda \delta_{ij}
\]

or

\[
V(\mathbf{x}) = \frac{\lambda}{2} (x^2 + y^2)
\]

Write \( \lambda = \frac{m \omega^2}{2} \),

and

\[
L = \frac{m}{2} (\dot{x}^2 + \dot{y}^2) - \frac{m \omega^2}{2} (x^2 + y^2).
\]
The 2 normal modes are degenerate. The mass behaves like a 2D isotropic harmonic oscillator. This is an example of how multidimensional maps give rise to degeneracy.

Note: Group theory tells you there is a degeneracy, it doesn't tell you what \( \omega \) is. For that you have to go beyond symmetry, and calculate \( \omega \) in terms of the properties of the potential \( V(x) \).

Further questions to think about:

1. Why is the origin an equilibrium?
2. Why (or under what circumstances) is the equilibrium stable?
3. We proved \( V(x) \) was invariant under \( C_3 \), but we didn't prove that it is still invariant when \( V(x) \) is replaced by its quadratic approximation. Is the quadratic approximation also invariant under \( C_3 \)? What if we went to cubic order?
4. Speaking of cubic order, Schur's lemma tells us that \( V_{ij}'' = \lambda \delta_{ij} \).

What does it (or anything else) say about the cubic coefficients \( V_{ijk}''' \)?

Now consider a more complicated problem (still with \( C_3 \) symmetry).
1. This is still in the plane.

2. The origin $O$ of coordinates $x,y$ is shown.

3. The $3$ masses are identical; the $3$ springs connecting the masses to the vertices of the $\Delta$ are identical; and the $3$ springs connecting the masses to each other are identical. The $\Delta$ is equilateral.

4. The masses are shown in their equilibrium position, but can vibrate around these.

5. The masses are labelled $1,2,3$.

\[ \text{or } (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3). \]

The coordinates of the $3$ masses are $(x_1, y_1, x_2, y_2, x_3, y_3)$. These are the coordinates on the $6D$ configuration space of the system, which is $\mathbb{R}^6$.

[Don't confuse configuration space with physical space.]

The potential is a function on configuration space, $V = V(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$.

Let $\alpha=1,2,3$ label the particles. Let $\mathbf{x}_{\alpha 0}$, $\alpha=1,2,3$ be the equilibrium positions of the particles, which we assume is the smaller equilateral $\Delta$ shown in the figure. We will be interested in small vibrations, so let's write $\delta \mathbf{x}_\alpha = \mathbf{x}_\alpha - \mathbf{x}_{\alpha 0}$ for the displacements about equilibrium.

Expand the potential about equilibrium,

\[
V(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = V(\mathbf{x}_{1 0}, \mathbf{x}_{20}, \mathbf{x}_{30}) + \sum_{\alpha=1}^{3} \sum_{i=1}^{2} \frac{\partial V(\text{equil})}{\partial x_{\alpha i}} \delta x_{\alpha i} \uparrow \text{const.} \quad \text{varies since equil.}
\]

\[ + \sum_{\alpha \beta} \sum_{i,j} \frac{\partial^2 V(\text{equil})}{\partial x_{\alpha i} \partial x_{\beta j}} \delta x_{\alpha i} \delta x_{\beta j}. \]

Useful notation: let $\mathbf{q} = (\delta x_1, \delta y_1, \delta x_2, \delta y_2, \delta x_3, \delta y_3)$.

or $q_\mu$, $\mu=1,\ldots,6$ for short.
Then the potential energy becomes,

\[ V(q_1, \ldots, q_6) = \text{const.} + \frac{1}{2} \sum_{\mu, \nu=1}^{6} V_{\mu\nu} q_{\mu} q_{\nu} \]

where \( V_{\mu\nu} = \frac{\partial^2 V}{\partial q_{\mu} \partial q_{\nu}} \) (equil) = a constant, 6x6 matrix.

As for the kinetic energy, it is

\[ T = \frac{m}{2} \sum_{\alpha=1}^{3} \dot{q}_\alpha^2 = \frac{m}{2} \sum_{\mu=1}^{6} \dot{q}_\mu^2. \]

So the Lagrangian overall is

\[ L = \frac{m}{2} \sum_{\mu=1}^{6} \dot{q}_\mu^2 - \frac{1}{2} \sum_{\mu, \nu} V_{\mu\nu} q_{\mu} q_{\nu}. \]

The normal modes of the system are obtained by diagonalizing \( V_{\mu\nu} \).

This is straightforward linear algebra, but let’s look at it from the standpoint of group theory. It seems obvious that the potential is invariant under \( C_{3v} \), but \( V \) is a function on the 6D config space and we have to define what we mean by the action of \( C_{3v} \) on this space (since the 2D rep. of \( C_{3v} \) used in the last problem only applies to (xy) space, the plane config space of a single particle).

Let \( \{ R_n \} \) stand for the 2x2 rep. (actually irrep) of \( C_{3v} \) as used in the previous problem. Now, is the potential invariant if you simply map

\[ \delta x^2 \rightarrow R_n \delta x^2 \]?

Answer is no, as you see from a picture. Suppose \( \delta x_1 \neq 0, \delta x_2 = \delta x_3 = 0 \), and apply \( R_1 = R(\frac{\pi}{3}, 2\pi/3) \).
It's intuitively clear that the potential energy in the new configuration is not the same as the old. But, if we rotate the equilibrium point along with the small displacement, then the potential is invariant:

This is because $R_1$ maps equilibrium point 1 into equilibrium point 2. It also maps equilibrium point 2 into e.p. 3, e.p. 3 into e.p. 1. So the rule we want (to keep the potential invariant) is:

\[
\begin{pmatrix}
\delta \vec{x}_1 \\
\delta \vec{x}_2 \\
\delta \vec{x}_3
\end{pmatrix}
\rightarrow
\begin{pmatrix}
R_1 \delta \vec{x}_1 \\
R_1 \delta \vec{x}_2 \\
R_1 \delta \vec{x}_3
\end{pmatrix}
= \begin{pmatrix}
0 & 0 & R_1 \\
0 & R_1 & 0 \\
0 & 0 & R_1
\end{pmatrix}
\begin{pmatrix}
\delta \vec{x}_1 \\
\delta \vec{x}_2 \\
\delta \vec{x}_3
\end{pmatrix}
\]

Thus we obtain a 6x6 matrix, call it $R_1^{(6)}$, that acts on the 6D configuration space and preserves the potential.
This matrix contains information about how the rotation permutes the equilibrium points, and how it rotates small displacements about the equilibrium points. Doing this for the other 5 rotations in $C_{3v}$, we get a set of $6 \times 6$ matrices:

\[
R_0^{(6)} = E^{(6)} = \begin{pmatrix}
E & 0 & 0 \\
0 & E & 0 \\
0 & 0 & E
\end{pmatrix} \quad R_3^{(6)} = \begin{pmatrix}
R_3 & 0 & 0 \\
0 & 0 & R_3 \\
0 & R_3 & 0
\end{pmatrix}
\]

\[
R_1^{(6)} = \begin{pmatrix}
0 & 0 & R_1 \\
R_1 & 0 & 0 \\
0 & R_1 & 0
\end{pmatrix} \quad R_4^{(6)} = \begin{pmatrix}
0 & 0 & R_4 \\
0 & R_4 & 0 \\
R_4 & 0 & 0
\end{pmatrix}
\]

\[
R_2^{(6)} = \begin{pmatrix}
0 & R_2 & 0 \\
0 & 0 & R_2 \\
R_2 & 0 & 0
\end{pmatrix} \quad R_5^{(6)} = \begin{pmatrix}
0 & R_5 & 0 \\
R_5 & 0 & 0 \\
0 & 0 & R_5
\end{pmatrix}
\]

These matrices form a 6D representation of $C_{3v}$, and specify a linear action of that group on the configuration space of the system. All matrices are partitioned into 2D matrices.

Now granting that the potential is invariant under this action, and that the invariance holds for the quadratic approximation as well as the exact potential, we have

\[
R_n^{(6)} V'' = V'' R_n^{(6)}, \quad n=0,\ldots,5 \quad \text{i.e.}
\]

for all $R_n \in C_{3v}$.

However, $R_n^{(6)}$ is not irreducible, so we can't conclude that $V''$ is a multiple of the identity.
Indeed, we want to go to a symmetry adapted basis, in which \( R^{(6)}_n \) becomes block diagonalized.

So the first question is, what irreps occur in this block diagonal form, and with what multiplicity? Use characters to answer this. We need the characters of \( R^{(6)}_n \). These can be expressed in terms of the characters of the 2D \((E)\) rep. of \( C_{3v} \),

\[
\begin{array}{c|ccc}
\text{class} & \{E\} & \{R_1, R_2\} & \{R_3 R_4 R_5\} \\
E & 2 & -1 & 0
\end{array}
\]

\[\chi^{(6)}(C)\]

So from the matrices above we have:

\[
\begin{array}{c|ccc}
\chi^{(6)}(C) & \{E\} & \{R_1, R_2\} & \{R_3 R_4 R_5\} \\
& 6 & 0 & 0
\end{array}
\]

Notice that in computing \( \chi^{(6)} \) we have

\[
\chi^{(6)}(E) = 3 \cdot \chi^{(2)}(E)
\]

\[
\chi^{(6)}(R_1, R_2) = 0 \cdot \chi^{(2)}(R_1, R_2)
\]

\[
\chi^{(6)}(R_3 R_4 R_5) = 1 \cdot \chi^{(2)}(R_3 R_4 R_5)
\]

where the numbers 3, 0, 1 are the number of times the 2D rep of \( C_{3v} \) occurs on the diagonal of the 6D rep. And this number in turn is the number of particles whose equilibrium positions are not permuted by the rotation. [Useful rule for later when we deal with molecules.]

Anyway, we use the character table to determine multiplicities, and we find that \( \{ R^{(6)}_n \} \) has one copy each of the \( A_1, A_2 \) irreps, and two copies of the \( E \) irrep.
We write it like this:

\[ 6D - 6^{\text{rep}} = A_1 \oplus A_2 \oplus 2E. \]

It means that in the symmetry adapted basis, the block structure of the \( R_n^{(6)} \) is

\[ R_n^{(6)} = \]

\[ M^{A_1}(R_n) \quad (1 \times 1) \]

\[ M^{A_2}(R_n) \quad (1 \times 1) \]

\[ M^{E}(R_n) \quad (2 \times 2) \]

\[ M^{E}(R_n) \quad (2 \times 2) \]

\[ M^{E}(R_n) \quad (2 \times 2) \]

\[ M^{E}(R_n) \quad (2 \times 2) \]

\[ 1 + 1 + 2 + 2 = 6. \]

This means that \( V'' \) has 2 eigenvalues \( \omega^{A_1}, \omega^{A_2} \) corresponding to 2 normal modes with \( A_1, A_2 \) symmetry. These frequencies are not expected to be equal, \( \omega^{A_1} \neq \omega^{A_2} \) (more precisely, there is no reason based on the C3v symmetry we have examined why they should be equal). Then \( V'' \) has 2 more eigenvalues \( \omega^{E_1}, \omega^{E_2} \), each of which is 2-fold degenerate, corresponding to 4 normal modes with \( E \) symmetry. The frequencies \( \omega^{E_1}, \omega^{E_2} \) are not expected to be equal, to each other or to either of the frequencies \( \omega^{A_1}, \omega^{A_2} \).
Notice that the multiplicities of the irreps in the decomposition of the 6D rep. of \( C_{3v} \) has given us information about the degeneracies of the normal modes. This is without knowing any details about the potential, except that it is symmetric under \( C_{3v} \).

(The degeneracies are equal to the dimensionalities of the irreps.)

Group theory alone does not give us the values of the eigenfrequencies.

This is what makes group theory useful in nuclear and particle physics, where the Hamiltonian is unknown (or very complicated), but symmetry groups are known. In addition, group theory allows us to calculate the normal modes themselves (at least sometimes).

A question: is it possible that the frequencies \( \omega^1, \omega^2, \omega^E, \omega^E \) might be equal? (This would make the degeneracy higher than predicted above.) The answer is yes, but it's unlikely if \( C_{3v} \) is really the largest symmetry group of the system. If you change the parameters of the potentials (the spring constants etc.) the frequencies move around and you may be able to bring them into coincidence.

This would be called an accidental degeneracy. For a “randomly chosen” potential, accidental degeneracies occur with probability zero.

On the other hand, it could happen that the symmetry group we are working with is not actually the largest symmetry group of the problem, maybe because we were not clever enough to see all the symmetry operations. Then we might observe degeneracies of another kind.
that go beyond the predictions of the theory based on the smaller symmetry group. This happens in the hydrogen atom.

In the problem with 3 masses with springs it turns out that we can find the normal modes of the system corresponding to the symmetry types $A_1, A_2, E$ by using group theory alone (still no information about the potential needed, apart from the fact that it has the required symmetry). To do this we return to general considerations of representation theory.

Let $g \mapsto T(g)$ be a representation of a group $G$ by means of unitary operators $T(g) : V \rightarrow V$ where $V$ is the carrier space of the rep. Let $\dim V = d$. Then we know that in a symmetry adapted basis, the matrices $M(g)$ for operators $T(g)$ are block diagonal.

\[
M(g) = \begin{bmatrix}
M^{(0)}(g) \\
& M^{(1)}(g) \\
& & \ddots \\
& & & M^{(d-1)}(g)
\end{bmatrix}
\]

etc. This follows from the definition of an irrep and not much else. So far we have said very little about how to find the symmetry